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This issue is edited with the aim to introduce our research activities from April 1997 to March 1998, under the four categories.

A. Current Research Fields
B. Original Articles
C. Review Articles
D. Books

本誌はエネルギー科学研究科における研究活動の紹介をおもな目的とし、次のA、B、CおよびDに分けて編集されたものである。

A．研究現況(テーマ)

B．研究発表

C．総説

D．著書(学術図書)

Contents

目次

Contents

A. Current Research Fields

Ａ．研究現況

Chapter 1

Current Research Fields

I Department of Socio-Environmental Energy Science

a1-1	Pursuit of happiness	幸福論
a1-2	New material for energy saving	低環境負荷材料の開発
a1-3	Recycle process	リサイクルプロセス
a2-1	Analysis of Energy Supply and Demand in Japan	日本のエネルギー需給分析
a2-2	Analysis of Optimal Generation Mix under Uncertainty	不確実性を考慮した最適電源構成の分析
a2-3	Life Cycle Analysis of Electric Vehicle	電気自動車のライフサイクル分析
a2-4	Economic Analysis of Energy Efficient Technologies	省エネルギー技術の経済性分析
a3-1	Chemical conversions of biomass and plastics wastes to their liquified fuels by the supercritical fluids	超臨界流体によるバイオマスおよび廃プラスチックスの液体燃料化に関する研究
a3-2	Bioconversion of lignocellulosics to ethanol by the supercritical water	超臨界水によるリグノセルロースのエタノールへの酵素変換に関する研究
a3-3	Pyrolysis of lignocellulosics to value-added chemicals	リグノセルロースの熱分解による有用物質への変換
a3-4	Topochemistry of biocarbon-inorganic composites for their property-enhancement	無機質複合化バイオカーボンの諸機能発現に関するトポ化学
a3-5	Long-living of wood enhanced by antimicrobial treatments	防菌・防黴性付与による木材のロングライフ化に関する研究

a3-6	Forest soil and carbon cycling in earth ecology	地球生態系での炭素循環と森林土壌に関する研究
a4-1	Environmentally clean renewable energy production by biological systems	生化学システムによるクリーンエネルギー生産
a4-2	Exploration of bioremediation systems for environmental toxic molecules	生化学システムによる除去
a4-3	Biochemical and chemical studies on the interaction of nitric oxide with gene and its regulation in the transcription process	一酸化窒素による遺伝子損傷とその制御
a4-4	Structural studies on nucleic acids by magnetic resonance spectroscopy	核酸の構造化学
a4-5	Electlical and thermodymanic phenomena on the metal/metal and metal/semiconductor diamond interfaces	金属／金属、金属／半導体界面の電気的・熱力学的性質
a5-1	Development of Mutual Adaptive Interface with Eye-Sensing HMD	アイセンシングＨＭＤによる相互協調型インタフェースの開発
a5-2	A Study on a Human Model based on Artificial Intelligence	ＡＩによるヒューマンモデルの構築
a5-3	Adaptive Interface based on Recognition of Facial Expression and Verbal Protocol	顔表情･発話認識を用いた適応型インタフェース
a5-4	A Study on Integrated CAI system	統合型教育支援システムの構築
a5-5	Development of Maintenance Training System based on Networked Virtual Environment	共有仮想空間を用いた保修訓練システムの構築
a5-6	Optimal Planning of Autonomous Decentralized Energy System	自律分散型エネルギーシステムの計画
a6-1	Characterization of Physical and Chemical Properties of Atmospheric Aerosols	大気エアロゾルの物理・化学的性状の特性化
a6-2	Application of PIXE Analysis to Atmospheric Sciences	PIXE 分析法の大気環境科学への応用
a6-3	Analysis and Modelling of Deposition of Air Pollutants	大気汚染物質の沈着機構の解析とモデル化
a6-4	Long-Range Transport of Gaseous and Particulate Air Pollutants Combined with Chemical Transformation and Removal	沈着、変質を伴う大気汚染物質の長距離輸送モデルの開発

a6-5	Evaluation of Radiative Forcing by Atmopsheric Aerosols	大気エアロゾル粒子の放射収支への影響評価
a6-6	Analysis of Environmental Loads in Energy Systems	エネルギーシステムにおける環境負荷評価
a7-1	Scientific consideration about best mixture of electricity sources in future	将来における電力源のベストミックス（最適組合せ）に関する科学的考察
a7-2	Investigation on nuclear subjects including non-proliferation, safeguards, physical protection, transportation, criticality safety, radioactive waste management, etc.	核不拡散、保障措置、核物質防護、核燃料輸送、臨界安全、放射性廃棄物管理などの核問題に関する研究
a7-3	Study on application of reactor neutrons to medicine	原子炉中性子の医学への利用に関する研究
a7-4	Neutron radiography	中性子ラジオグラフィ
a7-5	Experimental study on neutron-induced fission	中性子核分裂に関する実験的研究
a7-6	Evaluation of fluence and absorbed dose for neutrons and gamma-rays	中性子、ガンマ線のフルエンス及び吸収線量の評価
a8-1	Formation and evolution of nuclear-safety culture	原子力安全文化の醸成
a8-2	Transmission of information and public relations on energy problems	エネルギー問題に関する情報伝達と公報
a8-3	Formation of public attitudes on nuclear energy or radioactivity issues	原子力・放射線／放射能問題に関する社会の態度形成
a8-4	Neutron Activation Analysis of Ivory of African Elephants	アフリカ像の象牙の中性子放射化分析
a8-5	Physical Interpretation of Adjoint Flux in Reactor Physics	原子炉物理における随伴中性子束の物理的意味
a9-1	Japanese Strategy for Mitigating Global Environmental Issues (Global Warming)	地球環境問題、地球温暖化に対する日本の政策
a9-2	Analysis on Heat Cascading among Industrial Customers	産業需要家間のヒートカスケード化の分析
a9-3	Analysis on Wheeling in Electric Power Network	電力における託送の分析

a9-4	Effective Utilization of Uranium by Using High Burn-up Fuel Technology in Light Water Reactors	軽水炉用高燃焼度燃料によるウラン資源有効活用利用
a9-5	Plutonium Utilization in Light Water Reactors	軽水炉でのプルトニウム有効利用

II Department of Fundamental Energy Science

b1-1	Electrochemical Energy Conversion by Fuel Cells and Hydrogen Systems	燃料電池、水素エネルギーシステムによる電気化学的エネルギー変換
b1-2	Phyiscal Chemistry of Molten Salts and Applications to Energy Conversion Processes	溶融塩の物性・化学とエネルギー変換プロセスへの応用
b1-3	New Functional Materials and Their Applications	マテリアル・テーラリングによる新規な機能材料の創製と応用
b1-4	Development of Interdisciplinary Fields of Electrochemistry and Plasmas/Ion Beams	プラズマ、イオンビームなどと電気化学の境界領域の開拓
b1-5	Determination of Molecular and Solid Structures by Vibrational Spectroscopies and Diffractions	ラマン分光、中性子回折などによる物質構造の解明
b1-6	Inorganic Halgen Chemistry and Applications to Energy Processes	フッ化物、塩化物の化学とエネルギープロセスへの応用
b2-1	Dynamics of the conduction electrons in chalcogenide semiconductors and the related optical properties	カルコゲン化合物半導体における伝導電子の動的挙動と分光特性
b2-2	The transport processes and the percolative critical phenomena in structurally complicated media	複雑系における伝導プロセスとパーコレーション臨界現象
b2-3	Superconductivity in nano-metrically disordered high-T_c cuprates	乱れたナノ構造を持つ高温超伝導体における超伝導
b2-4	Thermoelectric and galvanomagnetic effects in semimetals and semiconductors	半金属と半導体における熱電効果と低温強磁場電流磁気効果
b2-5	Synthesis of High Performance Materials by DC Arc Plasma	ＤＣアークプラズマによる高機能材料の合成
b2-6	Micro-Characterization at the Interface of High Performance Materials	高機能材料界面のマイクロキャラクタリゼーション

b3-1	Analysis and Design of Ceramic Energy Materials	セラミックスエネルギー材料の解析と設計
b3-2	Studies on Rechargeable Lithium Battery Materials	リチウム２次電池の材料開発
b3-3	Development of Solid Oxide Fuel Cell Systems	固体酸化物型燃料電池の開発
b3-4	Sysnthesis of Functional Ceramic Thin Film from Aqueous Solution	水溶液からの機能性セラミックス薄膜の合成
b3-5	Design and Analysis of Novel Optical Energy Materials	新規光エネルギー材料の設計と解析
b3-6	Development of Hydrogen Energy System Materials	水素エネルギーシステム材料の開発
b4-1	fusion plasma	核融合プラズマ
b4-2	MHD theory	ＭＨＤ理論
b4-3	plasma transport theory	プラズマ輸送理論
b4-4	optimization of stellarator field	ステラレータ磁場の最適化
b4-5	study of process plasma	プロセスプラズマの研究
b5-1	Studies on multiply-ionized impurity ions in high temperature plasmas.	高温プラズマ中の多価電離不純物イオンの研究
b5-2	Theoretical studies on equilibrium and stability in the 3-dimensional non-axis symmetric torus plasmas.	３次元非軸対称トーラスプラズマの平衡と安定性の理論的研究
b5-3	Studies on magnetohydrodynamic(MHD) equilibrium and plasma current in non-uniform magnetic field.	磁場測定による不均一磁場中の超高温プラズマの平衡および内部電流の研究
b5-4	Studies on radiation by bolometric and spectroscopic diagnostics from high temperature plasmas.	ボロメーターおよび分光による高温プラズマからの輻射の研究
b5-5	Studies on neutron energy spectrum by D-D reaction.	高温プラズマ中の D-D 反応による中性子のエネルギースペクトルの研究
b6-1	Electron cyclotron heating and current drive	プラズマの電子サイクロトロン加熱・電流駆動

b6-2	Control of MHD instabilities by LHCD	低域混成電流駆動による磁気流体不安定性の制御
b6-3	Control of MHD instabilities by ECH	電子サイクロトロン加熱による磁気流体不安定性の制御
b6-4	Plasma diagnostics (soft X-ray CT and ECE)	プラズマ診断法の開発（軟X線トモグラフィーと電子サイクロトロン輻射計測）
b6-5	Confinement and nonlinear waves in non-neutral plasmas	非中性プラズマの閉じ込めと非線形波動
b7-1	Confinement Study of High Temperature Plasma in Helical System	ヘリオトロン装置による高温プラズマの閉じ込め制御
b7-2	Study of Helical Magnetic Configuration	ヘリカル磁場構造の研究
b7-3	Control of Edge Plasma	プラズマ閉じ込め領域周辺部におけるプラズマ制御
b7-4	Divertor Study	ダイバータ基礎研究
b7-5	Study of Plasma Production and Heating by Electron Cyclotron Wave	電子サイクロトロン波によるプラズマ生成・加熱の研究
b7-6	Study of Plasma Heating by Neutral Beam Injection	高速中性粒子によるプラズマ加熱の研究
b8-1	Study on High Temperature Plasma Heating and Confinement	超高温プラズマの加熱・閉じ込めに関する研究
b8-2	Experimental Analysis of Vacuum Magnetic Field Structure	真空磁場配位の実験構造解析
b8-3	Development of Monte Carlo Calculation Scheme for the Simulation of Plasma Transport and Heating	プラズマの輸送と加熱のシミュレーションのための新しいモンテカルロ計算スキームの開発
b8-4	Theoretic Analysis on Charged Particle Orbit in the None-axisymmetrical Torus with Adiabatic Constants	非軸対称トーラスにおける荷電粒子軌道の断熱不変量をもちいた理論解析
b8-5	Study on the Advanced Heliotron Magnetic Field with the Control of Chaotic and Statistic Characteristics	磁力線のカオスや統計的性質の制御に基づいたヘリオトロン磁場の高性能化に関する研究
b8-6	Study on the Optimization of Ion Cyclotron Heating Antenna for Various Heating Modes	イオンサイクロトロン加熱の加熱モードによるアンテナ最適化の研究

b9-1	Infrared Photochemical Reaction of Haloalkanes.	ハロアルカン類の赤外光化学反応
b9-2	Hydrogen in and on Inorganic Solid Materials.	無機固体材料中の水素の挙動
b9-3	Photo Excitation, Relaxation, and Reactions on a Semiconductor Electrode.	半導体電極における光励起，緩和，および反応機構
b9-4	Microstructure of Porous Materials and Their Physicochemical Properties.	多孔質材料の微細構造と物理化学特性
b9-5	Laser Ablation of Inorganic Solid Surfaces.	固体材料表面のレーザーアブレーション
b10-1	Design of Functional Supramolecules Based on Amphiphilic Molecular Assembly and their Utilization for Chemical Reaction and Separation of Substances	両親媒性分子集合体を用いた超分子集合体の構造設計とその反応分離場への応用
b10-2	Construction of Advanced Materials with Nano-Meso Sized Structure Using Amphiphilic Molecular Assemblies as Template	両親媒性分子集合体を鋳型として用いたナノ-メゾ材料の構築
b10-3	Method to Integrate the Processes for Obtaining Materials with Hierarchal Structures	階層構造を持つ材料作成プロセスのインテグレート手法
b10-4	Interaction between Solutes in Aqueous and Nonaqueous Solvents	水溶液中及び非水溶媒中における溶質間相互作用
b10-5	Prediction of Ternary Structures of Proteins in Aqueous Solutions	水溶液中におけるタンパク質の 3 次構造予測
b11-1	Molecular design of plastic enzyme	プラスチック酵素の分子設計
b11-2	Molecular design of asymmetric photocatalyst	不斉光触媒の分子設計
b11-3	Photo-induced enzyme reaction	酵素による光触媒反応
b11-4	Creation of high quality enzyme by artificial evolution	人工進化高機能酵素の創製
b12-1	Research on high-temperature batteries for energy storage	エネルギー貯蔵用高温二次電池の研究
b12-2	Elucidation of electrochemical behavior of sulfur dioxide and nitrogen oxides as the environmental pollutants	二酸化硫黄や窒素酸化物などの環境汚染物質の電気化学的挙動の解明

b12-3	Electrodeposition of refractory metals in molten salts	溶融塩電解によるリフラクトリーメタルの析出
b12-4	Analysis of current and potential distributions in electrochemical cells	電気化学セルにおける電流・電位分布の解析
b13-1	Study on nuclear characteristics of high performance reactors in next-generation	次世代の高性能新型原子炉の核特性研究
b13-2	Development of high performance advanced research reactor as neutron source	高性能研究用中性子源炉の開発
b13-3	Nuclear reactors utilizing thorium-uranium fuel cycle	トリウム・ウラン燃料サイクル原子炉
b13-4	Hybrid reactor system of accelerator driven fission reactor	加速器と核分裂炉のハイブリッド炉
b13-5	Transmutation and incineration of high level nuclear waste	高レベル放射性廃棄物の消滅処理
b13-6	Criticality safety study of nuclear fuel facility	核燃料施設の臨界安全性研究
b14-1	Study on target cooling of a spallation neutron source	スポレーション中性子源のターゲット冷却に関する研究
b14-2	Flow and heat transfer characteristics of gas-liquid two-phase flow in narrow channels	狭小流路における気液二相流の流動と伝熱
b14-3	Characteristics of two-phase flow with a large liquid/gas density ratio	高密度比気液二相流の特性
b14-4	Basic study on steam explosion	水蒸気爆発に関する基礎研究
b14-5	Study on basic phenomena in post-CHF heat transfer	ポスト限界熱流束熱伝達の基礎的現象に関する研究
b14-6	Visualization and measurement of multiphase phenomena by neutron radiography	中性子ラジオグラフィによる混相流現象の可視化と計測
b15-1	Studies on TiO2 thin film photocatalysts under weak UV light illumination.	酸化チタン光触媒反応の研究
b15-2	Applications and coating of fine particles	微粒子で構成される薄膜の作成と応用
b15-3	Studies on conductive diamond electrodes	導電性ダイヤモンド薄膜電極の研究

III Department of Energy Conversion Science

c1-1	Mitigation of Pollutants in Thermal Energy Conversion Systems	熱エネルギー変換システムにおける汚染物質低減
c1-2	Mixture Formation and Combustion in Diesel and Spark-Ignition Engines	ディーゼル機関および火花点火機関の混合気形成と燃焼
c1-3	Spray Characteristics and Their Effects on Combustion	噴霧特性ならびにその燃焼への作用
c1-4	Prediction of Combustion Processes in Internal Combustion Engines	内燃機関内燃焼過程の予測
c1-5	Alternative Fuels in Combustion Systems	燃焼システムにおける代替燃料
c1-6	Optimum Design of Power Plants	動力プラントの最適設計
c2-1	Ignition and Combustion of Homogeneous and Heterogeneous Mixtures	均一および不均一混合気の着火と燃焼
c2-2	Chemical Reaction Kinetics of Pollutant Formation	汚染物質生成の化学反応動力学
c2-3	Structure of Turbulent Diffusion Flames	乱流拡散火炎の構造
c2-4	Laser Diagnosis and Image Analysis for Combustion Research	レーザ計測および画像解析による燃焼診断
c2-5	Numerical Simulation of Turbulent Flows and Combustion	乱流および燃焼の数値シミュレーション
c2-6	Mechanical Effects of Fluid Energy on Bio-Tissues and Cells	生体組織および細胞に及ぼす流体エネルギーの力学的作用
c3-1	Inelastic Constitutive Equation of High Temperature Materials and Construction of the Data Base	高温における非弾性構成式とそのデータベース化
c3-2	Foundation of Materio-Thermo-Mechanics and Computer Simulation of Some Processes Incorporating Phase Transformation	変態・熱・力学の基礎と相変態を伴う工学過程のコンピューターシミュレーション
c3-3	Analysis of Plastic Forming Process under Large Deformation Depending on Microstructural Evolution	大変形を伴う塑性加工過程の解析とそれに及ぼす組織の効果
c3-4	Development of Sheet Metal Bending Process by Line Heating Technology	線状加熱による板材の曲げ加工機の試作開発

c3-5	Molecular Dynamics Simulation of Thermo-Mechanical Fields under Phase Trandformation	分子動力学による相変態過程とそれに伴う熱・力学場のシミュレーション
c4-1	Mechanics of Electromagnetic Materials	電磁気材料の力学
c4-2	Mechanics and Application of Functional Materials	機能材料の力学と応用
c4-3	Nondestructive Evaluation of Stress, Damage and Inhomogeneity by Ultrasonic Waves and Electromagnetic Phenomena	超音波と電磁気現象による応力，損傷，非均質の非破壊評価
c4-4	Processing of Ceramic-Coated Materials and Analysis of Their Structure and Deformation	セラミックス・コーティング材料の創成とその構造および変形の解析
c4-5	Strength Evaluation of Advanced Ceramics and Its Numerical Simulation	先進セラミックスの強度評価とその数値シミュレーション
c4-6	Computer Simulation of Fatigue Strength in Metallic Materials	金属材料の疲労強度コンピュータ・シミュレーション
c5-1	Design of Intense 14 MeV Volumetric Neutron Source	強力 14 MeV 体積中性子源のデザイン
c5-2	Magnetic Confinement of Ultra-Cold Neutrons	超冷中性子の磁気閉じこめ
c5-3	Study of the Production Mechanism of Negative Hydrogen Ion in Plasmas	プラズマ中での負イオン生成メカニズムの解明
c6-1	Free Electron Laser	自由電子レーザーの研究
c6-2	Particle Simulation for Advanced Klystron Tube and RF Guns	クライストン及びＲＦガンの高性能化のための粒子シミュレーション研究
c6-3	D $-^3$ He Advanced Fuel Fusion	D $-^3$ He 先進燃料核融合炉の研究
c6-4	Beam-Beam Colliding Fusion (IECF)	ビーム衝突型核融合の研究（慣性静電閉じ込め方式核融合）
c6-5	Spherical Plasma Generation and Application	球状プラズマの生成及び応用の研究
c7-1	Radiation Effects on Fusion Materials	核融合炉材料の照射効果
c7-2	Evaluation of Performance of Nuclear Reactor Structural Materials	原子炉構造材料の特性評価

c7-3	Environmental Effects on Advanced Intermetallic Compounds	先進金属間化合物の環境効果
c7-4	First-Principles Calculation of the Total-Energy and the Interatomic Force of Solid and Its Surface	固体，固体表面の全エネルギー，原子間力の第一原理計算
c7-5	Surface Science of the Transition Metal-Light Element System	軽元素ー遷移金属系の表面科学
c7-6	Electronic Structures and Properties of Transition-Metal Hydrides	遷移金属の水素化物，酸化物，窒化物の電子構造と物性
c8-1	Nonlinear Continuum Mechanics	非線形連続体力学
c8-2	Nonlinear Wave Propagation in Solids	固体における非線形波動
c8-3	Free/Moving/Growing Boundary Problem	自由/移動/成長境界問題
c8-4	Mechanics in Ferromagnetic Materials	強磁性体の力学

IV Department of Energy Science and Technology

d1-1	Study on structure and process of VLSI	超ＬＳＩのデバイスプロセスに関する研究
d1-2	Study on electrical characteristics of scaled-down MOS devices	サブミクロンＭＯＳデバイスに関する研究
d1-3	Study on reliability physics and modeling on carrier transport in insulating films	ＭＯＳ界面の信頼性物理とモデリングに関する研究
d1-4	Investigation of local chemical bondings of ceramics by EELS	高空間分解能 EELS 法による局所化学結合状態の解明
d1-5	Material design of new functional ceramics through electronic calculations	新しい機能性セラミックス材料の量子設計
d1-6	Electronic states of ceramic interfaces	セラミックス界面の機能と電子状態
d2-1	Heat transfer characteristics of cryogenic liquids (LN2, LHe, HeII) in relation to the cooling of superconducting magnets.	超伝導マグネット冷却に関連した極低温流体 (LN2, LHe, 超流動 He) の熱伝達特性
d2-2	High density heat removal from plasma facing devices in nuclear fusion systems.	核融合装置プラズマ対向壁からの高密度除熱

d2-3	Non-boiling and boiling heat transfer in liquid metals.	液体金属の非沸騰及び沸騰熱伝達
d2-4	Superconducting magnet energy storage system in electrical power system.	超伝導エネルギー貯蔵装置の電力系統特性に関する研究
d2-5	Power system characteristics of superconducting fault current limiter.	超伝導故障電流限流器の電力系統特性に関する研究
d2-6	Energy transfer between superconducting magnets.	超伝導マグネット間のエネルギー転送に関する研究
d3-1	Iron-Based Device for Low Temperature Thermoelectric Generator.	低温用鉄基熱電素子の開発
d3-2	New Continuous Process for Production of Titanium Metal.	金属チタンの新しい連続精錬プロセスの開発
d3-3	Ammounium Gas Steel Making.	アンモニアガス製鋼法
d3-4	Production of Functional Materials by Ozone Gas.	オゾンガスによる機能材料創製
d3-5	Thermodynamics of Superconductive Oxides.	酸化物超伝導材料の熱力学
d3-6	Refining of Refractory Metals.	高融点金属の精錬
d4-1	Physical Chemistry of Radioactive Nuclear Waste Management	放射性廃棄物処理の物理化学
d4-2	Thermochemistry of steelmaking	製鋼プロセスの熱化学
d4-3	Chemical sensors for metallurgical processes	材料プロセス用化学センサ
d4-4	Oxidation-reduction equilibrium in molten salgs, fluxes and salts.	溶融スラグ、フラックス、ソルト中の酸化還元平衡
d4-5	Recovery of iron unit from waste generated at steel works	製鉄所起源の廃棄物からの鉄資源回収
d4-6	Thermochemitsry of zirconium-based alloys	ジルコニウム系合金の熱化学
d5-1	The Earth Energy and Mineral Resources	地球エネルギーと鉱物資源
d5-2	Trends and Forecasts for the Supply and Demand of Resources and Energy	資源エネルギーの需給動向と予測

d5-3	Geological Studies of Radioactive Waste Disposal	放射性廃棄物の地層処分
d5-4	Resources Development and Environmental Protection	資源開発と環境保全
d6-1	Theoretical Analysis of Air-Lift Pump System for Conveying Marine Mineral Resources from Deep-Sea Bed	深海底鉱物資源の揚鉱理論
d6-2	Analysis of Heat Transfer by Impinging Jet	衝突噴流による熱伝達解析
d6-3	Numerical Simulation of Working Processes	数値加工プロセス
d6-4	Behaviour of Liquid Droplets on Super-High Temperature Metal Surface	超高温金属表面における液滴の挙動
d6-5	Combined Simulation of Fluid Flow and Heat Transfer	流動・伝熱複合シミュレーション
d6-6	Prediction of Forming Limit in Sheet Metal Forming Processes	板材成形における成形限界予測
d7-1	Hydrometallurgical Traetment of Rare Earth Magnet Scrap	希土類磁石スクラップの湿式処理
d7-2	Liquid-liquid Extraction of Oxide Fines in Metal Salts Solutions	液-液抽出法による金属酸化物微粒子の回収に及ぼす金属イオンの影響
d7-3	Adsorption of Inorganic Depressants on Inherently Hydrophobic Mineral l Surfaces	疎水性鉱物表面への無機抑制剤の吸着に関する研究
d7-4	Injection Smelting Operation for Environmentally Friend Process	地球環境調和型吹き込み溶錬プロセスに関する基礎的研究
d7-5	Electrochemical Processing for Compound Semiconductor Solar Cell	化合物半導体太陽電池の電気化学プロセシング
d7-6	Non-equilibrium Electrochemical Interfacial Phenomena in Space Station	宇宙ステーションにおける非平衡電気化学界面現象に関する基礎的研究
d8-1	NMR study of quantum spin-gap in low dimensional spin system	低次元スピン系における量子スピンギャップの核磁気共鳴
d8-2	NMR Study of Magnetic Frustration	フラストレートするスピン系における核磁気共鳴
d8-3	Generation of high-brightness electron beam	高輝度電子ビームの発生

d8-4	Generation of free-electron lasers	自由電子レーザーの発生
d8-5	Application of free-electron lasers	自由電子レーザーの応用
d8-6	Generation of novel high-brightness radiation	次世代の高輝度放射の発生
d9-1	R&D of Advanced Reduced-Activation Materials	先進低放射化材料の開発及び基礎研究
d9-2	Ceramic Composite Materials for Advanced Energy Systems	セラミクス系複合材料の開発と先進エネルギーシステムへの応用
d9-3	Physics and Irradiation Effects in Energy Conversion Materials	エネルギー変換材料の照射効果と物理
d9-4	Small Specimen Testing Technologies for Energy Materials Research	微小試験片による材料強度特性評価法の研究
d9-5	Joining of Materials for Nuclear Energy Systems	先進核融合・原子力材料等の接合の科学
d9-6	Fundamental Processes of Irradiation Creep	粒子線場における静的塑性変形挙動基礎過程の研究
d10-1	Development of advanced lasers	高機能レーザー開発
d10-2	Coherent interaction of lasers with atoms, molecules and solids	レーザーと原子・分子・固体とのコヒーレント相互作用
d10-3	Strong-field phenomena and their applications	高強度レーザー誘起現象とその応用
d10-4	Advanced energy transportation processes	先端エネルギー輸送プロセス
d10-5	Heat transfer in normal liquids, liquid sodium and cryogenic liquids	通常流体、液体ナトリウム及び低温液体中での熱伝達

B. Original Articles

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B．研究発表

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Chapter 2

Original Articles

I Department of Socio-Environmental Energy Science

(エネルギー社会・環境科学専攻)

1: * Bulk metallic multilayers produced by repeated press-rolling and their perpendicular magnetoregistance

K.Yasuna, M.Terauchi, A.Otsuki, K.N.Ishihara, and P.H.Shingu

Journal of Apllied Physics Vol.82, No.5, P.2435, 1997

Bulk Fe/Ag multilayers with layer thickness of about 10nm have been successfully fabricated by repeated press-rolling directly from macroscopic stack of metal sheets. The press-rolled multilayers exibited giant magnetoresistance of 13% in the current perpendicular to the plane geometry and 4% in the current in the plane geometry at 5K.

2: Synthesis of near net shape high density TiB/Ti composite

T.Yamamoto, A.Otsuki, K.N.Ishihara, and P.H.Shingu

Material Science and Engineering Vol.A239-140, P.647, 1997

TiB/Ti composite were produced by SHS (self propagating high temperature synthesis) under conditions of PHIP (pseudo-hot isostatic pressing). The synthesis conditions were optimized to produce high dense materials conforming a high volume fraction of TiB. Self-propagating reaction of the Ti and B powders occurred above the α- and β-Ti tranformation temperature (1155K). The compostites consist of Ti matrices with dispersed TiB reaction products of 2-30 μm size. Near fully dense composites with a TiB/Ti volume ratio of 33-44 vol.% were synthesized for B/Ti atomic ratios of 0.3-0.4 at pseudo isostatic

pressures of 100 MPa. THe Vickers hardness and fracture stress fo the composites are 5.6-7.1 and 2.1-2.3 GPa, respectively, and the wear of hte composites is approximately 7-9% of the Ti and Ti-6Al-4V.

3: Beate Certe Omnes Vivere Volumus

幸福論

P.H.Shingu

Development Engineering, Vol.3, p.1, 1997

開発技術学会 Vol.3, p.1

"We all want to live happily." This famous expression by Cicero so plinly descrives the aim of the Development Engineering. Then, naturally, comes the question, "What is happiness?". This paper first reviews various old and new writeing about happiness. Happiness is then classified into four stages. The first is the attainment of simplw pleasures. Second is the continuation of that pleasure to the time of one's death or beyound. Third is the experience of hardship or sorrow for the sake of intnsification. The last stage is to find the real and supreme happiness in the hardship or sorrow itself with out expectation of any compensation. (in Japanese)

4: The US/Japan comparison of energy intensity. Estimating the real gap

Yutaka Nagata

Energy Policy, Vol.25, No.7-9, pp.683-691, June/July 1997

Total primary energy requirement (TPER) divided by gross domestic product (GDP) is a commonly used indicator that measures national energy efficiency. However, this indicator is too approximate to represent actual efficiency and is misleading. This paper suggests a new method of comparing national energy efficiencies. A case study between the U.S. and Japan indicates that the U.S. consumes only 23shows that the U.S. consumes 72

5: * Cellulose triacetate prepared from low-grade hardwood dissolving pulp and its insoluble residues in acetylation mediums

Shiro Saka, Keiko Takanashi

Journal of Applied Polymer Science 67, 289-297, 1997

As cellulose triacetate was prepared from low-grade hardwood dissolving pulp, a considerable amount of the insoluble residue was present in the acetylation medium of the acetic acid/acetic anhydride/sulfuric

acid system. The charactrization of this residue indicated that the insoluble residue is composed of cellulose triacetate and xylan diacetate, retaining a fiber structure of swollen form. To reduce the insoluble residues, reaction conditions for acetylation were investigated. As one of the remedies of reducing the insoluble residues, 17 different solvents were selected to add to the acetylation medium, and among these, dichloroacetic acid was found to be very effective for its reduction. The obtained cellulose triacetate could then reveal good thermal properties similar to that from high-grade dissolving pulps. Therefore, acetylation systems with an addition of an appropriate solvent can have a potential to industrially manufacture a high- quality cellulose triacetate from even low-grade hardwood dissolving pulps, as observed in low-grade softwood dissolving pulps.

6: * Antimicrobial TMSAC-added wood-inorganic composites prepared by the sol-gel process.

Fumie Tanno, Shiro Saka, Keiji Takabe*
***(Grad. School of Agr.)**

Materials Science Research International 3(3), 137-142, 1997

One of the antimicrobial alkoxysilanes, 3-(trimethoxysilyl)propyldimethyloctadecyl ammonium chloride (TMSAC), was applied to the sol-gel reaction to prepare the antimicrobial wood-inorganic composites from tetraethoxysilane (TEOS). The obtained TMSAC-SiO_2 composites revealed some antimicrobial activities, but the use of the property-enhancer, 2-heptadecafluorooctylethyltrimethoxysilane (HFOETMOS) in a small quantity could provide water-repellency to the composites which has, further, improved its activities against both white-rot and brown-rot fungi. In addition, after a prolonged soil burial test, TMSAC woods have lost antimicrobial properties, whereas the TMSAC-SiO_2, particularly, HFOETMOS-(TMSAC-SiO_2) composites could have its high activities maintained. Therefore, it may be concluded that HFOETMOS-(TMSAC-SiO_2) and TMSAC-SiO_2 composites can provide sustainably high antimicrobial properties in wood.

7: * Several SiO_2 wood-inorganic composites and their fire-resisting properties

Shiro Saka, Tomonori Ueno

Wood Sci. Technol. 31, 457-466, 1997

In a study on the SiO_2 wood-inorganic composites prepared by the sol-gel process with tetraethoxysilane (TEOS), it is more appropriate to use safer agents than TEOS, considering the operational and processing environments. In this study, therefore, methyltrimethoxysilane (MTMOS) was used to prepare the SiO_2 wood-inorganic composites, and comparative studies were made with TEOS. Resultingly, SiO_2 wood-inorganic composites could be successfully prepared from MTMOS reaction system, as in TEOS system,

with its lower concentration, and both composites had SiO_2 gels specifically formed within the cell walls from moisture-conditioned wood specimens. On this SiO_2 composites, the water-repellent properties were added most effectively with a molar ratio of 2-heptadecafluorooctylethyltrimethoxysilane (HFOETMOS) to alcohol being 1/250 and 1/180 for TEOS and MTMOS reaction system, respectively. On the other hand, fire-resisting properties were tried to be added to SiO_2 composites with several fire-resisting agents. The fire-resisting agents in the obtained composites are not, however, stable and learched out readily. Therefore, a small addition of HFOETMOS was tested to the MTMOS and TEOS reaction system with fire-resisting agents. The obtained results clearly indicated that HFOETMOS could restrain the fire-resisting agents to be learched from the composites, and that composites from MTMOS system were superior to TEOS system on the antileachability. Therefore, MTMOS can be appropriate for displacement of TEOS as a chemical agents to prepare SiO_2 wood-inorganic composites.

8: * Fire-resisting properties in several TiO_2 wood-inorganic composites and their topochemistry.

Hisashi Miyafuji, Shiro Saka

Wood Sci. Technol 31, 449-455, 1997

A study of the wood-inorganic composites prepared by the sol-gel process with a metal alkoxide indicated that an inorganic modification of wood with TiO_2 gel from tetraisopropoxytitanium (TPT) can not improve its properties due to the formation of the gels in the cell lumina by high hydrolysis rate of TPT. In this study, therefore, titanium alkoxides or titanium chelates which have the lower rate of hydrolysis and subsequent polycondensation than TPT were used for preparing TiO_2 wood-inorganic composites to study the topochemical effects of TiO_2 gels for the property enhancement of wood. As a result, it was found by SEM-EDXA analysis that the TiO_2 gels deposited within the cell walls could improve the properties of wood in dimensional stability and fire-resistance, whereas for the gels in the cell lumina, property enhancement could not be achieved, as observed in SiO_2 wood-inorganic composites.

9: Synthesis of high molecular mass condensed tannin by cationic polymerization of flavan 3,4-carbonate

Satoshi Yoneda*, Haruo Kawamoto, Fumiaki Nakatsubo*
***(Graduate School of Agriculture)**

J. Chem. Soc. Perkin Trans. 1, 1997, 1025

A new synthetic method for the preparation of high molecular mass (the highest Mn 10200) condensed tannin has been developed. Polymerization of 3',4',5,7-tetrabenzyloxyflavan 3,4-carbonate and subsequent debenzylation gives a condensed tannin having high molecular mass. Molecular mass of the

synthetic tannin increases up to a degree of polymerization (DPn) of ~35 with an increase in the reaction time. This high molecular mass condensed tannin, synthesized for the first time, is useful as a model compound for natural condensed tannins with high molecular mass, such as that from Japanese persimon fruit.

10: Binding nature and denaturation of protein during interaction with galloylglucose

Haruo Kawamoto, Kayo Mizutani*, Fumiaki Nakatsubo*
***(Graduate School of Agriculture)**

Phytochemistry, 46(3), 473, 1997

Analysis of insoluble complexes between tetragalloylglucose and protein following a series of successive washes with buffer indicated (1) heterogeneity of binding between galloylglucose and protein and (2) irreversible denaturation of protein during interaction with galloylglucose. Relatively large amounts of tetragalloylglucose were removed by initial washes, indicating weak, low affinity binding, whereas smaller amounts removed by subsequent washes suggest bonds with a higher affinity. Although the maximum number of binding sites, calculated per 10000 MW of protein, was similar for BSA, myoglobin and lysozyme, the proportion of these sites that appeared to have high affinity, varied from 8 to 29%. The low proportion of strong binding sites in lysozyme explains its relatively low tannin-complexing ability. Solubility decrease in protein during successive washing and decrease in the β-glucosidase activity indicate that irreversible denaturation of protein occurs, which progresses with an increase in the incubation time with galloylglucose and galloylglucose/ protein molar ratio in the mixture. Relative affinity of galloylglucose is directly related to the ability to cause irreversible denaturation.

11: Effects of environmental factors on two-stage tannin-protein co-precipitation

Haruo Kawamoto, Fumiaki Nakatsubo*
***(Graduate School of Agriculture)**

Phytochemistry 46(3), 479, 1997

Effects of environmental factors on two-stage co-precipitation of tetragalloylglucose with three different proteins (BSA, lysozyme, myoglobin) were investigated. Factors such as pH, temperature, and ionic strength, mainly affected the second precipitation stage. On the other hand, protein concentration mainly affected the initial complexation stage. Precipitability of the galloylglucose-protein complexes is directly related to the solubility of the original protein under each environmental condition.

12: Solubility of protein complexed with galloylglucoses

Haruo Kawamoto, Fumiaki Nakatsubo*
***(Graduate School of Agriculture)**

Phytochemistry 46(3), 485, 1997

Solubility of bovine serum albumin (BSA) (P) precipitated with tetragalloylglucose (T) was investigated by successive washing over the pH range of 3-7. The solubility was highly dependent on pH ($4 < 5 < 6 < 7 < 3$), and these results were comprehensible with the interrelation between T/P ratio required for the precipitation [T/P(R)] and number of the strong binding sites on a BSA molecule (NSB); when NSB > T/P(R) (pH 4 and 5), the precipitates were very stable, while when NSB < T/P(R) (pH 3, 6, and 7), precipitated BSA was easily solubilized by washing. Galloylglucose structure also affected the solubility of the precipitates at pH 4 (penta- < tetra- < 2,3,6-tri- < 2,3,4-tri-galloylglucose). These differences were explainable mainly with their NSBs, which increase dramatically with an increase in the number of galloyl groups in a galloylglucose molecule [35(penta) > 15(tetra) > 0(tri)].

13: Spectroscopic evidence for the formation of four-stranded solution structure of oligodeoxycytidine phosphorothioate

H. Kanehara, K. Tajima, K. Kanaori, M. Mizuguchi, and K. Makino

Biochemistry, 36, 1790-1797 (1997)

Oligodeoxycytidine phosphorothioate (PS-dCn, n = chain length), known to show virus inhibition ability by the mechanism other than the antisense one when $n \approx 20$, was explored for its solution structure by circular dichroism (CD) and ultraviolet (UV) absorption spectroscopy. For S-dC_4, when the strand concentration was higher than 10 μM, the respective 288 nm positive and 265 nm negative Cotton effects appeared in the CD spectra at slightly acidic pHs and 0°C in the absence of salt, which is indicative of a four-stranded structure (namely i-motif). Strand concentration-dependent CD spectroscopy indicated that intermolecular association is responsible for this i-motif. The formation of i-motif was also characterized by UV absorption spectroscopy, in which the dissociation of this structure caused sharp increase in the absorbance at 275 nm and decrease at 305 nm. By plotting this change, the Tm values were estimated to be respectively ca. 11 and 13°C at 20 and 50 μM strand concentrations. Stability of i-motif was compared between S-dC_4 P-chiral diastereoisomers, and Sp configuration found to produce more stable structure than Rp. S-dC_{20} was also investigated at physiological temperature, and the respective 288 nm positive and 265 nm negative Cotton effects appeared at slightly acidic pH, and the concentration-independent behavior was observed above ca. 1 μM, suggesting intermolecular folding while intramolecular folding was predominant at the low strand concentration such as 0.05 μM. Gel filtration chromatography and nondenaturing gel electrophoresis provided the supporting data for the

four-stranded folding of S-dC20.

14: Deglycosilation susceptibility and base-pairing stability of 2'- deoxyoxanosine in oligodeoxynucleotide

T. Suzuki, Y. Matsumura, H. Ide, K. Kanaori, K. Tajima, and K. Makino

Biochemistry, 36, 8013-8019 (1997)

We have demonstrated recently that nitrous acid or nitric oxide converts 2'-deoxyguanosine (dGuo) into 2'- deoxyoxanosine (dOxo) [Suzuki, T., Yamaoka, R., Nishi, M., Ide, H. & Makino, K.(1996) J. Am. Chem. Soc. *118*, 2515-2516]. In the present study, we have measured susceptibility of the *N*-glycosidic bond of dOxo to spontaneous hydrolysis and its base-pairing stability to evaluate the biological significance of dOxo as a new lesion of DNA. When oligodeoxynucleotide d(T_5OT_6) (O = dOxo), isolated from nitrous acid-treated d(T_5GT_6), was incubated at pH 4.0 and 70°C, hydrolysis of the *N*-glycosidic bond of dOxo occurred with a first-order rate constant. Comparison of the rate constants with those of dGuo and dXao indicates that the *N*-glycosidic bond of dOxo was as stable as that of the dGuo in d(T_5GT_6) and hydrolyzed 44-folds more slowly than that of 2'-deoxyxanthosine (dXao), a simultaneously generated damage by nitrous acid and nitric oxide. For the estimation of the base-pairing stability, UV melting curves were measured for the duplexes of d(T_5OT_6)·d(A_6NA_5) (N = A, G, C, and T) at neutral pH. The Tm values obtained were 15.3, 14.1, 19.3, and 16.3°C for N = A, G, C, and T, respectively, which are much lower than that of intact duplex containing a G·C pair at the same position [d(T_5GT_6)·d(A_6CA_5), Tm=32.8°C] but comparable with those of d(T_5XT_6)·d(A_6NA_5) (X = dXao, Tm=14.8-22.3°C). CD spectra of the four duplexes containing dOxo showed preservation of the intact duplex at low temperature. UV and NMR pH-titration studies indicated the p*K*a for the ring-opening and -closing equilibrium to be 9.4, implying that dOxo is in the ring-closed form at physiological pH. This structure appears to be not suitable geometrically for the hydrogen bond formation with a specific counter base, thus causing equally low Tm values for all the counter bases. Consequently, these results imply that dOxo, a novel DNA lesion, may have an important and unique role in mutagenic events in cells.

15: Mechanism for the formation of six-coordinate Fe(III)TPP-peroxide complexes studied by simultaneous ESR and optical measurements.

K. Tajima, K. Tada, J. Jinno, H. Makino, N. Azuma, and K. Makino

Inorg. Chim. Acts, 254, 29-35 (1997)

ESR and optical absorption measurements were performed for six- coordinate Fe(III)TPP-butyl peroxide complexes formed in the reaction system composed of Fe(III)TPPCl, $NaOCH_3$, and $t-$ or $n-$butyl hydroperoxide. The presence of four paramagnetic iron complexes was detected in the reaction system.

Based on the spectroscopic parameters, the spin state and the axial ligand of these species were deduced as follows: Fe(III)TPP-($HOCH_3$)-OCH_3) (A), -($^-OCH_3$)$_2$ (B), - ($^-OCH_3$)($^-$OO-butyl) (C), -($^-$OO-butyl)$_2$ (D). The coordination reactions of $t-$ and $n-$butyl hydroperoxide and complexes A and B were monitored on changing the molar ratio of [$t-$ or $n-$butylperoxide]/ [Fe(III)TPPCl]. The observed spectral changes justified that complexes A and B were successively changed to complex D through complex C. The concentration of these four paramagnetic complexes was estimated by means of the duplicate integration of the observed ESR spectra at 4.2K. The molar distribution of complexes A, B, C and D was simulated by taking into account the formation constants relating to the generation of the peroxide complexes C and D. By comparison of the formation constants, the possible mechanisms for Fe(III)TPP-peroxide complex formation were discussed.

16: DMPO spin trapping of superoxide anion in strong alkaline DMSO solution

M. Hashimoto, Y. Nakai, M. Kohno, K. Tajima, K. Kanaori, N. Endo, and K. Makino

Chem. Lett., 1997, 71-72 (1997)

Superoxide anion ($O_2^{\cdot -}$) is generated in living bodies *via* electron transfer reactions and scavenged by superoxide dismutases forming H_2O_2, which is further converted into much more toxic hydroxyl radicals (·OH). Therefore, an assay system for clinically applicable $O_2^{\cdot -}$ scavenger has been required to be established. In the present study, 5,5-dimethyl-1- pyrroline-N-oxide (DMPO) was examined in alkaline DMSO solution, which is potent to be used as $O_2^{\cdot -}$ pool, to see if DMPO/$O_2^{\cdot -}$ generated by the reaction between DMPO and $O_2^{\cdot -}$ is successfully detected by EPR. We found that $O_2^{\cdot -}$, generated in the solution, can be trapped with DMPO and the resultant nitroxide radical, DMPO/$O_2^{\cdot -}$, is sufficiently stable for the subsequent EPR detection.

17: Replication bypass and mutagenic effect of α-deoxyadenosine site-specifically incorporated into single-stranded vectors.

H. Shimizu, R. Yagi, Y. Kimura, K. Makino, H. Terato, Y. Ohyama, and H. Ide

Nucleic Acids Res., 25, 597-603 (1997)

α-2'-Deoxyadenosine (α) is a major adenine lesion produced by γ-ray irradiation of DNA under anoxic conditions. In this study, single- stranded recombinant M13 vectors containing a were constructed and transfected into *Escherichia coli* to assess lethal and mutagenic effects of this lesion. The data for a were further compared with those obtained with M13 vectors containing normal A or a model abasic site (F) at the same site. The transfection assay revealed that α constituted a moderate block to DNA replication. The *in vivo* replication capacity to pass through α was ~20% relative to normal A, but 20-fold higher

than that of F constituting an almost absolute replication block. Similar data were obtained by *in vitro* replication of oligonucleotide templates containing α or F by *E.coli* DNA polymerase I. The mutagenic consequence of replicating M13 DNA containing α was analyzed by direct DNA sequencing of progeny phage. Mutagenesis was totally targeted at the site of α introduced into the vector. Mutation was exclusively a single nucleotide deletion and no base substitutions were detected. The deletion frequency associated α was dependent on the 3'- nearest neighbor base: with the 3'-nearest neighbor base T mutation (deletion) frequency was 26%, whereas 1% with the 3'-nearest neighbor base G. A possible mechanism of the single nucleotide deletion associated with α is discussed on the basis of the misinsertion-strand slippage model.

18: Factors governing the sequence-selective DNA binding of geometrically constrained peptide dimers

T. Morii, Y. Saimei, M. Okagami, K. Makino, and Y. Sugiura

J. Am. Chem. Soc., 119, 3649-3655 (1997)

Peptide dimers of the basic leucine zipper protein with non-native monomer arrangements were synthesized by using C_2 chiral templates as a synthetic dimerization module. The amino acid sequence of the peptide is derived from the DNA contact region of the basic leucine zipper protein GCN_4. These peptide dimers are designed to possess different geometrical constrains from that of native GCN_4 with respect the orientation of two DNA-containing peptides. Peptide dimers constrained at the 6th position from N-terminus recognized novel palindromic DNA sequences in which the polarity of each half-site of the parent GCN_4 binding sequence is reversed. This is in contrast with dimers that are constrained at the $N-$terminus which failed to recognize the reversed DNA sequences. Sequence-specific recognition of these palindromic DNA sequence was confirmed by DNase I footprinting. Circular dichroism spectral analyses revealed that dimers constrained at the 6th position bind in the helical conformation to the reversed palindromic sequences, whereas the dimers constrained at the $N-$terminus bind the same sequence with less helical contents. The stability of specific binding complexes was not affected by the difference in the chirality of the template. However, the stability of the half-specific complex was dramatically affected by the particular enantiomer of the templ

19: Pterin-6-aldehyde, an inhibitor of xanthine oxidase, has superoxide anion radical scavenging activity.

K. Watanabe, T. Arai, H. Mori, S. Nakao, T. Suzuki, K. Tajima, K. Makino, and K. Mori

Biochem. Biophys. Res. Commun., 233, 447-450 (1997)

Superoxide anion radical ($O_2^{\cdot -}$) scavenging activity of neopterin (NP) and its photodegraded products was studied. NP did not affect $O_2^{\cdot -}$ release in hypoxanthine/xanthine oxidase (HPX/XOD) reaction system, but pterin-6-aldehyde (P6A), one of photodegraded products of NP, suppressed it. The identification of P6A was successful by confirming inhibiting property of xanthine oxidase. In neutrophil/phorbol myristate acetate reaction system, NP did not affect the $O_2^{\cdot -}$ release but P6A suppressed it. The suppression by P6A was not associated with oxygen uptake, which indicated that P6A did not inhibit the generation of $O_2^{\cdot -}$ but directly scavenged it. These findings suggest that P6A has ameliorating effects on ischemia- reperfusion injury in which $O_2^{\cdot -}$, which is generated both in HPX/ XOD reaction and in activated neutrophil, is one of the major substances to damage the tissues.

20: Substrate and mispairing properties of 5-formyl-2'-deoxyuridine 5'- triphosphate assessed by *in vitro* DNA polymerase reactions

M. Yoshida, K. Makino, H. Morita, H. Terato, Y. Ohyama, and H. Ide

Nucleic Acids Res., 25, 1570-1577 (1997)

5-Formyluracil (fU) is one of the thymidine lesions produced by reactive oxygen radicals in DNA and its constituents. In this work, 5-formyl-2'-deoxyuridine 5'-triphosphate (fdUTP) was chemically synthesized and extensively purified by HPLC. The electron withdrawing 5-formyl group facilitated ionization of fU. Thus, p*Ka* of the base unit of fdUTP was 8.6, significantly lower than that of parent thymine (p*Ka*=10.0 as dTMP). fdUTP efficiently replaced dTTP during DNA replication catalyzed by *Escherichia coli* DNA polymerase I (Klenow fragment), T7 DNA polymerase (3'-5' exonuclease free) and *Taq* DNA polymerase. fU-specific cleavage of the replication products by piperidine revealed that when incorporated as T, incorporation of fU was virtually uniform, suggesting minor sequence context effects on the incorporation frequency of fdUTP. fdUTP also replaced dCTP, but with much lower efficiency than that for dTTP. The substitution efficiency for dCTP increased with increasing pH from 7.2 to 9.0. The parallel correlation between ionization of the base unit of fdUTP (p *Ka*=8.6) and the substitution efficiency for dCTP strongly suggests that the base-ionized form of fdUTP is involved in mispairing with template G. These data indicate that fU can be specifically introduced into DNA as unique lesions by *in vitro* DNA polymerase reactions. In addition, fU is potentially mutagenic since this lesion is much more prone to form mispairing with G than parent thymine.

21: Mechanistic study on *meso*-hydroxyoctaethylporphyrin formation from an FeIII(oep)-H_2O_2 complex

K. Tajima, K. Tada, M. Shigematsu, K. Kanaori, N. Azuma, and K. Makino

Chem. Commun., 1997, 1069-1070 (1997)

The benzoyl ester of an iron(III) *meso*-hydroxyoctaethylporphyrin complex, containing ^{18}O derived from molecular oxygen, is isolated from the reaction solution of the complex $[Fe^{III}(oep)(OOH)(OH)]^-$ which is prepared by reduction of $[Fe^{II}(oep)(py)(^{18}O_2)]$ with sodium ascorbate.

22: Interaction of pyrylium dye with self-complementary DNA oligomer as studied by ^1H NMR spectroscopy.

K. Kanaori, K. Yokoyama, K. Tajima, N. Yamamoto, T. Okamoto, and K. Makino

Nucleosides & Nucleotides, 17, 603-611 (1998).

Interaction of 2-methyl-4,6-bis-(4-*N,N*$^-$ dimethylaminophenyl)pyrylium salt (P2) with $[d(CGACGTCG)]_2$ was investigated by ^1H NMR spectroscopy. The aromatic signals of P2 and the oligomer were shifted to the upfield by forming the complex, and intermolecular NOEs were also observed between P2 and the terminal CpG base steps but not between P2 and the central CpG. These results indicate that P2 binds to the weakly stacking CpG steps in an intercalation manner.

23: * Carrier transport mechanisms through the metal/p-type diamond semiconductor interfaces

Y.Koide, M.Yokoba, A.Otsuki, F.Ako, T.Oku, M.Muarakami

Diamond and Related Materials, 6, 847-51(1997).

The carrier transport mechanisms through the p-diamond/metal interface were studied by analyzing the dependences of the specific contact resistivities (ρ_c) on the measurement temperature and the acceptor concentration (N_A). A variety of metals such as Ti, Mo, and Cr (carbide forming metals) and Pd and Co (carbon soluble metals) were deposited on boron-doped polycrystalline diamond films, and ρ_c values were measured by a transmission line method. A constant Schottky barrier heights(SBH) of around 0.5eV was measured for these annealed contacts, and the reason was believed to be due to phase transformation from metastable diamond to a stable conductive graphite layer in the vicinity of the diamond/metal interface. By controlling the crystal structure at the diamond/metal interface, non-annealed ohmic and high-voltage Schottky contacts were successfully develpoped.

24: Carrier transport mechanisms of Ohmic contact to p-type diamond

M.Yokoba, Y.Koide, A.Otsuki, F.Ako, T.Oku, M.Muarakami

J.Appl.Phys., 81(1997)pp.6815-21.

The carrier transport mechnism through the p-diamond/metal interface was studied by measuring specific contact resistance (ρ_c) using a transmission line method for Ti, Mo, and Cr (carbide forming metals) and Pd and Co (carbon soluble metals) metals contacting to the boron-doped polycrystalline diamond films. Schottky barrier heights(ϕ) of around 0.5eV were measured for the annealed contacts. The present result indicates that formation of thermally stable graphite layers at the diamond/metal interfaces upon annealing would pin the Fermi level of the p-diamond. This model led to the preparation of *in situ* Ohmic contacts by depositing a thin diamond like carbon on the p-diamond suface prior to metal deposition, and also to excellent Scottky contacts with breakdown voltages higher than 900V. The present experiment concluded that the existence of a graphite layer at the diamond/metal interface controlled the electrical properties through the p-diamond/metal interface.

25: Temperature dependence of energies of [001] tilt boundaries in aluminum

A.Otsuki

Proceedings of JIMIS-8, The Japan Institute of Metals, (1996), pp.323-326.

The temperature dependence of energies of [001] tilt boundaries in the aluminum is measured by a dihedral angle method. The boundary energies are estimated relatively with respect to solid aluminum/liquid tin interfacial energies, which are caluculated by using of Eustathopoulos-Joud-Desré (ECD) model as a function of temperature. The temperature dependence of the boundary energies, i.e. the entropy, is found to be dominated by the temperature dependence of elastic constants.

26: Stored Energy and electromotive-force of mechancally milled copper

A.Otsuki,P.H.Shingu and K.N.Ishihara

Materials Science Forum, 235-238, 949-53(1997).

The electromotive-force(EMF) of mechanically milled copper relative to the annealed copper was measured by using a solid state super ionic conductive cell at 30°C. The measured EMF values reached -19mV after 100 h milling. This value corresponds to an excess free energy of 1.8kJ/mol for the milled

Cu powders relative to well annealed Cu. The enthalpy released from stored energy due to annealing measured by DSC was larger than the free energy change with the same annealing measured by EMF.

27: Development of Nuclear Power Plant Operator Simulator for Man-Machine Interface Evaluation

マンマシンインタフェース評価のための原子力運転員行動シミュレータの開発

NAKAGAWA Takashi*, NAKATANI Yoshio*, SASAKI Kazunori*, YOSHIKAWA Hidekazu, TAKAHASHI Makoto, FURUTA Tomihiko, HASEGAWA Akira****

(Industrial Electronics & System Development Laboratory, Mitsubishi Electric Corporation), *(Institute of Human Factors, Nuclear Power Engineering Corporation)**

Journal of the Society of Instrument and Control Engineering, Vol.33, No.8, pp.834-842, 1997

計測自動制御学会論文集、３３巻、８号、８３４－８４２、１９９７

The operational safety in nuclear power plants depends strongly on man machine interfaces (MMI), such as assignment of equipment on control boards and operation procedures in emergency situations. Therefore, the evaluation and analysis methods for the MMI are important. In order for the methods to be practical, the methods should be executed in each step of design and be easy for designers to use. We aim to develop SEAMAID system: a computer supported system for evaluating and analyzing the MMI by simulating the interaction between the operator and the machine. In this paper, we discuss problems of the conventional methods and the required functions of the operator simulator for the SEAMAID. The operator simulator executes not human errors but correct behavior which follows the operational procedure. The SEAMAID evaluates the MMI by finding potential human errors which could occur in the simulated interactions and points out the problematic interaction parts which could induce human errors.(in Japanese)

28: Simulation of Machine-Maintenance Training in Virtual Environment

仮想空間における機器保修訓練シミュレーション

YOSHIKAWA Hidekazu, TEZUKA Tetsuo, KASHIWA Ken-ichiro, ISHII Hirotake

Journal of the Atomic Energy Society of Japan, Vol.39, No.12, pp.1078-1089, 1997

日本原子力学会誌、３９巻、１２号、１０７８－１０８９、１９９７

The periodical inspection of nuclear power plants needs a lot of workforces with a high degree of technical skill for the maintenance of various sorts of machines. Therefore, a new type of maintenance training system is required, where trainees can get training safely, easily and effectively. In this study we developed a training simulation system for disassembling a check valve in virtual environment (VE). The features of this system are as follows: Firstly, the trainees can execute tasks even in wrong order, and can experience the resultant conditions. In order to realize this environment, we developed a new Petri-net model for representing the objects' states in VE. This Petri-net model has several original characteristics, which make it easier to manage the change of the objects' states. Furthermore, we made

a support system for constructing the Petri-net model of machine-disassembling training, because the Petri-net model is apt to become of large size. The effectiveness of this support system is shown through the system development. Secondly, this system can perform appropriate tasks to be done next in VE whenever the trainee wants even after some mistakes have been made. The effectiveness of this function has also been confirmed by experiments.(in Japanese)

29: A study on VR-based Mutual Adaptive CAI system for Nuclear Power Plant

FUKUSHIMA Shogo*, TAKAHASHI Makoto, YOSHIKAWA Hidekazu
***(Matsushita Electric Works, Ltd.)**

Proc. of NUTHO-5 (FIFTH Topical Meeting on Nuclear Thermal Hydraulics, Operation & Safety), pp.DD3/1-DD3/6, 1997

A novel framework of human-computer-interaction for computer aided instruction (CAI) system is presented which aims at introducing a new off-the-job training environment to master nulear power plant monitoring skill by more user-friendly manner than by present. The framework is based on the following two new ideas: one is mutual adaptive interface (MADI) concept, and the other is virtual reality (VR). In order to realize a hardware mechanism of mutual adaptive interface based on VR, a new head-mounted-display (HMD) was developed which can not only provide the user with virtual environment conventionally but also detect the user's eyes images for in-situ analysis of various ocular information. The information are expected to utilize for realizing advanced human-computer-interaction in the CAI system.

30: Application of a Newly Developed Eye Sensing Head-Mounted-Display to a Mutual Adaptive CAI for Plant-Diagnosis

FUKUSHIMA Shogo*, YOSHIKAWA Hidekazu
***(Matsushita Electric Works, Ltd.)**

Proc. of HCI'97 (Human Computer Interaction), No.21B, pp.225-228, 1997

An innovative framework of mutual adaptive CAI system is proposed in this paper for teaching plant diagnosis knowledge by more human friendly than by conventional CAI method. In order to realize such CAI, a new head-mounted-display, i.e., Eye-Sensing Head-Mounted-Display (ES-HMD), has been developed which will not only provide the user with virtual environment through visual and auditory stimuli but will also monitor the user's both eyes and calculate ocular information such as pupil size, eyeblink or eye gaze. The obtained ocular information will be utilized for on-line analysis of user's mental workload, cognitive state and longtime fatigue, because user's ocular information will reflect on such psychological factors unconsciously while watching display image. Some experimental results are also presented to test eye tracking capability by using the developed ES-HMD.

31: Development of Eye-Sensing HMD and its Application Experiments for Observing Human Ocular Information Processing Characteristics

YOSHIKAWA Hidekazu, SHIMODA Hiroshi, FUKUSHIMA Shogo*, MORIKAWA Daisuke, FUJIYAMA Hiroaki

***(Matsushita Electric Works, Ltd.)**

Proc. of AROB 3rd '98 (Artificial Life and Robotics), pp.7-10, 1998

A new Head-Mounted Display (HMD), "Eye-Sensing HMD (ES-HMD)" was developed as a VR-based human interface. The basic experiments are conducted to apply ES-HMD for the study of eye movement characteristics of stereoscopic view imposed by VR.

32: Modeling of Diagnosis Behavior of Nuclear Power Plant Operator

WU Wei, YASUTA Akira, TAKAHASHI Makoto, YOSHIKAWA Hidekazu

Proc. of NUTHO-5 (FIFTH Topical Meeting on Nuclear Thermal Hydraulics, Operation & Safety), pp.DD1/1-DD1/6, 1997

Using Nuclear Power Plant(NPP) simulator, a laboratory experiment was conducted for several experts in NPP operation, in order to construct a computer model on operators diagnostic process. The derived operator model was organized so that it could model and interpret the cognitive behavior of each subject during experiment. The numerical simulation by the model was compared with the experimental results with respect to its accuracy.

33: A Study on Constructing a Machine-Maintenance Training System Based on Virtual Reality Technology

ISHII Hirotake, KASHIWA Ken-ichiro, TEZUKA Tetsuo, YOSHIKAWA Hidekazu

Proc. of NUTHO-5 (FIFTH Topical Meeting on Nuclear Thermal Hydraulics, Operation & Safety), pp.DD2/1-DD2/6, 1997

The development of a VR based training system is presented for teaching disassembling procedures of mechanical machines used in nuclear power plant. The methods of Petri net model for describing trainees' plausible actions in the disassembling process and reducing a right sequence of action sequence are developed as well as realization of the related Petri net editor and the demonstration of the developed VR based training system was demonstrated by example practice of disassembly simulation of check valve. Moreover, the needed future works are also discussed.

34: An Experimental Study on Estimating Human Error Probability (HEP) Parameters for PSA/HRA by Using Human Model Simulation

YOSHIKAWA Hidekazu, WU Wei

Proc. of CSAPC'97 (Cognitive Science Approach to Process Control), pp.60-65, 1997

A framework of Human Error Probability (HEP) parameters is first proposed, which is needed for Human Reliability Analysis (HRA) within a practice of Probabilistic Safety Assessment (PSA) of Nuclear Power Plant (NPP). Then, a laboratory experiment has been conducted for constructing a computer simulation model (human model) which describes human cognitive behavior on detecting and diagnosing plant anomaly cause. Inter-comparison between experimental data and human model simulation has been made to estimate Human Cognitive Reliability (HCR) curves , in order to confirm the applicability of human model for estimating such HEP parameters for PSA/HRA practice.

35: A Pilot Study on Human Cognitive Reliability (HCR) by Human Model Simulation

WU Wei, YOSHIKAWA Hidekazu

Proc. of IIS'97 (Intelligent Information Systems), pp.95-99, 1997

Based on human model simulation, an estimation method for basic Human Error Probability(HEP) parameters is presented, for Probability Safety Assessment (PSA) / Human Reliability Assessment(HRA) in Nuclear Power Plant(NPP). A framework of HEP parameters needed for PSA/HRA is firstly described, and then in order to construct a human model on plant anomaly diagnosis at NPP, methods of laboratory experiment are briefly explained. An experiment was conducted for obtaining information about operators' cognitive behavior. Two kinds of Human Cognitive Reliability(HCR) curves for detecting and diagnosing an anomaly were derived from the experimental data and the characteristics of both curves were analyzed with respect to the nature of time dependency of the HEP. The human model was constructed for simulating the operators' cognitive behaviors during the detection and diagnosis phase. Using the human model, HCR curves for anomaly detection phase were deduced by computer experiments. The inter-comparisons of the HCR curves with the experimental data resulted in that the application of human model simulation would be feasible for the estimation of HEP parameters needed for PSA/HRA.

36: Integrated Design Support Systems for Conceptual Design of a Space Power Reactor

SHIMODA Hiroshi, YOSHIKAWA Hidekazu, NAGAMATSU Tadashi, TAKEOKA Satoshi

Proc. of IIS'97 (Intelligent Information Systems), pp.298-302, 1997

The conceptual design of a space power reactor core requires cooperative work by a group of experts from various fields. It is necessary to implement mechanisms to realize an effective computerized support system for group activity by different engineers. We aimed at incorporating tasks into a workable human interface system based on virtual reality technology with the full usage of advanced information technology on 3D graphics, numerical calculation and AI processing. We also aimed at developing a WWW-based design support system for the same work domain for higher levels of flexibility in cooperative work using distributed computer systems. In this paper, we describe the structure of the space reactor as a conceptual design target, a VR-based design support system to realize an effective human interface and WWW-based design support system for effective cooperative work.

37: A Basic Study on Exploring Real-time Verbal Protocol Analysis System for Analyzing Diagnostic Cognitive Process of Nuclear Power Plant Operators

OZAWA Takahisa, UMEDA Naoki, SHIMODA Hiroshi, TAKAHASHI Makoto, YOSHIKAWA Hidekazu

Journal of Tsinghua University (Science and Technology), Vol.37, No.S3, pp.183-194, 1997

This paper presents two types of cognitive experiments and one developing system for realization of the mutual adaptive interface (MADI). Effectiveness of Verbal Protocol and Operational Sequence History for the cognitive behavior analysis has been evaluated from the experimental data obtained by first type of cognitive experiments using nuclear power plant simulator. Effectiveness of our proposed systematic analysis method to trace subjects' cognitive processes has been evaluated from the second type of experiments similar to the first one but using a voice recognition device. Based on the both results, a future development plan of the real-time cognitive process estimation system is discussed in relation to MADI.

38: A Study on VR-based Plant-Maintenance Training System

TEZUKA Tetsuo, YAMAMOTO Michiya, ISHII Hirotake, YOSHIKAWA Hidekazu

Journal of Tsinghua University (Science and Technology), Vol.37, No.S3, pp.53-64, 1997

We have developed new types of plant-maintenance training systems by using virtual reality (VR). One is the training system for disassembling a check- valve, and the other is that for detecting the failure part in the logic card of the control-rod driving-mechanism control system. VR-based training system is expected to have salient features as an experience-oriented CAI system, and these two training simulation systems showed its promising applicability in the area of plant maintenance. In this paper, the functions necessary for the VR- based experience-oriented training system are first discussed, and then explained is the way how they were realized in the two training systems we developed. The future developmental works are also discussed, for realizing the effective training simulation system.

39: * Numerical Simulation of Below-Cloud Scavenging of Gaseous and Particulate Matters

Susumu Tohno, Junji Ueda*, Mikio Kasahara
*** (Graduate School of Engineering)**

Journal of Aerosol Science, Vol.28, No.S1, pp.S455-S456, 1997

One-dimensional and time-variant model was presented for simulating below-cloud scavenging of gaseous and particulate matters. The model includes gas absorption, particle capture and aqueous chemical reactions in rain water. We calculated and analyzed the effects of below-cloud acidification on precipitation chemistry at the surface. Contribution of aerosols to sulfate and nitrate concentrations in rain was extremely small in our calculation conditions. Simulation results of S(VI) and Ca^{2+} concentrations (C) in rain at ground level indicated that C/r-dependence (relation between C and raindrop size) was different between the two compounds after long precipitation times. The difference can be explained by the fact that Ca^{2+} in rain attributes from the scavenging of coarse calcium aerosols, while aqueous phase oxidation of SO_2 is the major contribution to S(VI) in ran water.

40: Analysis of Acid Rain 1991-1995 and Regional Climate in South China

Yintang Li*, Mikio Kasahara
***(Xi'an Jiaotong University)**

J. Japan Soc. Atmos. Environ., Vol.33, No.1, pp.50-59, 1997

大気環境学会誌, 33 巻, 1 号, pp.50-59, 1997

The distributions of acid rain* with the annual mean pH of rainfalls and acid rain frequency of yearly precipitation in South China are described for the period of 1991-1995. The areas suffering from heavy acid rain were the Sichuan Basin, Guizhou, Hunan and Jiangxi (SGHJ) where is the center of South China. Some climate features in SGHJ are summarized about cloud, precipitation, and wind. The formation reasons of acid rain are discussed. The lowest annual mean pH of rainfalls was 3.8, and the acid rain frequency of yearly precipitation exceeded 90% in several cities. The most flourishing districts where the

energy consumption is greatest is not in SGHJ but in the coastal area. The climate characters in SGHJ such as cloudy, moist and weak wind, must be the important factors for the acid rainfall, although SO_2 emission is the original cause. The maximum annual mean of total cloudiness canopies the main part of Sichuan-Guizhou where the acid rain originated in China and is a part of acid rain region all along. The annual rainfall amount in SGHJ is large but slightly less than that of the southeast coast. However, its annual mean of rainy days is higher than that of the coast. The prevailing wind speeds, directions and frequencies in SGHJ, and its geographical features, are unfavorable to diffusion.

41: Comparison between Equilibrium Cycle and Successive Multicycle Optimization Methods for In-Core Fuel Management of Pressurized Water Reactors

ＰＷＲ炉心燃料管理における平衡サイクル及び連続複数サイクル最適化手法の比較

Akio Yamamoto, Keiji Kanda

J. Nucl. Sci. and Technol., Vol.34, no.9, p.882-892, 1997

Analysis of an equilibrium cycle are useful for evaluating newly designed fuels, defining an envelope of core operating parameters, and so on. However, generation of a loading pattern for the equilibrium cycle is much more difficult than that of a single cycle. Therefore, a loading pattern optimization code for the equilibrium cycle of pressurized water reactors, OPAL, had been newly developed on the basis of the simulated annealing method. In order to verify the capability of the OPAL code, comparison with successive multicycle optimizations was performed while fixing the number of fresh fuel in each cycle. Through benchmark calculations, it was found that the result of the equilibrium cycle optimization was almost compatible with that of the successive multicycle optimization, when the definition of each objective function was similar. However, successive multicycle optimization includes some ambiguity due to limits on the number of calculated cycles, since it requires much computation time. Consequently, the equilibrium cycle optimization has advantages including the quantitative comparison of the core neutronic performances.

42: New Method of Estimating Electric Power Plants Planning Taking Security into Consideration

エネルギーセキュリティを考慮にいれた電源構成計画を評価するための手法の開発

Hiroshi Yamagata, Keiji Kanda

日本リスク研究学会誌　第９巻、　第１号、　43頁－50頁、　1997年

When we make an electric power plant construction plan, we have to take into consideration the four view points: cost, technology, environment, and security. The purpose of this paper is to define security quantitatively, and to develop a new model that takes security into consideration. We proposed to define security as variance of cost and expected cost of the future combination of power plants. We developed the new model that calculate variance of cost by a Monte Carlo method.

43: Establishment of Nuclear Liability Regime in the Developing Countries - Examples of China and Indonesia -

発展途上国における原子力損害賠償制度の整備ー中国とインドネシアの例ー

Kenkichi Hirose, Keiji Kanda

J. At. Energy Soc. Japan, Vol.39, No.12, pp.1028-1034, 1997

日本原子力学会誌、 第39巻、第12号、 1028頁－1034頁、 1997年

While the nuclear developed countries has been establishing the nuclear liability regime in the form of national law and international treaty, establishment of the nuclear liability regime in the devolping countries which try to actively promote nuclear development is desired. In the Asian area in which a large-scale nuclear development is expected in the future, China which has already started nuclear development showed a basic policy of nuclear liability regime in the form of "reply" instead of establishing a legal framework, and Indonesia which will start a nuclear development in the future has made a high-level legal framework covering nuclear liability regime. To develop nuclear liability regime in the developing countries it is important to give consideration to establishment of national law in each country, increase in amount of liability and international cooperation and linkage in the area.

44: * Measurement of Level Density Parameters of Fission Fragments Following Thermal Neutron Induced Fission of Uranium-235

ウラン-235の熱中性子核分裂に伴う核分裂片の準位密度パラメータの測定

Katsuhisa Nishio*, Itsuro Kimura*, Yoshihiro Nakagome
***(Graduate School of Engineering, Kyoto Univ.)**

J. Nucl. Sci. and Technol., Vol.34, No.5, pp.439-444, 1997

Level density parameters of fission fragments following the thermal neutron induced fission of 235U were determined as function of the fragment mass by measuring the energy and multiplicity of prompt neutrons from a specified mass. This measurement gave the absolute values of the parameters for the neutron-rich nuclei covering the mass range from 80 to 155u except the region from 115 to125u. The obtained parameters showed a saw-tooth trend against the mass with the minimum value around the double magic number, 132u, and this trend was close to that for 252Cf(s.f) by Budtz-Jorgensen et al. The analysis by a phenomenological description of the level density parameters including the shell and collective effects suggested the existence of a collective motion of the fission fragemnt at the moment of prompt neutron emission.

45: Role of Effective Distance in the Fission Mechanism Study by the Double-energy Measurement for Uranium Isotopes

ウラン同位体の二重エネルギー測定による核分裂機構研究における実効距離の役割

Hiroshi Baba*, Tadashi Saito*, Naruto Takahashi*, Akihiko Yokoyama*, Takahiro Miyauchi*, Sigehisa Mori*, Daisaku Yano*, Teruyuki Hakoda*, Koichi Takamiya*, Kiyoshi Nakanishi*, Yoshihiro Nakagome

***(Faculty of Science, Osaka Univ.)**

J. Nucl. Sci. and Technol., Vol.34, No.9, pp.871-881, 1997

Fission product kinetic energies were measured by the double-energy method for thermal-neutron fission of 235,233U and proton-induced fission of 238U at the 15.8-MeV excitation. From the obtained energy-mass correlation data, the kinetic-energy distribution was constructed from each mass bin to evaluate the first moment of kinetic energy for a given fragment mass. The resulting kinetic energy was then converted to the effective distance between the charge centers at the moment of scission. The effective distances deduced for the proton-induced fission was concluded to be classified into two constant values, one for asymmetric and the other for symmetric mode, irrespective of the mass though an additional component was further extracted in the asymmetric mass region. This indicates that the fission takes place via two well-defined saddles, followed by the random neck rupture. On the contrary, the effective distances obtained for thermal-neutron induced fission turned out to lie along the contour line at the same level as the euilibrium deformation in the two-dimensional potential map. This strongly suggests that it is essentially a barrier-penetrating type of fission rather than the over-barrier fission.

46: Minimizing Energy Consumption in Industries by Cascade Use of Waste Energy

Naoki Hayakawa and Yoichi Kaya

IEEE/PES Winter Meeting, 98WM266, 1998

47: Effect Analysis of Wheeling in Electric Power Network

Hideki Katsumata and Yoichi Kaya

The 14th Conference on Energy System Economics, 1998

48: Estimation of Global Energy Future Scenario Using the DNE 21 Model

Kae Takase and Yoichi Kaya

The 14th Conference on Energy System Economics, 1998

II Department of Fundamental Energy Science

(エネルギー基礎科学専攻)

49: Electrochemical behavior of a graphite anode in fluorosulfonic acid at -78°C

Rika Hagiwara, Yasuhiko Ito

Journal of Fluorine Chemistry, Vol. 87, pp.185–188, 1998

Electrochemical oxidation of fluorosulfate ion (SO_3F^-) on a graphite anode gives peroxydisulfuryl difluoride at -78°C in KSO_3F/ HSO_3F solution. Continuous electrolysis finally results in a potential jump of the graphite anode, which is quite similar to the anode effect found in the molten KF·2HF electrolysis to produce elemental fluorine. The formation of a metallic blue graphite fluorosulfate, $C_xSO_3F{\cdot}n(HSO_3F)$, is mainly achieved by the chemical reaction of graphte with $S_2O_6F_2$ as the electrolyte solution is warmed up to room temperature after the electrolysis.

50: * Reactions of graphite hexafluoroarsenates with fluorobases in anhydrous hydrogen fluoride

Rika Hagiwara, Kazukiyo Tozawa, Yasuhiko Ito

Journal of Fluorine Chemistry, Vol.88, pp.201–206, 1998

A first-stage graphite intercalation compound of a strong fluoroacid, graphite hexafluoroarsenate ($C_{10}AsF_6$) reacts with fluorobases such as potassium fluoride in anhydrous hydrogen fluoride (AHF) to give a second-stage compound. X-ray diffraction adn XPS analyses revealed that the compound is covered with planar-sheet graphite fluoride, C_xF. $C_{10}AsF_6$ also reacts with the solvent hydrogen fluoride, liberating AsF_5 to give a mixture of the first- and second-stage compounds. Surface coverage of the material with graphite fluoride protects the bulk graphite fluoroarsenates from the attack of moisture in air.

51: * Electrocehemical hydrogen absorbing behavior of Pd and Pd-Li alloys in a molten LiCl-KCl-LiH system

Toshiyuki Nohira, Yasuhiko Ito

Journal of the electrochemical society, Vol. 144, pp. 2290–2295, 1997

Electrochemical hydrogen absorption and desorption into/from Pd and Pd-Li alloys were studied in a molten LiCl-KCl-LiH system (5 mol% LiH added) at 673 K. A cyclic voltammogram for a Pd electrode indicates that the current is largely due to a hydrogen related reaction and partly due to a Li related reaction. Pd spontaneously changes into $PdLiH_x$ merely by immersion into the molten LiCl- KCl-LiH system, because the anodic hydrogen absorption and the cathodic lithium deposition occurs on the same surface. By chronopotentiometry, H/Pd ratios were estimated for Pd, Pd_7Li, Pd_2Li and PdLi electrodes after hydrogen charging at 0.6 V for 0.5 hour as 0.05, 0.08, 0.27 and 0.74, respectively. These results show that the hydrogen absorbing ability of the alloys increases as the Li concentration increases. These characteristics can be explained by the stronger interaction of Li-H than of Pd-H.

52: * Thin-film quantitative microanalysis of the cation composition in ceramics with ultrathin-window-type energy-dispersive X-ray spectroscopy in a transmission electron microscope

Junya Kondoh, Shiomi Kikuchi, Yoichi Tomii, Yasuhiko Ito

Philosophical magazine B, Vol. 76, No. 1, pp. 23-45, 1997

Quantitative elemental microanalysis of the cation composition in ceramics was examined by ultrathin-window-type energy-dispersive X-ray spectroscopy (EDS) in a transmission electron microscope. One object of this investigation was the development of a quantitative analysis method by which absorption correction can be carried out. Another was to determine how anions in ceramics are treated in quantitative elemental analysis. The two-beam intensity ratio method was improved for ceramics and the method by which the absorption effect of anions is taken into consideration and the concentration of anions is not analyzed was developed. This method is the best way to determine the composition of cations of and foil thickness. It was shown that the quantitative accuracy of anions is not very good and that quantitative elemental analysis of anions is somewhat difficult using EDS, in a transmission electron microscope.

53: * Stress on a reaction vessel by the swelling of a hydrogen absorbing alloy

K. Nasako, Y. Ito, N. Hiro*, M. Osumi**
***(Mechatronics Research Center,Sanyo Electric Co.Ltd.),**
****(Mechatronics Research Center,Sanyo Electric Co.Ltd.)**

Journal of Alloys and Compounds , 264 , 271-276 , (1998)

There is a possibility that hydrogen absorbing alloys will generate unexpected stress in an alloy bed and deform or destroy hte vessel because the alloys expand when they absorb hydrogen.The amount of stress generated on the vessel surface by alloy swelling was measured with the object of elongating the life time of the reaction vessel in heat utilization systems that use hydrogen absorbing alloys.As a result,it

was found that 1)localized stress is generated at the bottom of the vessel due to hydrogen ab-/desorption cycles with an alloy packing fraction of 50 vol%, and this stress not only increases with each cycle,but also continues to increase even after plastic deformation of the vessel,2)stress accumulation depends on the amount of hydrogen ab-/desorption and on the initial packing fraction,and 3)the mechanism for stress accumulation can be estimated as a two-step process in which agglomeration between the hydride particles occurs when the packing fraction of hydride is higher than 61 vol% in the initial cycles(Step1),and then fine powder generated by pulverization during the cycles falls in gaps at the bottom of the vessel and causes the hydride packing fraction at the bottom of the vessel to gradually increase(Step2).

54: * Thermodynamic properties of Pd-Li alloys

Toshiyuki Nohira, Yasuhiko Ito

Journal of the electrochemical society, Vol. 145, No. 3, pp. 785-790, 1998

The potentials for various Pd-Li alloys in coexisting phase states were investigated in LiCl-KCl eutectic melt in the temperature range of 673-773 K. The activities and the relative partial molar Gibbs free energies of Li were calculated from the measured potentials for various Pd-Li alloy phases, i.e., Pd_7Li, Pd_2Li, PdLi, $PdLi_2$ and the liquid phase. The relative partial molar entropies and enthalpies of Li were also calculated for the Pd-Li alloys by using the temperature dependence of the potentials. Using the Gibbs- Duhem relation, the activities and the relative partial molar properties of Pd were calculated from the activities of Li for the Pd-Li alloy phases. Finally, the standard Gibbs free energies of formation were calculated for the Pd-Li alloy phases.

55: * Electrochemical Behavior of Nitride Ions in a Molten Chloride System

Takuya Goto, Masayuki Tada, Yasuhiko Ito

Journal of the Electrochemical Society, Vol. 144, No. 7, p. 2271-2276, 1997

The electrochemical behavior of nitride ions in a LiCl-KCl eutectic melt has been studied by cyclic voltammetry, chronopotentiometry, chronoamperometry and gas analysis. Nitride ions are oxidized to form nitrogen gas almost quantitatively on nickel electrodes according to the following reaction: $N^{3-} = 1/2\ N_2 + 3\ e^-$. This reaction is reversible, one-step, three-electron reaction governed by a simple diffusion- controlled charge-transfer process. The diffusion coefficient of nitride ion was found to be 1 X 10^{-5} cm^2 s^{-1} at 450 C.

56: * Characterization of Two-Phase Composites in Terms of the Percolation Phenomenon

Katsukuni Yoshida

Proc. 5th Japan International SAMPE Symposium, pp. 999-1002 (1997)

Electric properties such as conductivity and dielectric constant have been investigated for two types of composites: metal-insulating ceramics and metal-conducting ceramics (cuprates). These composites show some difference between them in the critical behavior peculiar to the percolation transition, which is analogous to the well-known phase transition. The composite Nb-Al_2O_3 has the exponent t very closed to the universal value, while the composite Ag-doped cuprate has t much smaller than the universal one. However, another exponent s observed does not show significant difference between these composites, having the value proximate to the universal one. This discrepancy between t and s can be explained in terms of the scaling model considering a role of the specific-resistivity ratio of the constituent phases. Those factors describing the critical behavior are fond to be effective for characterizing the composites.

57: Thermal Conductivity of the c-Axis Aligned $(Bi,Pb)_2Sr_2Ca_2Cu_3O_y$ in the Superconducting and Mixed States

M. Matsukawa*, K. Iwasaki*, K. Noto*, T. Sasaki*, N. Kobayashi, K. Yoshida, K. Zikihara*** , M. Ishihara*****

***(Iwate Univ.), **(Tohoku Univ.), ***(Sumitomo Heavy Industries Ltd)**

Cryogenics, Vol. 37, pp. 255-262 (1997)

The thermal conductivity of a c-axis aligned BPSCCO polycrystal in the superconducting and mixed states has been studied as a function of temperature and magnetic field up to 14 T along the c-axis. Comparing the κ data of a semiconducting sample with those of a metallic sample, an observed anomaly in κ below T_c is attributed to the electric thermal conductivity κ_e, and seems to be explained by the electron-electron interaction model based on a strong suppression of the quasiparticle scattering rate in the superconducting state. A peak value in κ decreases and its position shifts to higher temperatures with increasing field strength. This behavior in $\kappa(T)$ is roughly described by the Kadanoff-Martin expression in κ taking into account quasiparticle scattering by quasiparticles in the normal core at several fixed fields. The K-M expression extended to the mixed states qualitatively explains an observed nonlinear filed dependence of $\kappa(H)$ at several fixed temperatures.

58: * Critical Behavior of the Resistivity of Sintered $(Bi,Pb)_2Sr_2Ca_2Cu_3O_y$ on Varying Composition Ratio

Katsukuni Yoshida, Michiaki Matsukawa*, Shizumasa Ueda**
(Iwate Univ.), *(Institute of Advanced Energy, Kyoto Univ.)**

Materials Science Research International, Vol. 3, pp. 190-191 (1997)

We have investigated the clustering process in Ag-added (Bi, Pb)-Sr-Ca-Cu-O 2223 composites with the critical temperature $T_c \approx 110$K. Main attention was focused on the difference in the particulate shape of Ag- and cuprate-grains, expecting that this difference results in variance between their ways of clustering. As T is lowered, the contribution from the cuprate phase is to be enhanced, since the phase finally becomes superconducting. However, this contribution is uncovered only at extremely low temperature, much lower than 77K. This implies superconducting clusters are constructed by the interfacial weal-link among the cuprate grains. The percolation power law for the cuprate phase shows that the spatial extension of the cuprate clusters is two-dimensional. This variance between the Ag phase and the cuprate phase is ascribable to the difference in the original grain shape of two phases.

59: * Hydrothermal Synthesis and Structure Refinements of Alkali-Metal Trivanadates AV_3O_8(A = K, Rb, Cs)

Yoshio Oka*, Takeshi Yao and Naoichi Yamamoto**
***(Faculty of Integrated Human Studies)**
****(Graduate School of Human and Environmental Studies)**

Materials Research Bulletin Vol. 32, pp. 1201-1209, 1997

Hydrothermal methods for growing single crystals of alkali-metal trivanadates AV_3O_8 for A = K, Rb, Cs and their single-crystal structural studies are presented. Plate- shaped orange crystals were hydrothermally grown at 250°C from V_2O_5 powders dispersed in $A(NO_3)$ solutions. RbV_3O_8, the structure of which has remained undetermined, was found to be isostructural with KV_3O_8 and CsV_3O_8: the monoclinic system $P2_1/m$ with a = 4.9864(8) Å, b = 8.442(1) Å, c = 7.8621(7) Å, β = 96.064(9)°, and Z = 2. The crystallographic data for KV_3O_8 and CsV_3O_8 have been revised; in particular, the data of KV_3O_8 has been greatly improved. AV_3O_8 adopts a layered structure with V_3O_8 layers consisting of VO_6 octahedra and VO_5 square pyramids. The oxygen coordination around interlayer A atom is AO_8 for A = Rb, Cs but is regarded as AO_6 for A = K from the anomalous variation of A–O distances with A^+ ionic radii.

60: On the Layer Structure of Vanadium Pentoxide Gels — Comment on "Molecular Dynamic Simulation of the Vanadium Pentoxide Gel Host"

Takeshi Yao and Yoshio Oka*
***(Faculty of Integrated Human Studies)**

Solid State Ionics vol. 96, pp. 127-128, 1997

A comment on the article entitled "Molecular dynamic simulation of the vanadium pentoxide gel host" [J. Linde and J. O. Thomas, Solid State Ionics 85, (1996) 1] is presented concerning the model structure of the V_2O_5 layer of vanadium pentoxide gels. The double-layer structure used in the simulation was derived from the crystalline V_2O_5. This model structure significantly differs from the double-sheet type determined by the X-ray Rietveld method. The simulation should be recalculated based on the double-sheet type V_2O_5 layer.

61: Synthesis of $LaMeO_3$ (Me = Cr, Mn, Fe, Co) Perovskite Oxides from Aqueous Solutions

Takeshi Yao, Akira Ariyoshi and Takashi Inui

Journal of the American Ceramic Society Vol. 80, pp. 2441-2444, 1997

$LaMeO_3$ (Me = Cr, Mn, Fe, Co) perovskite oxides have many functional uses, and methods for forming films from aqueous solutions are advantageous compared with CVD, sputtering, sol-gel methods, etc., because of lower cost, no requirement for a vacuum or high temperature, and applicability to films with wide areas and/or complicated shapes. A novel method for synthesizing $LaMeO_3$ from aqueous solutions at ordinary temperature and pressure has been discovered. $LaMeO_3$ powder produced by solid-state reaction was dissolved in hydrofluoric acid. Boric acid was added to shift the chemical equilibrium, then $LaMeO_3$ was synthesized. This method promises to lead to applications for preparing perovskite films for various uses.

62: * Crystal Structures of Hydrated Vanadium Oxides with δ-Type V_2O_5 Layers: δ-$M_{0.25}V_2O_5 \cdot H_2O$, M = Ca, Ni

Yoshio Oka*, Takeshi Yao, Naoichi Yamamoto**
***(Faculty of Integrated Human Studies)**
****(Graduate School of Human and Environmental Studies)**

Journal of Solid State Chemistry Vol. 132, pp. 323-329, 1997

Single crystals of hydrated vanadium oxides with layered structures containing divalent Ca or Ni were hydrothermally grown, and their structural characterization was focused on the interlayer sites. Both compounds are formulated by $M_{0.25}V_2O_5 \cdot H_2O$, M = Ca, Ni and crystallize in the monoclinic system $C2/m$ with $Z = 4$: $a = 11.692(2)$, $b = 3.564(1)$, $c = 10.986(2)$ Å, $\beta = 105.42(1)°$ for M = Ca; $a = 11.756(1)$, $b = 3.649(1)$, $c = 10.364(2)$ Å, $\beta = 95.03(1)°$ for M = Ni. The structures consist of δ-type V_2O_5 layers stacking along the c axis and interlayer hydrated M^{2+} ions; the δ refers to the V_2O_5 layer of δ-$Ag_{0.68}V_2O_5$ after which the compounds are designated δ-$M_{0.25}V_2O_5 \cdot H_2O$. The M atoms partially occupy interlayer sites of the $2c$ position for M = Ni and the $4i$ position for M = Ca, to each of which four water molecules (O_w) are attached forming MO_{w4} rectangles. M and O_w site occupancies indicate that the MO_{w4} rectangles are distributed so that they do not interact with each other, and the above stoichiometric formula correspond to the maximum occupancies. Bonding to three apical oxygens of the V_2O_5 layers, the Ca atom forms a CaO_7 polyhedron, and to two apical oxygens the Ni atom forms a NiO_6 octahedron, due to the Ca^{2+} ion being larger than that of Ni^{2+} ion. This is the first single-crystal study on the structures of hydrated δ-type vanadium oxide bronzes.

63: Coordination of Yttrium in RF-Sputtered Amorphous Films in the System SiO_2-Y_2O_3

Takuya Shinoda*, Teiichi Hanada*, Setsuhisa Tanabe and Takeshi Yao**
***(Graduate School of Human and Environmental Studies)**
****(Department of Integrated Human Studies)**

Journal of Non-Crystalline Solids Vol. 221, pp.302-306, 1997

Extended X-ray absorption fine structure near the Y K-edge was measured to determine the coordination state of yttrium ions in amorphous films in the system SiO_2-Y_2O_3 prepared by rf-sputtering. The coordination number of yttrium ions in the amorphous films with ¡ 30 mol% Y_2O_3 content was greater than six, but it approached six, dependent on the Y_2O_3 content, in the region ¿ 35 mol% Y_2O_3 content. That is, the region between about 35 mol% and about 50 mol% Y_2O_3 content is the transition stage of the change of the coordination number of yttrium ions. This result of the coordination state of yttrium ions has given a direct proof for the prediction that the coordination state of yttrium ions changes at about 45 mol% Y_2O_3 content in SiO_2-Y_2O_3 amorphous films, which was obtained from our previous study about their physical properties, such as density and elastic moduli.

64: * Crystal Structure of $Cs_2V_4O_{11}$ with Unusual V-O coordinations

Yoshio Oka*, Fumihiko Saito, Takeshi Yao and Naoichi Yamamoto**
***(Faculty of Integrated Human Studies)**
****(Graduate School of Human and Environmental Studies)**

Journal of Solid State Chemistry Vol. 134, pp. 52-58, 1997

Single crystals of $Cs_2V_4O_{11}$ were obtained in the hydrothermal $CsVO_3$-$VO(OH)_2$ system and its structural characterization was performed. $Cs_2V_4O_{11}$ crystallizes in the C-centered orthorhombic system: $Cmm2$ with $a = 5.571(2)$ Å, $b = 9.639(2)$ Å, $c = 5.222(2)$ Åand $Z = 1$. Structure refinements based on 402 reflections converged to $R = 0.037$ and $R_w = 0.044$. The structure has V_4O_{11} layers and interlayer Cs atoms. The V_4O_{11} layer exhibits an unusual V-O network structure consisting of VO_4 tetrahedra and VO_5 trigonal bipyramids in a random distribution. The structure is derived from that of a fictive V_4O_{10} layer made up of vertex-sharing VO_4 tetrahedra. That is, one-fourth of the shared vertices in the V_4O_{10} layer are converted into shared edges by adding extra oxygens leading to the V_4O_{11} layer; actually a vertex-sharing VO_4 dimer changes to an edge-sharing VO_5 dimer. Consequently the V atom in a single crystallographic site shows two different V-O coordinations of VO_4 tetrahedra and VO_5 trigonal bipyramids in a one-to-one ratio.

65: Preparation of Perovskite-Type $La_{1-x}Sr_xMnO_3$ films by Vapor-Phase Processes and Their Electrochemical Properties

Tsutomu Ioroi*, Tatsunori Hara*, Yoshiharu Uchimoto, Zempachi Ogumi* and Zen-ichiro Takehara*

***(Graduate School of Engineering)**

Journal of the Electrochemical Society Vol. 144, pp. 1362-1370, 1997

Dense and thin $La_{1-x}Sr_xMnO_3$ film electrodes were prepared on yttria-stabilized zirconia (YSZ) electrolyte by vapor-phase processes. In order to construct the electrochemical system, the YSZ film was first deposited by a chemical vapor deposition-electrochemical vapor deposition method on porous $La_{0.85}Sr_{0.15}MnO_3$ substrate. Then the $La_{1-x}Sr_xMnO_3$ film was deposited on the YSZ film by using a vapor mixture of $LaCl_3$, $SrCl_2$ and $MnCl_2$ as metal sources and humidified oxygen gas as an oxygen source. The as-prepared $La_{1-x}Sr_xMnO_3$ thin film were uniform and pinhole-free, and adhered strongly to the YSZ film. The electrochemical conductivity of the $La_{1-x}Sr_xMnO_3$ thin film was comparable to that of sintered $La_{1-x}Sr_xMnO_3$. The electrode interface resistance of the deposited $La_{1-x}Sr_xMnO_3$ film, which was determined by ac impedance measurements, was proportional to the $La_{1-x}Sr_xMnO_3$film thickness, and the inverse of the electrode interface resistance was proportional to the electrode surface area of the $La_{1-x}Sr_xMnO_3$ thin film. In the $La_{1-x}Sr_xMnO_3$ thin-film electrode, it was concluded that oxygen is reduced to oxide ions at the electrode surface and they are transported through the electrode thin film to the electrolyte.

66: Photovoltaic Effect in Titanium Dioxide/Polythiophene Cell

Koichi Kajihara, Katsuhisa Tanaka*, Kazuyuki Hirao* and Naohiro Soga*
***(Graduate School of Engineering)**

Japanese Journal of Applied Physics Vol. 36, pp. 5537-5542, 1997

The photovoltaic effect has been observed in a titanium dioxide (TiO_2) and polythiophene (PT) composite cell, ITO/TiO_2/PT/Au. The TiO_2/PT junction forms a rectifying contact and the ideality is better than that of the TiO_2/ZnPc junction reported previously. There exists a good correlation between the optical absorption spectrum of the PT layer and collection efficiency of the cell with illumination from the ITO side. This indicates that the TiO_2 layer effectively works as a wide-gap window material. Photovoltaic and electrical properties of the cell are varied considerably by changing the undoping potential of the PT layer. These phenomena are interpreted in terms of the band theory taking into consideration the contribution from surface states.

67: Crystal Structure of Zinc Hydroxide Sulfate Vanadate(V), $Zn_7(OH)_3(SO_4)(VO_4)_3$

K. Kato*, Y. Kanke*, Y. Oka and T. Yao**
***(National Institute for Research in Inorganic Materials)**
****(Faculty of Integrated Human Studies)**

Zeitschrift für Kristallographie Vol. 213, p. 26, 1998

Source of material: The title compound was obtained as by-product of a hydrothermal synthesis, in which a suspension of $VO(OH)_2$ powder in $ZnSO_4$ aqueous solution was sealed in a Pyrex glass ampoule and was treated in an autoclave at 553K for 48 hours. The crystals grew on the wall of the ampoule. The main products were σ-$Zn_{0.25}V_2O_5 \cdot H_2O$ (see ref. 1) and VO_2(A) (see ref. 2). The $VO(OH)_2$ powder was prepared in advance hydrothermally at 423K from a mixture of $VOSO_4$ and NaOH. Attempt to synthesize the title compound from V_2O_5 or $VOSO_4$ was not successful.

68: * Chaotic behaviour in PIC simulation and its relation to computational errors

Y. Idomura, S. Tokuda* and M. Wakatani
***(Japan Atomic Energy Research Institute)**

Computer Physics Communications 102 (1997) 68-80

For a parallelized one-dimensional electrostatic PIC simulation code, and increase of separation of test

particle orbits has been observed between numerical results with a single node and multiple nodes under the same initial and boundary conditions. The PIC simulation treats the many body Hamiltonian system which is characterized by positive Lyanpunov exponents. In order to check the accuracy of simulation results at microscopic level, we have evaluated the chaotic property of the dynamical system realized in these two calculations. By measuring the maximum Lyapunov exponent, it is shown that the separation of particle orbits is not caused by accumulation of numerical errors, but caused by the origin of chaos that the solution is sensitive to initial conditions. Therefore, both results obtained with the single node and the multiple nodes are considered as the realization of an ensemble and equally reliable. We also discuss the relation between breakdown of energy conservation and stochasticity in the particle simulation.

69: * Generation of Sheared Flow and its Effect on Transport Based on Nonlinear Interchange Mode

A. Takayama, M. Wakatani

Journal of Korean Physical Society (Proc. Suppl.), Vol.31, August 1997, pp.S167-S170

Nonlinear evolution of interchange mode is investigated in a scrape-off layer plasma with unfavorable magnetic curvature using both a direct numerical simulation on nonlinear MHD model and a low-order dynamical model. Both results show that when the Reyleigh number exceeds a critical value, the zonal counter-streaming flow is generated in the perpendicular direction to the ambient magnetic field, which makes the fluctuation level suppress. The reduction of transport is not stationary, but oscillatory or intermittent, which resembles the behavior of the Edge Localized Mode observed in tokamak H-mode experiments. The low-order model is usable to investigate mechanism of sheared flow generation during the nonlinear evolution of interchange mode.

70: * Plasma Size for Ignition Experiment

M. Wakatani, M. Furukawa

Journal of Plasma and Fusion Research Vol.73, No.5 (1997), pp.526-528

An estimation for a plasma size to realize ignition in a magnetically confined toroidal plasma is given by using similar assumptions for Lawson criterion. If the anomalous transport governs the edge region, it is difficult to obtain an ignited plasma with a plasma radius of about 1(m).

71: Behavior of pellet injected Li into Heliotron E plasmas

ヘリオトロン Eプラズマにペレットで入射されたリチウムの挙動

Katsumi Kondo, Katsumi Ida*, C.Christou, V.Yu.Sergeev, K.V.Khlopenlov*, S.Sudo*, F.Sano, H.Zushi, T.Mizuuchi, S.Besshou, H.Okada, K.Nagasaki, K.Sakamoto, Y.Kurimoto, H.Funaba, T.Hamada, T.Kinoshita, S.Kado, Y.Kanda, T.Okamoto, M.Wakatani, T.Obiki**

(NIFS), *(St.Petrsburg Technical Univ. St.Petersburg, Russia)**

Journal of Nuclear Materials, 241-243, 956-960

Li pellet injection has provided a complex plasma with a large fraction of Li ions. The spatial profiles of the fully ionized Li ions are measured by charge exchange recombination spectroscopy with a resolution of 13 mm and local decay time of the injected Li ion has been estimated.

72: Complete Integral Suppression of Pfirsch-Schluter Current in a Stellarator Plasma in Heliotron E

Sakae Besshou, Vladimir.D.Pustovitov*, Norito Fujita, Katsumi Kondo, Tohru Mizuuchi, Kazunobu Nagasaki, Masahiko Nakasuga, Tokuhiro Obiki, Hiroyuki Okada, Fumimichi Sano, Hideki Zushi**

(Russian Research Centre 'Kurchatov Institute'), *(Institute for Advanced energy, Kyoto University)**

Physics of Plasmas, Vol.5, No. 2, pp481-485, 1998

The Poloidal magnetic field was measured to detect the plasma boundary position. It was found that the pressure-induced plasma shift, an observable characteristic of the Pfirsch-Schluter current, depends strongly on the initial position of the magnetic axis. When the axis was moved by the vertical field inside the torus, the finite-beta shift became smaller. Complete suppression of the finite-beta plasma shift was achieved in a deeply inward shifted configuration: 7cm from the standard position Raxis=2.20m. This effect is explained by magnetohydrodynamic(MHD) equilibrium theory for stellarator toroidal plasmas with a large magnetic hill and deep inward shift.

73: Suppression of Pfirsch-Schuluter Current in the Inward-Shifted Stellarator Plasma on heliotron-E

Sakae Besshou, Norito Fujita, Katsumi Kondo, Tohru Mizuuchi*, Kazunobu Nagasaki, Masahiko Nakasuga, Hiroyuki Okada, Fumimichi Sano, Hideki Zushi, Tokuhiro Obiki

***(Institute for Advanced Energy, Kyoto university),**

Proceedings of the 24th European Physical Society Conference on Controlled Fusion and Plasma Physics (9-13 June 1997, Berchtesgarden, Germany) Vol. 1, p2.082, 1997

The experimental observation of the suppression of Pfirsch-Schluter current in a finite pressure stellarator plasma on Heliotron-E is reported. The poloidal magnetic flux was measured to determine the finite beta free boundary shift as an observable of the dipole Pfirsch-Schluter current. It was found that the measured finite beta free boundary shift depends strongly on the initial magnetic axis positions which are controlled with the vertical field. When the magnetic axis position is shifted inward toward the major axis by 7cm (Raxis=2.13m) form the original position(Raxis=2.20m), the complete suppression of the finite beta shift and the dipole Pfirsch-Schluter current was observed for the finite pressure plasma with the magnetic hill and the deep inward shift.

74: Evolution of the Tearing Mode During LHCD Induced Mode Locking in WT-3

Takashi Maekawa, Yasushi Terumichi*, Makoto Asakawa*, Satoshi Yoshimura*, Yoshio Yoshizawa*, Mitsunari Sukegawa*, Keisa Matsunaga*, Akira Yamazaki*, Kazuya Uno*, Tomoyuki Izuhara*, Masahiko Nakamura**

(Fac. of Science, Kyoto Univ.),*(Osaka Institute of Technology)**

Proc. 16th Int. Conf. on Fusion Energy Vol.1, pp.771-775, 1997

Through the application of lower hybrid current drive, toroidal rotation of the tearing mode excited in OH plasmas is slowed down, and finally mode locking is artificially induced. The time evolution of the plasma internal structure during mode locking is investigated by using soft X ray (SX) cameras, and it is found that SX bursts appear intermittently at the plasma periphery in accordance with overlapping of the m = 1 and m = 2 structures in the inner part of the plasma before disruption. Through the application of second harmonic electron cyclotron heating, the mode locking comes untied, the toroidal rotation frequency increases and no disruption takes place.

75: Electron Cyclotron Current Drive in a Lower Hybrid Current Drive Plasma

Tsunehiro Maehara*, Satoshi Yoshimura, Takashi Minami***, Kazuaki Hanada****, Masahiko Nakamura*****, Takashi Maekawa, Yasushi Terumichi******
*(Fac. of Science, Ehime Univ.), **(Fac. of Engineering, Osaka Univ.), ***(National Institute for Fusion Science), ****(Institute for Applied Mechanics, Kyushu Univ.), *****(Osaka Institute of Technology), ******(Fac. of Science, Kyoto Univ.)**

Nucl. Fusion, Vol.38, No.1, pp.39–57, 1998

Electron cyclotron (EC) current drive experiments were carried out in lower hybrid current drive (LHCD) plasmas on the WT–3 Tokamak. Using oblique injection of EC waves, plasma current is ramped up in a frequency range $\omega/\Omega_e \simeq 1.2 - 1.4$, where Ω_e is the EC frequency at the plasma centre. This ramp-up is ascribed to selective EC heating of fast electrons in LHCD plasmas via the fundamental EC resonance at the upshifted frequency due to the Doppler effect. Fast electron momentum distributions are estimated from bremsstrahlung hard X ray spectra. These distributions indicate that the parallel momentum input to the fast electrons in the relativistic energy range from oblique EC waves is effective for efficient EC current drive. Current ramp-up is also observed in the second harmonic frequency range $\omega/\Omega_e \simeq 1.9 - 2.2$. In this case, bulk electrons are heated as well as fast electrons and no definite cause of current ramp-up is clarified.

76: * Confinement of Nonneutral Spheroidal Plasmas in Multi–Ring Electrode Traps

Akihoro Mohri*, Hiroyuki Higaki, Hitoshi Tanaka, Youhei Yamazawa**, Masayuki Aoyagi**, Tetsumori Yuyama*, Toshinori Michishita***
*(Fac. of Integrated Human Studies, Kyoto Univ.), **(Grad. School of Human and Environmental Studies, Kyoto Univ.)**

Jpn. J. Appl. Phys. Vol.37, No.2, pp.664–670, 1998

A nonneutral spheroidal plasma can be settled in a rigid rotor equilibrium inside a closed conducting cell independently of induced image charges on the cell wall if the electrostatic potential distribution on the wall surface is set equal to the sum of the external hyperbolic potential $(r^2 - 2z^2)$ and the self-potential produced by the plasma. A confinement system equipped with a train of properly biased ring electrodes can approximately generate any axisymmetric potential, including the above field. Experiments on confinement of electron spheroids in such a system showed that the confinement time became the longest when the condition to diminish the image charge effects was satisfied. The observed frequency of the centre-of-mass harmonic oscillation of the plasma in this configuration was in good agreement with the estimated one.

77: Effects of ECH on NBI Plasma in Heliotron E

T.Obiki, F.Sano, K.Kondo, H.Zushi, K.Hanatani, T.Mizuuchi, S.Besshou, H.Okada, K.Nagasaki, M.Wakatani, Y.Nakamura, M.Nakasuga, C.Christou, Y.Ijiri, T.Senju, K.Yaguchi, S.Kobayashi, K.Toushi, K.Sakamoto, Y.Kurimoto, H.Funaba, T.Hamada, S.Sudo, M.Sato, K.Ida, B.J.Peterson, K.Muraoka, S.Kado, H.Sugai, H.Toyoda, K.Sasaki, H.Okura, K.Matsuo, G.Denisov, A.Goldenberg, V.Kurabatov, V.Orlov, D.Vinogradov, V.Yu.Sergeev, K.V.Khlopenkov, V.V.Chechkin, V.S.Vojtsenya

16th Conference Proceedings, Fusion Energy (IAEA, Montreal, 1996), Vol.2, pp.13-26, 1997

Propagation and absorption of second harmonic electron cyclotron resonance microwaves are investigated in Heliotron E. A highly focused beam with good single pass absorption allows a centrally peaked high electron temperature profile to be obtained. It is experimentally confirmed that the linearly polarized beam should be launched at a proper angle to the sheared field line and cross the resonance layer at the magnetic axis to obtain the best plasma production in heliotron/torsatron devices. The effects of ECH on NBI plasmas are studied by using two ECH systems with different absorption and resonance conditions. The superposition of ECH pulses on NBI plasmas has shown that $\Delta T_i > 0$ for ECH overlapping with a rather broad ECH power deposition profile but $\Delta T_i < 0$ for a centrally focused deposition profile. A key to an explanation of these different observations is the balance between the gain from $\Delta T_e > 0$ (and from $\Delta E_r > 0$, possibly) and the loss from the particle 'pump-out' and the resultant flattening of the density profile, both of which are caused by the ECH overlapping.

78: Waveguide Transmission Line for 106-GHz Electron Cyclotron Heating in Heliotron-E

K.Nagasaki, S.Kobayashi, K.Sakamoto, H.Zushi, T.Obiki, K.Ohkubo, M.Kawaguchi, G.G.Denisov, A.L.Goldenberg, V.I.Kurbatov, V.B.Orlov, D.V.Vinogradov

Fusion Technology, Vol.32, pp.287, 1997

A 106-GHz electron cyclotron heating system is in stalled and operated for plasma production and heating of the Heliotron-E helical device. The Gaussian beam radiated from the gyrotron is coupled to the HE_{11} waveguide mode by the matching optics unit (MOU), then transmitted through 15-m corrugated waveguides and four miter bends. The system is closed for safety to prevent spurious modes from radiating into the free space and is operated at atmospheric pressure. The transmitted wave is launched from the outside of the torus, and the launched beam is focused on the magnetic axis so that the power deposition is expected to be localized at the desired resonance region. The measured transmission efficiency from the MOU output to the launcher output is 86%, which is in good agreement with the theoretical estimate. The power losses arise mainly at the waveguide mouth where the Gaussian beam is coupled to the HE_{11} mode, at the miter bends and in the launching system.

79: Second Harmonic ECH Experiment on Heliotron-E

K.Nagasaki, S.Kobayashi, K.Sakamoto, F.Sano, T.Mizuuchi, H.Okada, K.Kondo, H.Zushi, S.Besshou, Y.Kurimoto, H.Funaba, T.Obiki, A.Ejiri, K.Ohkubo, M.Kawaguchi, G.Denisov, A.Goldenberg, V.Kurbatov, V.Orlov, D.Vinogradov

Strong Microwaves in Plasmas, 1996 (Nizhny Novgrod University Press), Vol.1, pp.89-108, 1997

A new 106.4GHz electron cyclotron resonance heating (ECH) system has been installed and operated for second harmonic extraordinary-mode plasma heating in the Heliotron-E helical device. The waveguide transmission line is effective for high power and high frequency ECH as well as the quasi-optics transmission line. Plasma experiments using this 106.4 GHz ECH showed that the accessible electron density was doubled, and plasma parameters such as electron temperature and energy confinement time were improved. Focused Gaussian beam and good single pass absorption allow us to study the plasma response to the change in the power deposition profile and the effect of magnetic shear on the wave propagation. Plasma production is also discussed in terms of the difference between fundamental and second harmonic ECH breakdowns.

80: Dynamics of Ion Temperature in Heliotron-E

K.Ida, S.Hidekuma, K.Watanabe, K.Kondo, H.Zushi, S.Besshou, K.Nagasaki, F.Sano, T.Mizuuchi, H.Okada, T.Obiki, T.Hamada, H.Funaba, Y.Kurimoto

16th Conference Proceedings, Fusion Energy (IAEA, Montreal, 1996), Vol.2, pp.151-156, 1997

The ion temperature dynamics as related to the density profile is studied in the Heliotron-E plasma. The density profiles can be peaked by the H_2/D_2 pellet injection or can be flattened by second harmonic electron cyclotron heating (2nd ECH). Higher ion temperature and better ion transport are observed, associated with the density peaking, and the large density gradient results in radial electric field shear. The improvement of ion transport is related to the radial electric field shear rather than to the bulk velocity shear.

81: Study of the Fast Ion Slowing-Down Process and ECRH Effects in Heliotron E

Y.Kurimoto, H.Zushi, F.Sano, K.Kondo, T.Mizuuchi, H.Okada, K.Nagasaki, T.Obiki

Journal of the Physical Society of Japan, Vol.66, pp.2033-2043, 1997

In the Heliotron E device, combining a neutral beam injection (NBI) with an electron cyclotron resonance heating (ECRH) system, new physical issues are applied to the investigation of fast ion behavior. Especially, the slowing-down (deceleration and parallel diffusion) and the loss processes are studied experimentally through measurements of the temporal change of charge-exchange neutral particle energy spectra. As results, first, in the longer slowing-down time ($\tau_s \sim 200$ ms) plasma realized by ECRH, discrepancies from the theoretical values are detected in the deceleration and the parallel diffusion processes, whose factors are $4 \sim 6$ for the former, $6 \sim 13$ for the latter. Second, the fast ion loss cone is reduced by the ECRH on the NBI plasma, of which cause is discussed associated with the modification of the radial electric field, E_r.

82: Experimental Investigation of the Fast Ion Orbit Shift and Loss Cone in Heliotron E

Y.Kurimoto, H.Zushi, F.Sano, K.Kondo. T.Mizuuchi, H.Okada, K.Nagasaki, T.Obiki

Journal of the Physical Society of Japan, Vol.66, pp.2702-2714, 1997

The inward shift and the toroidal precession of the deeply trapped ion orbit in Heliotron E plasmas are measured using the charge exchange analysis, and found to be consistent with the classical drift orbit theory. Depletion structures on energy spectra are observed during limiter insertion or pellet injection. Furthermore, the rapid change of the depletion structures by additional beam injection or limiter bias is also investigated. These depletion structures can be explained by an effect of the resonant loss due to the negative radial electric field, E_r. Theoretical analysis of the E_r profile shows that a positive E_r in the vicinity of the loss boundary disturbs the resonant condition of deeply trapped particles locally, and can reduce the resonant loss cone.

83: Field line measurements in the divertor of Heliotron E under boronized conditions

F.Sano, T.Mizuuchi, T.Hamada, H.Funaba, M.Nakasuga, K.Kondo, H.Zushi, S.Besshou, H.Okada, K.Hanatani, K.Nagasaki, T.Obiki

Journal of Nuclear Materials, Vol.241-243, pp.961-966, 1997

Vacumm magnetic field line structure of Heliotron E has been studied experimentally with special reference to the edge plasma physics of the helical system (heliotron/torsatron). A new approach for measuring the vacuum impedance between the magnetic surface and the chamber wall under the boronized conditions was attempted in order to extract the detailed field line topology efficiently. Measurements have revealed the position of the experimental last closed surface and the nesting and folding structure of the divertor field lines. In conclusion, an advanced 2D visualization of Heliotron-E divertor field lines was obtained as compared with the previous one using the stainless-steel wall conditions. In addition, the relationship between the edge plasma distribution and the relevant field line topology is discussed.

84: A new approach for vacuum surface mapping in Heliotron E

F.Sano, T.Mizuuchi, T.Hamada, M.Nakasuga, H.Matsuura, K.Kondo, H.Zushi, S.Besshou, H.Okada, K.Hanatani, K.Nagasaki, K.Tohshi, B.J.Peterson, C.Christou, Y.Kurimoto, S.Kado, H.Funaba, T.Kinoshita, K.Yaguchi, H.Sugai, T.Obiki

Fusion Engineering and Design, Vol.34-35, pp.807-809, 1997

Wall boronization was applied in Heliotron E with special reference to the study of impurity and recycling control in the helical sysftem. However this technique was also found to work as an advantageous tool to enhance the diagnostic sensitivity of the beam impedance method for measuring the edge and divertor field line structure. In this paper we describe a new approach to the beam impedance method that utilizes the wall boronization.

85: * Thermal lensing study on the kinetics of IR multiphoton dissociation

Tetsuo Sakka, Takashi Tsuboi, Yukio H. Ogata

Journal of Chemical Society, Faraday Transactions, 93 (7), 1305 (1997).

Thermal lensing (TL) signals from $CClF_2CHCl_2$ gas undergoing infrared multiphoton dissociation (IRMPD) were observed. The rising rate of the TL signals increases with increasing laser energy fluence above the reaction threshold fluence, while it is constant below the threshold fluence. An explanation is given to this result by comparing the result with a kinetic model, in which the rate of the vibrational deactivation of both the reactant and product molecules and a unimolecular reaction rate of the vibrationally excited molecules are taken into account. The applicability of the TL method to investigations of the IRMPD is mentioned.

86: * Thermal lensing study on the vibrational relaxation of highly excited chlorofluoroethane

Tetsuo Sakka, Kenichi Matsumura, Takashi Tsuboi, Yukio H. Ogata

Chemical Physics Letters, 286 (1-2), 107 (1998).

Vibrational relaxation rate of $CClF_2CHCl_2$ gas excited by TEA CO_2 laser in the presence of various addition gases was measured by thermal lensing (TL) technique. The collision efficiency was calculated to be the order of $10^{-2} - 10^{-3}$. The vibrational relaxation rate was higher for large molecules, implying that off-resonant vibrational energy transfer is playing a role in the relaxation process. The relaxation

was fast for high fluence irradiation, indicating that the relaxation in a quasi-continuum region is faster than a discrete region. By comparing the present results with the product yield measurement of infrared multiphoton dissociation (IRMPD) it seems that the collision partner effect of the vibrational relaxation rate measured by the TL technique is correlated to the addition gas effect in the IRMPD rate.

87: Analysis of Salt Effects on Solubility of Noble Gases in Water Using the Reference Interaction Site Model Theory

Masahiro Kinoshita and Fumio Hirata*
***(Department of Theoretical Studies, Institute for Molecular Science)**

The Journal of Chemical Physics, Vol.106, No.12, pp.5202-5215, 1997.

We have developed robust and very efficient algorithms for solving the reference interaction site model (RISM) equations for salt solutions in the bulk and near a solute atom of noble gases. The theory of dielectric consistency recently developed for solutions at finite salt concentrations is employed in the formalism. The change in water structure in the bulk caused by addition of salts have been examined for model 1-1 salt solutions (LiCl, NaCl, KCl, KF, KBr, KI and CsI). The density and orientational structures of each salt solution near a solute atom have been analyzed. The water model employed is the extended simple point charge (SPC/E) model. Ions characterized by positive hydration (F^-, Li^+ and Na^+) are strongly hydrated in the bulk and stay significantly far from the atom. Those of negative hydration (Cl^- and Br^-) or hydrophobic hydration (Cs^+ and I^-) are excluded from the bulk to the atom. Due to a specific orientational order of water molecules adjacent to the solute atom, there is a trend that cations stay less closer to the atom than anions. Overall, cations indirectly affect the solubility of noble gases via the change in water structure induced by addition of those ions. On the other hand, anions affect the solubility not only indirectly but also directly by interacting with solute atoms. The agreement between the calculated and experimental values for the salting coefficient is excellent for He. However, the discrepancy becomes larger as the number of electrons of the solute atom increases (the calculated value is larger), which implies that the ion-induced dipole interaction neglected has significantly large effects.

88: Calculation of Hydration Free Energy for a Solute with Many Atomic Sites Using the RISM Theory

Masahiro Kinoshita, Yuko Okamoto*, and Fumio Hirata*
***(Department of Theoretical Studies, Institute for Molecular Science)**

Journal of Computational Chemistry, Vol.18, No.10, pp.1320-1326, 1997.

We have developed an algorithm for solving the reference interaction site model (RISM) equations for

water near a solute molecule with many atomic sites (interaction sites). It is a hybrid of the Newton-Raphson and Picard methods which is judiciously constructed. Various considerations are given so that the computer time can be saved as greatly as possible. The robustness and high efficiency of the algoritm has been demonstrated for calculating hydration free energies of Met-enkephalin (a peptide with 75 sites) with different conformations. The Jacobian matrix is treated as part of the input data, and it has been found that the same matrix can be used for a considerably large set of different conformations of the solute molecule.

89: Solvation Structure and Stability of Peptides in Aqueous Solutions Analyzed by the Reference Interaction Site Model Theory

Masahiro Kinoshita, Yuko Okamoto*, and Fumio Hirata*
***(Department of Theoretical Studies, Institute for Molecular Science)**

The Journal of Chemical Physics, Vol.107, No.5, pp.1586-1599, 1997.

We report results of numerical analyses on solvation structure and conformational stability of a dipeptide and Met-enkephalin in the extended simple point charge (SPC/E) model water. The reference interaction site model (RISM) theory is fully solved using our robust, highly efficient algorithm. It is shown that water structure near the peptides and the hydration free energy are greatly dependent on the peptide conformations. Stability of Met-enkephalin is examined in terms of the total energy defined as the sum of the conformational energy and the hydration free energy of the peptide. We test several different conformations including that with the minimum energy in gas phase, which takes rather compact form due to an intramolecular hydrogen bond. It is shown that a fully extended conformation has the highest stability in water. Our results are in qualitative accord with the recent nuclear magnetic resonance (NMR) experiments which suggest fully extended conformations with large fluctuations for the solution structure of the peptide. A conformation which is similar to that obtained from the NMR experiments in miceller solutions, is much less stable when it is put in water. Thus, the peptide conformations are greatly sensitive to microscopic solvent environment, and any native treatment of the solvent such as the continuum model will end in failure.

90: Structure of the Metal-Liquid Interface: Self-Consistent Combination of the First-Principles Metal Calculation and an Integral Equation Method

Masahiro Yamamoto and Masahiro Kinoshita

Chemical Physics Letters, Vol.274, No.5,6, pp.513-517, 1997.

This letter contributes to development of microscopic theories for the metal/liquid interface. We report results of the first attempt to combine the first-principles calculation for the metal and the reference

hypernetted-chain method for the liquid in a fully self-consistent manner. The dipolar liquid/Pt(111) interface is considered. The electron density, liquid structure, and electrostatic potential across the interface are briefly discussed.

91: Fractal-Like Behavior of a Mass-Transport Process

Masahiro KINOSHITA, Makoto HARADA, Yasuo SATO, Kyoichi TSUBATA and Yasutaka NAKAMURA

AIChE Journal, Vol.43, No.9, pp.2187-2193, 1997.

After an aqueous solution containing Sr^{2+} was made flow through a bed packed with particles of activated charcoal for a very long time, the flow was abruptly switched to deionized water. The variation of the ionic concentration at the outlet with time was characterized by the power law, $C_{out} \sim t^{-\alpha}$, for sufficiently large t. This fractal- like behavior reported in our previous note has further been studied theoretically and experimentally. A major concern is to examine dependency of α on experimental conditions. Adsorption sites predominate over dead- end pores or spaces as "trappers" in our case where Sr^{2+} or Ba^{2+} are adsorbed on activated charcoal. The experimental results can well be explained by our theoretical model. It has been found, however, that the response curve for Sr^{2+} deviates from the power law after a very long time. This deviation can be explained by introducing the assumption that there exists a maximum value of the activation energy for the desorption process. The curve for Ba^{2+}, on the other hand, exhibits no such deviation until Cout decreases to the detection limit of the analytical device used.

92: Structure of the Metal-Aqueous Electrolyte Solution Interface

Daniel R. Berard*, Masahiro Kinoshita, Natalie M. Cann, and Grenfell N. Patey****

(Department of Chemistry, University of Utah), *(Department of Chemistry, University of British Columbia)**

The Journal of Chemical Physics, Vol.107, No. 12, 4719-4728 (1997).

Theoretical results are given for aqueous electrolyte solutions in contact with uncharged metallic surfaces. The metal is modeled as a jellium slab and is treated using the local density functional theory. The solution structure is obtained using the reference hypernetted-chain theory. The two phases interact electrostatically and the coupled theories are iterated to obtain fully self-consistent results for the electron density of the metal and surface- particle correlation functions. The metal- induced structure of pure water and aqueous electrolyte solutions as well as the electrostatic potential drop across the interface are discussed in detail. The results are compared with those for ions in simple dipolar solvents. It is found that the water molecules are ordered by the metal field and that the surface- induced solvent structure

strongly influences the ion distributions.

93: Analysis on Fractal-Like Behaviour Expected for Migration of Radionuclides in Geologic Sorbing Media

Masahiro KINOSHITA, Makoto HARADA, Kyoichi TSUBATA and Yasuo SATO

Journal of Nuclear Science and Technology, Vol.35, No.1, pp.40-48, 1998.

In earlier work, we showed that within nonhomogeneous sorbing media the desorption process becomes fractal-like. In migration of radionuclides in geologic media, the adsorption is an essential factor retardating the migration. Moreover, geologic media is inherently nonhomogeneous. It is therefore probable that the migration is significantly influenced by the fractal-like feature. Based on this idea, we have analyzed migration behaviours by employing a new model and compared the results with those obtained using conventional models. The nuclides migrate in the media with the flow of ground water being continually trapped on adsorption sites and released (desorbed) to the flow. The concept of the overall residence-time distribution function for nuclides on the adsorption sites is introduced in the new model. This function obeys the power form, $\sim t^{-1-\alpha}$ ($\alpha > 0$), for sufficiently large t (t denotes time). The migration behaviours predicted by our theory are qualitatively different from those by conventional theories, and the details of the differences are greatly dependent on the exponent α. In particular, the migration behaviour in cases of $0 < \alpha < 1$ is characterized by far larger retardation effects.

94: First-Principle Determination of Peptide Conformations in Solvents: Combination of Monte Carlo Simulated Annealing and RISM Theory

Masahiro Kinoshita, Yuko Okamoto*, and Fumio Hirata*
***(Department of Theoretical Studies, Institute for Molecular Science)**

Journal of the American Chemical Society, Vo.120, No.8, pp.1855-1863, 1998.

This paper contributes to development of a microscopic approach to predicting stable conformations of proteins in solvent. We report results of the first attempt to combine Monte Carlo simulated annealing, a powerful conformational sampling technique, and the reference interaction site model (RISM) theory, a statistical-mechanical treatment for molecular fluids. In solvent the key function is the total energy defined as the sum of the conformational energy and the solvation free energy, and the RISM theory is employed to calculate the latter. Starting from an initial conformation given, our computer program samples many conformations, and then finds the conformation with the minimum total energy. Met-enkephalin in the two different solvents, a model water and a simple, repulsive-potential system, are considered. In water the solvation free energy varies greatly from conformation to conformation, while in the simple solvent it remains almost unchanged against conformational changes. In water most of the conformations with

larger solvation free energies are strongly rejected and the number of probable conformations is drastically reduced, which is suggestive that Met-enkephalin is forced to take conformations favored by water far more rapidly than in gas phase and in the simple solvent. The set of stable conformations obtained in water are quite different from those in gas phase and the simple solvent: they are characterized by almost fully extended backbone structure with large fluctuations in side-chain structure, which are in qualitatively good agreement with those determined by the recent nuclear magnetic resonance (NMR) experiments.

95: * Bioaffinity Separation of Trypsin Using Trypsin Inhibitor Immobilized in Reverse Micelles Composed of a Nonionic Surfactant

Motonari Adachi, Masaru Yamazaki, Makoto Harada, Akihisa Shioi and Shigeo Katoh*
***** (Kobe Univ.)**

Biotechnology Bioengineering, Vol. 53, No. 4, pp. 406-408, 1997

Trypsin inhibitor was converted to hydrophobic states by covalently combining cholesteryl groups using acylation reaction and was immobilized in reverse micelles composed of a nonionic surfactant. Using this reverse micellar phase containing trypsin inhibitor as an affinity ligand, trypsin was selectively separated with high recoveries from a mixture of several kinds of contaminating proteins by forward and backward extraction. No loss of activity of the recovered trypsin was observed through these operations.

96: * Anomalous Water Extraction Rate and Mechanism between Sodium Bis(2-ethylhexyl) Sulfosuccinate Water-in-Oil Microemulsion Phase and Co-existing Aqueous Solution

Motonari Adachi, Akihisa Shioi and Makoto Harada

Langmuir, Vol. 13, No. 16, pp. 4280-4286, 1997

Anomalous behavior of hydrodynamic process in water extraction was observed in the two phase system; sodium bis(2- ethylhexyl)sulfosuccinate(AOT) w/o- microemulsion(ME) phase and co-existing aqueous solution. The main factors causing the anomalous behavior were elucidated due to the experimental results and an analysis based on the following water extraction model: (1) rapid formation of equilibrium droplets at the liquid/liquid macro-interface due to the fast permeation of water through the bilayer which is formed between a ME droplet and the surfactant monolayer at the liquid/liquid macro-interface, (2) dependence of the diffusion coefficient of ME droplets on their size, (3) change in the ME droplet size due to coalescence and redispersion of ME droplets. The increase in thickness of the diffusion boundary layer due to formation of heavier droplets at the macro-interface also played an important role in the extraction rates of water, especially in forward extraction of water at low agitation speed.

97: * Protein Extraction in a Tailored Reverse Micellar System Containing Nonionic Surfactants

Akihisa Shioi, Makoto Harada, Hiroki Takahashi and Motonari Adachi,

Langmuir, Vol. 13, No. 4, pp. 609-616, 1997

Protein solubilization was studied for two kinds of reversed micellar systems with the aid of two phase transfer methods. The first system was composed of nonionic surfactant, poly (oxyethylene) alkyl ether (CiEj) and sodium bis(2-ethylhexyl)sulfosuccinate (AOT). Proteins used were α- chymotrypsinogen A (ctn) and cytochrome c (cytc). In the absence of AOT, protein was solubilized in the micelles by the entropic effect. Then, the fraction E of the protein extracted to the micellar phase was very low. The E increased with the addition of AOT due to the electrostatic interaction between AOT-anion and proteins. The denaturation of proteins in the micelles was restrained by controlling the electrostatic interaction. The solubilization mechanism was simplified by using this extraction system. The second system was composed of CiEj and alkylglucopyranoside (AGn), which worked as an amphiphilic affinity ligand to concanavalin A (conA). ConA was not extracted to the reverse micelles consisting of CiEj alone. With the addition of AGn, conA was taken up to the reversed micelles through the biospecific interaction. The reverse micelles tailored by controlling the interactions with proteins provide an ideal extraction system for proteins.

98: * Reactivity of α-Chymotrypsin in Reverse Micelles Containing Nonionic Surfactants

Akihisa Shioi, Tsukuru Kishimoto, Motonari Adachi and Makoto Harada

Journal of Chemical Engineering of Japan, Vol. 30, No.6, pp. 1130-1133,

The characteristics of the hydrolysis of oil- soluble substrate 2-naphthylacetate by α-chymotrypsin CT are examined in reversed micellar systems containing nonionic surfactant, polyoxyethylene alkyl ether CiEj. The rate of hydrolysis in CiEj-containing reverse micellar system is much higher than in sodium bis(2-ethylhexyl) sulfosuccinate AOT-stabilized reverse micelles. This higher rate constant in Michaelis-Menten kinetics compared with that for the AOT-reverse micellar system. The formation constant for CT-stabilized complex is unaltered compared with that in the aqueous phase. The activity of CT in the CiEj/AOT composite reverse micelles is almost unchanged after one week, whereas in the AOT system, the activity decreases substantially with time.

99: * Characteristics of Solute Transfer in Sodium Dioleyl Phosphate/Sodium Bis(2-ethylhexyl) Sulfosuccinate Microemulsion System

Makoto Harada, Gen Nonaka, Katsuya Kanaoka, Akihisa Shioi, Motonari Adachi, Noriaki Mizutani, Masahiro Goto and Fumiyuki Nakashio

Journal of Chemical Engineering of Japan, Vol. 31, No. 1, pp. 67-75, 1998

The behavior of solute transfer in sodium dioleylphosphate (SDOLP)/n-heptane and SDOLP-AOT/n-heptane systems was elucidated by focusing on the extraction process in Winsor II and the solute exchange process between microemulsion droplets. The extraction of tryptophan (Trp) between the organic and aqueous phases is rather fast for simultaneous extraction of water and Trp in the SDOLP and SDOLP/AOT systems, whereas in the extraction of Trp without water transfer between the microemulsion droplet and the aqueous phase, the rate slows down significantly with the addition of SDOLP in the AOT system. The rate of the interdroplet exchange process is insensitive to the presence of SDOLP. The reason for the difference in these two processes is discussed with the help of a model of the exchange processes.

100: Density functional study of NOx reduction in zeolite cage

Hisayoshi Kobayashi*, Katsutoshi Ohkubo
***(Kurashiki Univ.)**

Applied Surface Science 121/122, 111-115 (1997)

A density functional method was applied to investigate the electronic structure of Cu ion adsorbed ZSM-5 zeolite and the interactions of NO molecules with zeolite. Two types of models were considered, the pentameric cluster model and the 5-membered ring cluster model. In the former, the Cu ion was bound to the two O atoms with larger stabilization energy (52 kcal/mol) than the single O atom. For the 5-membered ring model, a much smaller stabilization energy (38 kcal/mol) was calculated. The deNOx reaction mechanism was simulated as the reactions between two NO molecules or between NO and HNO (or NOH) molecules. The former did not produce N_2 and O_2 smoothly due to the activation barrier, whereas the latter is found to lead to N_2O and OH more easily.

101: Cloning, Expression, and Characterization of a Novel Phospholipase D Complementary DNA from Rat Brain

Tsutomu Kodaki, Satashi Yamashita*
***(Gunma Univ.)**

J. Biol. Chem. 272, 11408-11413 (1997)

Phospholipase D (PLD) is implicated in important cellular processes such as signal transduction, membrane trafficking, and mitosis regulation. Recently, cDNA for human PLD1 (hPLD1) was cloned from HeLa cells. hPLD1 is stimulated by phosphatidylinositol 4,5-bisphosphate and the small GTP-binding protein known as ADP-ribosylation factor-1. Here we report the cloning and characterization of cDNA for a different type of PLD (rat PLD2 (rPLD2)) from rat brain. We synthesized highly degenerated amplimers corresponding to the conserved regions of eukaryote PLDs and performed polymerase chain reaction on a rat brain cDNA library. Using the amplified sequences as the probe, we cloned a rat brain cDNA clone that contained an open reading frame of 933 amino acids with a M_r of 105,992. The deduced amino acid sequence showed significant similarity to hPLD1 with a large deletion in the middle of the sequence. When the sequence was expressed in the fission yeast *Schizosaccharomyces pombe*, PLD activity was greatly increased. The activity was markedly stimulated by phosphatidylinositol 4,5-bisphosphate but not by ADP-ribosylation factor-1 and RhoA. Rat brain cytosol known to stimulate small GTP-binding protein-dependent PLD did not stimulate rPLD2 expressed in *S. pombe*. The transcript was detected at significant levels in brain, lung, heart, kidney, stomach, small intestine, colon, and testis, but at low levels in thymus, liver, and muscle. Only a negligible level was found in spleen and pancreas. Thus rPLD2 is a novel type of PLD dependent on phosphatidylinositol 4,5-bisphosphate, but not on the small GTP-binding proteins ADP-ribosylation factor-1 and RhoA.

102: Cloning, differential regulation and tissue distribution of alternatively spliced isoforms of ADP-ribosylation-factor-dependent phospholipase D from rat liver

Kazuhisa Katayama*, Tsutomu Kodaki, Yukio Nagamachi*, Satoshi Yamashita*
***(Gunma Univ.)**

Biochem. J. 329, 647-652 (1998)

An alternatively spliced isoform of ADP-ribosylation-factor-dependent phospholipase D (PLD1) was previously shown to occur in rat C6 cells and human HeLa cells. However, its complete sequence and the enzymological difference between the two PLD1 isoforms were unclear. Here we report the cloning, complete sequence, enzymological properties and tissue distribution of each of the two alternatively spliced PLD1 isoforms, a and b, from rat liver. The major difference between the two isoforms was the deletion of 38 amino acids in the b isoform, but otherwise the two cDNA sequences were 99.9 % identical. The a-isoform seqeunce was 91 % identical with the a form of human PLD1, and the 38- amino-acid deletion

in the b form occurred a the same site as in the b form of human PLD1. Both of the rat PLD1 isoforms expressed in the fission yeast *Schizosaccharomyces pombe* were dependent on ADP-ribosylation factor 1 and phophatidylinositol 4,5-bisphosphate. The a isoform was activated by RhoA in a synergistic manner with ADP-ribosylation factor 1, whereas the b isoform was less responsive to RhoA. Reverse transcription PCR showed that the b form was the predominant PLD1 isoform expressed in rat tissues. The b-form transcript occurred in various rat tissues, including lung, brain, liver, kidney, small intestine and colon, whereas the a-form transcript was only detectable in lung, heart and spleen. Both transcripts were hardly detectable in thymus, stomach, testis and muscle. Thus the two PLD1 isoforms were differently regulated and expressed in rat tissues.

103: * Cathodic Polarization of Copper Electrode in CuCN-KCN Solutions and the Current Distribution for Copper Deposition on Grooved Substrates

A. Katagiri, H. Inoue*, N. Ogure*
(*Ebara Corporation)

Journal of Applied Electrochemistry, Vol.27, pp.529-538, 1997

The cathodic polarization of a copper electrode in CuCN/KCN solution was interpreted by considering the diffusion and migration of all ionic species, chemical reactions involving cyano-copper(I) complexes, and the quasiequilibrium of charge transfer reaction. Experimental polarization curves were compared with theoretical ones, where the diffusion layer thickness was determined. The present model was applied to the prediction of thickness distribution of copper coating on grooved substrates. Two types substrates with grooves of different size (width × depth), (a) 5 mm × 5 mm and (b) 1 mm × 1 mm were used. Agreement between theory and experiments was satisfactory for substrate a, but not for substrate b. The effect of convective mass transfer in the groove was discussed.

104: * Electrochemical Behavior of Glassy Carbon and Some Metals in a $ZnCl_2$-NaCl (60 - 40 mole Percent) Melt

Y. Okano*, A. Katagiri
(*Graduate School of Human and Environmental Studies, Kyoto University)

Journal of the Electrochemical Society, Vol.144, pp.1927-1932, 1997

The stability and reactivity of glassy carbon, nickel, platinum, and tungsten in the $ZnCl_2$-NaCl (60 - 40 mole percent) melt at 450°C were investigated by cyclic voltammetry and constant-potential electrolysis. Glassy carbon was stable in the potential range of 0.23 - 1.8 V vs. Zn in $ZnCl_2$-NaCl(saturated). Nickel was oxidized and partially passivated at 0.8 - 0.9 V; X-ray diffraction analysis revealed the formation of γ-NiZn alloy at 0.20 - 0.25 V and γ_1-NiZn alloy at 0.30 - 0.35 V. Platinum was oxidized and partially

passivated at 1.7 - 1.8 V; it formed γ-PtZn alloy at 0.20 - 0.25 V, γ_1-PtZn alloy at 0.30 V, and β_1-PtZn alloy at 0.35 - 0.40 V. The voltammetric results were consistent with the thermodynamic activity data of Ni-Zn and Pt-Zn alloys. Tungsten was oxidized at potentials above 0.7 V, but no passivation occurred. A gaseous product, presumably WCl_5 or WCl_6, was formed at 1.2 V.

105: Nuclear Design Study on a Super High-burnup Fuel Assembly for Pressurized Water Reactors Using Transuranium

超ウラン元素を利用する超高燃焼度 PWR 燃料集合体の核設計

Masaaki Mori* , Masayuki Hijiya ** , Seiji Shiroya and Keiji Kanda***
(Nuclear Engineering , Ltd.),**(Nuclear Engineering , Ltd.),(Reserach Reactor Institute, Kyoto Univ.)**

Journal of Nuclear Science and Technology, Vol.34, No.7, p. 644-654 (1997)

A conceptual design study was carried out on a super high-burnup mixed-oxide (MOX) fuel assembly (SHB FA) for pressurized water reactors (PWRs) using transuranium (TRU). This study aims to avoid the surplus plutonium (Pu) accumulation and to reduce the accumulation of long-lived radioactive minor actinides (MAs) by utilizing the currently existing PWRs under the condition that the Japanese program to develop fast breeder reactors (FBRs) is tend to delay. For this purpose, an SHB FA with discharged burnup of about 80 GWd/t was investigated by utilizing MAs positively as both burnable absorbers and fissile suppliers and loading high-content Pu. It is possible to load the SHB FAs in a current PWR together with UO_2 FAs and to use 2.5 times as much as amount of Pu as that in a standard 1/3 MOX core. Moreover, it is found to be possible to reduce the total number of fresh FAs further from that of a high-burnup (55 GWd/t in maximum) UO_2 (4.9wt%) core and also to reduce the accumulation of MAs in the nuclear fuel cycle significantly.

106: Present Status and Prospect of KUCA Experiment

ＫＵＣＡ実験の現状と展望

Seiji Shiroya

核データニュース、No.57, p.2-10 (1997)

107: Experimental Investigation on Secondary-Count Effect in Feynman-α Measurement by Fission Counter

Kengo Hashimoto* , Hiroshi Shirai*, Tetsuo Horiguchi* and Seiji Shiroya
***(Kinki Univ.),**

Annals of Nuclear Energy, Vol.24, No.11, p.907-915 (1997)

The Feynman-α (variance-to-mean ratio) measurements were carried out by using fission counters, which contain fissile material of around 2 g, to investigate experimentally the secondary-count effect caused by fission events in the counter. The secondary-count effect observed when the fission counter was covered with graphite, whereas it was not observed when the bare counter was used and when the counter was surrounded by light-water. Therefore, it was concluded that the secondary-count effect depends not only on fission events in the counter but also on the surrounding material of the counter. A formula to correct the secondary-count effect was derived, and it was applied to obtain the inherent decay constant α. The validity of this formula was demonstrated through the comparison with the results obtained by using ^3He and BF_3 counters which are free from the secondary-count effect.

108: Analysis of First-Harmonics Eigenvalue Separation Experiments on KUCA Coupled-Core

Yoshiki Kato*, Toshihisa Yamamoto*, Takanori Kitada*, Toshikazu Takeda*, Kengo Hashimoto, Seiji Shiroya, Hironobu Unesaki and Otohiko Aizawa*****
***(Osaka Univ.), **(Kinki Univ.), ***(Musashi Institute of Technology)**

Journal of Nuclear Science and Technology, Vol.35, No.3, p.216-225 (1998)

The first-harmonic eigenvalue separation, the difference between the fundamental and the first order eigenvalues of the higher harmonic neutron transport equations, which were measured at the Kyoto University Critical Assembly (KUCA) has been analyzed. A method was proposed to calculate the first order eigenvalue based on the discrete ordinate method. The 3-D effect, energy group effect, mesh size effect, and transport effect were investigated. Among these effects, the transport effect was significant and when it was taken into account, the calculated eigenvalue separation approached the measured value on the KUCA coupled-core.

109: * Measurement of $^{237}Np/^{235}U$ Fission Rate in Cores with Various Moderator-to-Fuel Volume Ratios at the Kyoto University Critical Assembly

Seiji Shiroya, Akio Kohashi, Hironobu Unesaki, Takashi Kato, Takanori Kitada*, Tomohiko Iwasaki and Keiji Kanda*****

(Osaka Univ.), *(Tohoku Univ.), *****(Research Reactor Institute, Kyoto Univ.)**

Proc. of International Conference on Future Nuclear Systems, held at Yokohama, Japan, Oct. 5-10, 1997, p1307-1310 (1997)

At the Kyoto University Critical Assembly, $^{237}Np/^{235}U$ fission rate ratios were measured by a back-to-back type double fission chamber to examine the nuclear data and the computational method for the transmutation of minor actinides in light water reactors. Neutron spectra of cores were systematically varied by changing moderator-to-fuel volume ratios. The measured data were compared with the calculated results by the SRAC code system on the basis of three different nuclear data for ^{237}Np fission cross sections. It was indicated from present result of comparison that the use of JENDL-3.2 better than that of JENDL-3.1 or ENDF/B-IV.

110: Measurement of Flux Tilt and Eigenvalue Separation in Axially Decoupled Core

Masaki Andoh* , Tsuyoshi Misawa, Kojiro Nishina and Seiji Shiroya**

(Nagoya Univ.), *(Nagoya Univ.)**

Journal of Nuclear Science and Technology, Vol.34, No.5, p.445-453 (1997)

A study on the nuclear characteristics of an axially decoupled core was performed through a series of experiments using the solid moderated core in the Kyoto University Critical Assembly (KUCA). In the axially decoupled core which has an internal blanket between the upper and lower cores, the measured differential reactivity worth of a control rod moving axially was apparently asymmetric between the two core regions. Since it was considered that this phenomenon was attributed to the neutron flux tilt caused by the axial movement of control rods during the measurement of differential worth, the axial reaction rate distributions were measured by gold wires with and without cadmium tube. It was found that the reaction rate distribution was remarkably tilted by changing the pattern of control rods inserted in the core to maintain the critical state, and that the flux distribution was tilted without energy dependency. The value of first-order eigenvalue separation based on the Explicit Higher-order Perturbation (EHP) method. This value agreed with the calculated results by the SRAC system.

111: Development of Perturbation Code Based on Modified Explicit Higher Order Perturbation Method with Two-Energy-Group

Cheol Ho Pyeon, Yoshihiro Yamane*, Tsuyoshi Misawa, Akio Yamamoto , Katsushi Kagehira*** and Seiji Shiroya**

(Nagoya Univ.), *(Nuclear Fuel Industry), *****(Nuclear Fuel Industry)**

Proc. of the Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications, held at Saratoga Springs, New York, U.S.A., Oct. 5-9, 1997, p. 1149~1158 (1997)

112: * Electronic States of Cobalt Iron Cyanides Studies by ^{57}Fe Mossbauer Spectroscopy

Y. Einaga, O. Sato, T. Iyoda, Y. Kobayashi, F. Ambe, K. Hashimoto, and A. Fujishima

Chem. Lett., 289-290 (1997)

The electronic states of cobalt iron cyanides were observed using ^{57}Fe Mossbauer. It was revealed that Prussian blue analogs $Co_{1.5}[Fe(CN)_6]6H_2O$ and $K_{0.5}Co_{1.25}[Fe(CN)_6]3.6H_2O$ have Fe^{III} (Iow spin) and Fe^{II} (low spin), respectively, at both room temperature and 4 K. In $Co_{1.5}[Fe(CN)_6]6H_2O$, a magnetic hyperfine inieraction was observed at low ternperature. Moreover, the Mossbauer spectra provided clear evidence for an internal electron transfer from $Fe^{III}$to Co^{II} in $K_{0.5}Co_{1.25}[Fe(CN)_6]3.6H_2O$ by red light illumination at low temperature.

113: * Spin Switching Effect in Nickel Nitoroprusside: Design of a Molecular Spin Device Based on Spin Exchange Interaction

Z. Z. Gu, O. Sato, T. Iyoda, K. Hashimoto, and A. Fujishima

Chem. Mater., 9(5), 1092-1097 (1997)

The mechanism of photocatalytic decomposition of ethanol in aqueous solution was studicd using a microelectrode technique. We employed a partially Pd-covered TiO_2 film as a model for the metal-deposited photocatalyst. We observed concentration changes of dissolved oxygen and H_2O_2 caused by the photocatalytic reaction in the absence and presence of ethanol separately above the bare TiO_2 and Pd-covered surfaces. It is clearly shown that dissolved oxygen is consumed even on oxidation sites of thc photocatalyst in the presence of ethanol, producing H_2O_2. On the basis of these results, we conclude that radical chain reactions procced at oxidation sites (i.e., bare TiO_2) but not at reduction sites (i.e.,

Pd-covered surface) on the photocatalyst.

114: * Photocataytic Reactions Involving Radical Chain Reactions JO

K. Ikeda, H. Sakai, R. Baba, K. Hashimoto, and A. Fujishima

J. Phys. Chem., B, 101, 2617-2620 (1997)

A new approach for designing optically switchable molecular communication devices based on spin-exchange interactions is proposed in the present paper. The device is constituted from two parts, i.e., a paramagnetic block (PMB) and a coupling control block (CCB). As a prototype of this model, nickel nitroprusside, $Ni[Fe(CN)_5NO]\cdot H_20$ was synthesized, in which the nickel ion acts as the PMB and the nitroprusside molecule does as the CCB. In this compound, as there is no spin on Fe, the magnetic interaction between the neighboring Ni cations is very weak. No magnetic phase transition can be observed until 1.8 K. Photoirradiation at 475 nm causes a charge transfer from the metal, Fe, to the ligand, NO, which induces two antiferromagnetically coupled spins on Fe and NO. Furthermore, the new spin on Fe interacts ferromagnetically with those on neighboring nickels. As a result, the spins on the Ni ions, which surround the Fe with spin, form a magnetic cluster with S=5.

115: * AFM Molecular Images during Tip-Induced Surface Modification on the (010) Surface of a KCP(Br) Single Crystal

T. Kawasaki, L. Jiang, T. Iyoda, T. Araki, K. Hashimoto, and A. Fujishima

J. Phys. Chem. B, 101, 2723-2729 (1997)

Molecular-resolution images of an electrochemically prepared single crystal of potassiurn tetracyanoplatinate bromide complex (KCP(Br)) were recorded by atomic force microscopy during a tip-induced surface-modification process in which the probing tip scraped off the topmost surface layer by layer. Two kinds of molecular images on the (010) face of the KCP(Br) crystal correspond to altemate layered structures consisting of tetracyanoplatinate layers and interstitial ions. One molecular arrangement was assigned to cyanide ligands and interstitial K^+ and Br^- ions, in good agreernent with that obtained from X-ray diffraction. The other corresponds to rearranged interstitial ion (K^+ and Br^-) layer. The rearrangement of the interstitial ions during the tip-induced surface modification involves both loss of half of the K^+ ions so as to preserve electroneutrality of the surface and to stabilize the dislocations of the rernaining ions. The present AFM imaging process during the tip-induced surface modification provides mechanistic information on molecular and ionic arrangements on the topmost surface.

116: * Characterization of Dye-Doped TiO_2 Films Prepared by Spray Pyrolysis

H. Yanagi, Y. Ohoka, T. Hishiki, K. Ajito, and A. Fujishima

Appl. Sur. Sci., 113/114, 426-431 (1997)

Thin films of TiO_2 were prepared by spray-pyrolysis of titanium (IV)-oxy-acetylacetonate onto indium-tin- oxide glass electrodes. Depending upon the substrate temperature, morphology of the deposited TiO_2 films changed from irregular aggregates at 200°C to homogeneous particles with a diameter of 50-100 nm above 400°C. Dye-doping was achieved at the substrate temperature below 260°C by dissolving phthalocyanine or rhodamine molecules into the oxy-acetylacetonate solution. Photoelectrochemical measurements indicated that anodic photocurrents at the wavelength range below 400 nm due to direct excitation of TiO_2 increased by formation of homogeneous fine particles at higher temperature. The electrode doped with phthalocyanine exhibited photocurrents in its visible absorption band at 600-700 nm whereas that doped with rhodamine yielded no sensitized photocurrent.

117: * Photoelectrorheology of TiO_2 Nanoparticle Suspensions

Y. Komoda, Tata N. Rao, and A. Fujishima

Langmuir, 13(6), 1371-1373 (1997)

The electrorheological pralperties of a TiO_2 (anatase) particle suspension in silicone oil were found to undergo changes during illumination, including an increased electrorheological effect, i.e., inclsased viscosity upon illumination. The increased viscosity is due to the polarization of photoinduced charge carriers under the influence of the imposed electric field. A small photocurrent was observed, which can be attiibuted to photoelectrophoretic conduction and leakage of photogenerated charge through field-induced columns. Microlscopic observation carried out under stationary conditions showed an increase in the number of field-induced columns upon illumination, consistent with increased viscosity.

118: * Surface Molecular Rearrangements on the (0001) Face of C_{70} Single Crystals

L. Jiang, T. Iyoda, D. A. Tryk, N. Kino, K. Kitazawa, A. Fujishima, and K. Hashimoto

Jpn. J. Appl. Phys. 36, Part 1 (6B), 3903-3908 (1997)

Surface molecular rearrangements on the (0001) face of C_{70} single crystals were investigated using atomic force microscopy (AFM). On the snrface of a freshly prepared crystal, the molecules are arranged

in a slightly distorted hexagonal close-packed (hcp) structure, with an average nearest- neighbor distance of 10.5 ±0.3A. After the samples were stored for two weeks in dry air, the surfaces of the crystals became relatively rough. A quasi-two-dimensional molecular rearrangement from a purely hexagonal structure to a mixture of hexagonal, cubic, and rhombic structures was observed over a several- nanometer region. For different crystal growth conditions, a superstructure resulting from a quasi-three-dimensional surface molecular rearrangement was grown and observed on the surface of the crystals. The superstructure appears as an ordered array of domain boundaries between surfaces regions with face-centered cubic (fcc)-type stacking (CBA) and hcp-type stacking (ABA) regions. The coexistence of the different phases in a nano-scale area is probably due to the similarity of the cohesive energies of the phases. The AFM images represent the direct observation of a transient state in a surface phase transformation on the C_{70} single crystals.

119: * Distribution of Componnents in Composite Two-Dimensional Arrays of Latex

S. Matsushita, T. Miwa, and A. Fujishima

Langmuir, 13(9), 2582-2584(1997)

We have successfully prepared conposite two-dimensional arrays, composed of polystyrene particles and carboxylate particles, on a solid surface in a highly oriented coating. The manner in which the particles assembled to form the arrays differed with the pH of the particle suspensions. Therefore, the pH is proposed as an effective means of controlling the distribution of particles in the array. In addition, the authors found that the fractal dimension is useful in characterizing quantitatively the distribution properties of these images.

120: * Cation-Driven Electron Transfer Involving a Spin Transition atRoom Temperature in a Cobalt Iron Cyanide Thin Film

O. Sato, Y. Einaga, T. Iyoda, A. Fujishima, and K. Hashimoto

J. Phys. Chem. B, 101(20), 3903-3905 (1997)

The electronic structure of a cobalt iron cyanide thin film, $Na_{0.4}Co_{1.3}[Fe(CN)_6]5H_20$, was switched from Fe^{III} (low spin)-CN-Co^{II} (high spin) to Fe^{II} (low spin)-CN-Co^{III} (low spin) by exchanging cations in interstitial sites from Na^+ to K^+. The reverse process was also induced by replacing Na^+ to K^+ .That is, the alkali cations in the interstitial sites dominate the electronic and spin states of the host compound. This type of switching phenomenon can be achieved by choosing a compound with both electronic degeneracy and zeolitic properties.

121: * Photo-Induced Structural Transformation on the Surface of Azobenzene Crystals

K. Nakayama, L. Jiang, T. Iyoda, K. Hashimoto, and A. Fujishima

Jpn. J. Appl. Phys., 36, Part 1 (6B), 3898-3902 (1997)

Atomic force microscopy (AFM) was used to investigate the surface structure and photo-induced surface morphological changes in azobenzene crystals. In large-scale images, a layered structure was observed. The thickness of the layer was 1.8 ± 0.2nm, corresponding to bilayers of azobenzene molecules. Molecular resolution images revealed that the molecular arrangement on the surface of the layers was a (001) face, with intermolecular distances of a = 1.32 ±0.02nm and b= 0.62 ± 0.02nm. By irradiating the crystal surface with UV or visible light, structural transformations were observed, which are considered to be the $trans - cis$ photoisomerization of surface azobenzene molecules.

122: * Photocatalytic Bactericidal Effect of TiO2 Thin Films: Dynamic View of the Active Oxygen Specied Responsible for the Effect

Y. Kikuchi, K. Sunade, T. Iyoda, K. Hashimoto, and A. Fujishima

J. Photochem. Photobiol.A: Chem., 106, 51-56 (1997)

The role of active oxygen species in the photocalalytic bactericidal effect was investigated using a thin transparent titanium dioxide (TiO_2) film. The viable number of *Escherichiacoli*(*E.coli*) significantly decreased on the illuminated TiO_2 film, and the bactericidal effect was observed even when *E.coli* was separate from the TiO_2 surface with a 50 μm porous membrane. Mannitol, a hydroxyl radical scavenger, inhibited the effect only in the absence of the membrane. In contrast, catalase inhibited the effect in all cases. On the basis of these results, the long-range bactericidal effect of hydrogen peroxide was proposed, together with a cooperative effect due to other oxygen species.

123: * Observation of Photocurrent from Band-to-Band Excitation of Semiconducting p-Type Diamond Thin Film Electrodes

L. Boonma, T. Yano, D. A. Tryk, K. Hashimoto, and A. Fujishima

J. Electrochem. Soc., 144(6), L142-L145 (1997)

High quality semiconducting boron-doped polycrystalline diamond thin films were prepared on Si substrates via microwave plasma chemical vapor deposition. The resistivities of the lightly doped films were

on the order of $10^2\Omega$ cm. The photoelectrochemical behavior was studied with excimer lasers of several different wavelengths, including ArF (193 nm, 6.4 eV), KrF (248 nm, 5.0 eV), and XeF (351 nm, 3.53 eV). The photocurrent observed using the ArF laser was significanily greater than those observed with the KrF and XeF lasers. We propose that, for the ArF laser, the suprabandgap illumination was able to excite electrons into the conduction band, while the KrF and XeF lasers were not.

124: * Preparation of a New Nanostructured TiO_2 Surface Using a Two-Dimensional Array-Based Template

S. Matsushita, T. Miwa, and A. Fujishima

Chem. Lett., 925-926 (1997)

Nanoporotis, nanostructured semiconducting films of photocatalytic titaniuin dioxide (TiO_2) were fabricated by molding from two-dimensionally ordered arrays. We were able to control the structures of the periodic surfaces by varying the annealing temperature of the films.

125: * A Kelvin Probe Force Microscopic Study of the Local Dopant Distribution in Conducting Polybithiophene

O. A. Semenikhin, L. Jiang, T. Iyoda, K. Hashimoto, and A. Fujishima

Dopant Distribution in Conducting Polybithiphene, 3321-3326 (1997)

Local dopant distribution in electrochemically deposited polybithiophene films as well as the effect of the electrochemical treatment were studied *exsitu* using the technique of Kelvin probe force microscopy (KFM). The doping- level distribution was found to be directly related to the polymer surface morphology. For the as-grown polymer, most or the doping anodic charge was found to be located at the grain tops. The polymer that was further electrochemically doped featured relatively higher doped grain periphery and less doped grain tops. On the contrary, undoping or the polymer resulted in no pronounced change in the dopant distribution pattern. The effect or the pretreatment or the HOPG support on the propeties or the polyrner films is also discussed. A model is proposed that relates the observed inhomogeneity the lateral ditribution or the primary polymer nuclei formed during the initial steps or the polymer deposition process. The results suggest that the KFM is a powerful tool for studying dopant distribution in conducting polymers.

126: * Nanometer-Size Cu Clusters Formed by Reversible Deintercalation on Layered Chalcogenides with Scanning Probe Techniques

L. Jiang, W. Jaegermann, C. Pettenkofer, Y. Tonum, T. Iyoda,K.Hashimoto, and A. Fujishima

Adv. Mater., 9(7), 578-581 (1997).

We have demonstrated that Cu can be reversibly intercalated on the van der Waals(0001) plane of 1T $TaSe_2$. This process allows formation and erasure of clearly defined Cu clusters on atomically flat substrates. In principle this process may hold the potential of a technologically feasible nanometer-scale reversible storage device working at ambient conditions.

127: * Charge Transport Processes in Electrochemically Deposited Poly(Pyrrole) and Poly(N-Methylpyrrole) Thin Films

J. J. Kim, T. Amemiya, D. A. Tryk, K. Hashimoto, and A. Fujishima

J. Electroanal, Chem., 416, 113-119 (1997)

Poly(pyrrolc) (pPy) and poly(*N*-methylpyrrole) (pNMePy) films that were electrodeposited under similar conditions were compared in terms of electronic conductivities and counterion diffusion coefficients. Films were prepared and compared both in aqueous electrolyte (CI^-, ClO_4^- counterions) and in non-aqueous (propylene carbonate) eleclrolytc (ClO_4^- counterion). Consistent with the range of values reported in the literarure, the electronic conductivities differed by a factor of ca. 5×10^3 , although this is lower than the often-cited value of los This smaller difference in the conductivities is more consistent with that expected on the basis of simple steric factors. A.c. impedance measurements were used to determine the counterion diffusion coefficienis. That for ClO_4^- was approximately one order of magnitude lower in pNMePy than that in pPy, possibly due either to differences in morphoiogy or to Stronger interactions of the counterion with the polymer chains.

128: * Light-Induced Amphiphilic Surfaces

R. Wang, K. Hashimoto, A. Fujisima, M. Chikuni, E. Kojima, A. Kitamura, M. Shimohigoshi, and T. Watanabe

Nature, 388(31), 431-433 (1997)

The ability to control the surface wettability of solid substrates is important in many situations. Here

we report the photogeneration of a highly amphiphilic (both hydrophilic and oleophilic) titanium dioxide surface. The unique character of this surface is ascribed to the microstructured composition of hydrophilic and olechilic phases, produced by ultraviolet irradiation. The result is a Tio_2-coated glass which is antifogging and self-cleaning.

129: * Electrochemical Modulation of Molecular Conversion in an Azobenzene-Terminated Self-Assembled Monolayer Film:An in Situ UV-Visible and Infrared Study

R. Wang, T. Iyoda, D. A. Tryk, K. Hashimoto, and A. Fujishima

Langmuir, 13(17), 4644-4651 (1997)

UV-visible absorption spectroscopy and Fourier transform infrared reflection absorption spectroscopy were utilized as in situ probes to investigate the electrochemical redox process in an azobenzene-terminated self- assembled monolayer (SAM) film in an aqueous electrolyte. The electrochemical reduction process, which is exceedingly slow due to disruption of the extremely densely packed SAM, prgduced the hydrazobenzene species. Upon reoxidation, the resulting hydrazobenzene is quickly converted back to trans-azobenzene. It appears that the electrochemical redox process is accompanied by a reversible orientational change in terms of the azobenzene terminal group. Therefore, by simply modulating the applied potential, a reprloducible electrochemical redox process together with a reversible orientational variation can be achieved in an organized monolayer film.

130: * Electrostatically Induced Isomerization of Azobenzene Derivatives in Langmuir-Blodgett Films

T . Enomoto, H. Hagiwara, D. A. Tryk, Z. F. Liu, K. Hashimoto, and A.Fujishima

J. Phys. Chem., 101(38), 7422-7427 (1997)

A novel electrochemically induced cis-to-trans isomerization process involving amphiphilic azobenzene derivatives in Langmuir-Blodgett monolayer films at electrode/electrolyte interfaces was examined using electrochemical and UV-visible absorption measurements. This isomerization proceeds electrostatically, i.e., with no Faradaic current and no discernible features in the double-layer capacitive charging current, when relatively positive electrode potentials are applied to the monolayer film. This electrostatically induced process is rather slow (first-order rate constants in the $10^{-2} - 10^{-1} s^{-1}$ range over the potential range of +0.65 to +0.85 V vs Ag/AgCI, respectively), but the highest rate constant measured (at +0.85 V vs Ag/AgCI) represents an increase of approximately 3 orders of magnitude compared to that of the thermal isomerization process. Surprisingly, the activation energy for the electrostatic process was found to be essentially potential independent and nearly the same as that for thermal isomelization. The rate constants for the cis-to-trans isomelization obtained at given potentials were also found to

depend sensitively on details of the molecular structure, such as the length of the alkyl chain connecting the carboxyl group to the azo glloup (spacer) and the length of the alkyl tail, which implies that the isomelization reaction involves an interaction between the intrinsic electric field of the molecules in the highly ordered film and the relatively strong electric field associated with the electrical double layer at the electrode surface.

131: * Molecularly Resolved Observation of Surface Reconstruction of C60 Epitaxial Films by Atomic Force Microscopy

Y. Kim, L. Jiang, T. Iyoda, K. Hashimoto, and A. Fujishima

Sur. Sci., 385, L945-L951 (1997)

Reconstructed surfaces of C_{60} epitaxial films on KBr(O01) substrates were directly observed by atomic force microscopy (AFM). AFM imnages showed ridge-like fringes running along the three equivalent [110] directions on the face-centered cubic (fcc) (111) face on the surfaces of C_{60} thick (¿500 nm) films. Molecular-resolution images revealed that the raised fringe region is contracted by ca 3vertical displacernent of the rringe is 0.30±0.02 nm. The observations suggest a stacking-fault-domain model involving periodic transitions between fcc (ABCABC...stacking) and hexagonal close-packed (hcp, ABAB...Stacking) structures. Fcc surface domains were proposed to exist on the wider areas between fringes on the C_{60} film surface based on the fact that the fcc bulk structure is energetically slightly more favorable than that of hcp.

132: * Photogeneration of Highly Amphiphilic TiO_2 Surface

R. Wang, K. Hashimoto, and A. Fujishima, M. Chikuni, E. Kojima, A. Kitamura, M. Shimohigoshi, and T. Watanabe

Adv. Mater., 10(2), 135-138 (1998)

We report the details of the photoconvertible surface wettability. The formation of a microstructured composite between hydrophilic and olephilic phases, which results from the photofenerated Ti^{3+} defects at definite sites, is considered to account for this unique feature.

133: * Kinetics of Photocatalytic Reactions under Extremely Low-Intensity UV Illumination on Titanium Dioxide Thin Films

Y. Ohko, K. Hashimoto, and A. Fujishima

J. Phys. Chem., A, 101(43), 8057-8062 (1997)

The photocatalytic decomposition efficiency of gaseous 2-propanol was studied using a titanium dioxide thin film under very weak UV light; the incident UV light intensity was 36nw- 45μW·cm^{-2}. Under such low-intensity UV illumination, the value of the quantum yield (QY) increased gradually with decreasing number of absorbed photons and finally saturated (28%) for a number of absorbed photons less than 4 $\times 10^{11}$ quanta ·cm^{-2}·s^{-1} for an initial 2-propanol concentration of 1000 ppmv. Thus, purely light-limited conditions were reached. For lower initial concentrations, the QY values decreased, but the same maximum QY value as that for 1000 ppmv was also approached with decreasing light intensity. We discuss these results in terms of the normalized absorbed photon number :' (I_{norm}/S^{-1}),a parameter that we have defined as the ratio of the number of absorbed photons ([photom]$_{ab}$) to the number of adsorbed 2-propanol molecules([M]$_{ad}$. When all of the experimental QY values were plotted as a function of I_{norm}, all of the points appeared on a single line for a wide range of initial 2-propanol concentrations. On the basis of these results, we conclude that either OH radicals or 2-propanol molecules must be able to diffuse at least ca. 11 nm on the titanium dioxide surface in order to react with each other. We also conclude that the maximum QY value of 28% represents the intrinsic charge-separation efficiency for this photocatalyst.

134: * Magnetic Properties of Charge Transfer Complexes of Manganese Porphyrin Derivatives and Tetracyanoethylene

K. Nagai, T, Iyoda, A. Fujishima, and K. Hashimoto

Synthetic Metals, 85, 1701-1702 (1997)

A series of charge transfer complexes between tetracyanoethylene and Inanganesc (II) tetraphenylporphyrin derivatives with redox potentials (E^0(Mn$^{3+/2+}$)) ranging frorn -0.23 through -0.08 V vs. SCE, were prepared. The magnitude of the charge transfer decreased with the more anodically shifted redox potentials of the porphyrins which have stronger electron withdrawing groups, in the order of phenyl, 4-methoxyphenyl, 2- thienyl, and 4-cyanophenyl substituents at meso positions. The rnagnitude of the charge transfer reflected in frequency shift of CN vibration of the TCNE. The magnetization curves at very low tempetature showed hystercsis. The salt with cathodically-shifted E^0(Mn$^{3+/2+}$ has a lower Curie temperature (Tc). In other words. the degree of the charge transfer between TCNE and Mn porphyfin responsible foi the high T_C

135: * A Soft-Hard-Tunable Molecule-Based Magnet Via Photo-Induced Spin-Flopping Transition in a MnTEtOPP-TCNE Charge Transfer Salt

K. Nagai, T. Iyoda, A. Fujishima, and K. Hashimoto

Sold State Commu., 102(11), 809-812 (1997)

A photo-induced spin-flopping transition was observed below 5 K, lower than the Curie temperature (T_c = 25 K), in a new charge- transfer-type magnet of manganese porphyrin derivative and tetracyanoethylene(TCNE). While the spin-flopping transition on interchain spin alignments takes place irreversibly in high external field, the transition is induced reversibly by the photoirradiation, depending on the external magnetic field. This transtion causes a drastic change in coercive force by four orders of magnitude (ca 0.5 mT to ca 2 T).

136: * Color Impendance and Electrochemical Impedance Studies of WO_3 Thin Films: Behavior of Thinner Films in Non-Aqueous Electrolyte

J. J. Kim, D. A. Tryk, T. Amemiya, K. Hashimoto, and A. Fujishima

J. Electroanal. Chem., 433, 9-17 (1997)

The electrochemical and color impedance behavior of thin (0.25 μm) amorphous WO_3 films was examined. In general, the two types of behavior match rather well over most of the frequency range,but ieviations were observed at high and low frequencies. The high frequency deviation involved a phase shift of greater than 90° due to a non- faradaic capacitance, which most likeiy invoives either ClO_4^- insertion or an ion exchange process in which Li^+ adsorbs on the surface of the film and displaces protons, which then jump into lattice sites associated with coloring. The low frequency deviation prohably involves a similar but much slower ion exchange process involving the bulk of the amorphous WO_3 structure.

137: * First-Order Hyperpolarizability of Oligo-Acene Derivatives by Hyper-Rayleigh Scattering

K. Ishibashi, T. Iyoda, K. Hashimoto, A. Fujishima, Y. Shirai,and J. Abe

Chem. Phys. Lett., 279, 107-111 (1997)

First-order hyperpolarizabilities β for a series of oligo-acene derivatives were estimated as a function of the conjugation length by means of the hyper-Rayleigh scattering (HRS) technique. Satisfactory

data acquisition and analyses gave the hyperpolarizabilities $(17 \mp 2)\times 10^{-30}$ and $(68 \mp 8)\times 10^{-30}$ esu for naphthalene-2,3- dialdehyde and anthracene-2,3-dial-dehyde, respectively. The pure β value of tetracene-2,3-dialdehyde (OA4) could not be determined because of multiphoton absorption induced fluorescence superimposed on the HRS signal. A large β value ($\approx 180 \mp 10^{-30}$ esu) is expected for OA4 by extrapolating the conjugation length dependence on β.

138: * Comparative Studies on the Photocatalytic Decomposition of Ethanol and Acetaldehyde in Water Containing Dissolved Oxygen Using a Microelectrode Technique

K. Ikeda, K. Hashimoto, and A. Fujishima

J. Electroanal, Chem., 437, 241-244 (1997)

Photocatalytic decomposition of ethanol and acetaldehyde in water containing dissolved oxygen was studied using a microelectrode technique. We employed a partially Pd-covered TiO_2 film as a model for the metal- deposited photocatalyst and observed concentrarion changes of dissolved oxygen above the TiO_2 surface due to the radical chain oxidation initiated by the photooxidation. The concentration change of dissolved oxygen was larger in acetaldehyde-containing aqueous solution than in ethanol-containing aqueous solution. In addition, we examined the role of superoxide radicals in the decomposition of ethanol and acetaldehyde using a biological enzyme, superoxide dismutase (SOD). The amount of oxygen consumed in the ethanol solution was much less in the presence of SOD than in the absence of SOD. However, the amount consumed in the acetaldehyde solution was greater in the presence of SOD than in the absence of SOD. Based on these results, we have suggested decomposition mechanisms for ethanol and acetaldehyde.

139: * Color Impendance and Electrochemical Impedance Studies of WO_3 Thin Films: H^+ and Li^+ Transport

J. J. Kim, D. A. Tryk, T. Amemiya, K. Hashimoto, and A. Fujishima

J. Electroanal. Chem., 435, 31-38 (1997)

Ac potential-modulated optical transmittance (color impedance) and electrochemical impedance measurements were employed in an in situ investigation of the electrochromic behavior of evaporated amorphous tungsten trioxide (a-WO_3) films in non-aqueous ($LiClO_4$ + propylene carbonate), aqueous acid (H_2SO_4) and mixed non- aqueous-aqueous acid (PC+$HClO_4$) electrolytes. The optical and electrochemical responses were essentially the same with the 0.8 μm thick films that were examined, indicating that all of the injected charge was involved in the faradaic process. The behavior of the WO_3 films in $LiCl0_4$ + PC and H_2S0_4 electrolytes was relatively simple compared to that of the PC +$HClO_4$ electrolyte, in which the charge transfer resistances and diffusion coefficients were found to vary considerably with potential,

probably due to a shift from proton insertion at more positive potentials to lithium ion insenion at more negative potentials. In all of the electrolytes, evidence was seen for two types of diffusion processes, a slower one, most likely due to diffusion within small clusters of WO_6 octahedra, and a faster one, due to diffusion in nanometer-scale spaces between these clusters.

140: * Surface-Enhanced Raman Imaging (SERI) of Patterned Self-Assembled Monolayers of Various Derivatized Thiophenols on Silver

D. A. Tryk, X. Yang, K. Hashimoto, and A. Fujishima

Bull. Chem. Soc. Jpn., 71(1) 31-39 (1998)

Surface-enhanced Raman imaging (SERI)

141: * Structural Investigation of Azobenzene-Containing Self-Assembled Monolayer Films

R. Wang, T. Iyoda, L. Jiang, D. A. Tryk, K. Hashimoto, and A. Fujishima

J. Electroanal. Chem., 438, 213-219 (1998)

An azobenzene-terminated long chain alkanethiol was used for self- assembly onto gold substrates. A remarkable lack of activity for trans-to- cis photoisomerization in the film was evaluated quantitatively using a combined photochemical-electrochemical method. The film structure was then examined in detail by means of UV-visible spectroscopy and atomic force microscopy (AFM). The results indicated that the azobenzene- containing molecules were extraordinarily densely packed in the SAM. A pinwheel structure, in which the long axes of the azobenzene moieties are parallel to each other and the neighboring short axes are mutually perpendicular to each other, was supported by UV-visible and IR evidence and was observed directly with AFM. This structure is consistent with the dense packing. By comparing with the structure of the same molecule in the crystalline state, it was found that the pinwheel struclure can be ascribed to a combination of the covalent bonding between the sulfur head-groups of the molecule and Au atoms of the substrate, the strong van der Waals interaction of the alkane chains, and interactions between neighboring azobenzene moieties.

142: * Two Types of Spiral Growth of C_{60} Films on KBr(001)

Y. Kim, L. Jiang, T. Iyoda, K. Hashimoto, and A. Fujishima

Appl. Phys. Lett., 71(24), 3489-3491 (1997)

Two types of spiral growth, single and double spirals, of C_{60} epitaxial films on a KBr(001) substrate were observed by atomic force microscopy (AFM). These single and double spirals were found on films grown at different rates. All spiral islands show the threefold symmetry of the face-centered-cubic (fcc) structure. In the case of single spifals, many fringes were observed in three equivalent [110] directions on the fcc (111) surface. From the AFM images, we concluded that the growth process of these spirals can be explained by the classical crystal growth theory of Burton, Cabrera, and Frank and that screw dislocations form without any direct influence of the substrate.

143: * Photoelectrorheological Phenomena Involving TiO_2 Particle Suspensions

Y. Komoda, N. Sakai, T. N. Rao, D. A. Tryk, and A. Fujishima

Langmuir, 14(5), 1081-1091 (1998)

Photoeffects on the electrorheological (ER) properties of various types of commercial TiO_2 powders dispersed in silicone oil were investigated. Two types of photoelectrorheological (PER) efrects (i.e., positive and negative) were observed in these fluids, the effect being dependent on the adsorbed water content of the powder. The positive PER effect of low-water-content (<2wt%) particle suspensions during illumination, associated with low photocurrents, is due to the polarization of photogenerated electrons and holes under the influence of the applied electric field, which facilitates the formation of particle cluster bridges between the electrodes under the relatively low flow rate conditions used in this work. The negative PER effect in the case of high-water-content (>3wt%) particle suspensions is correlated with the high degree of photoelectrophoretic (PEP) oscillatory motion of particle clusters between the electrodes that was directly observed and measured using microvideo techniques under stationary conditions (i.e., no net flow). This circulation of clusters is responsible for the high photocurrents that are observed even under flowing conditions, that is, when there are few bridges. The enhancement of the PEP effect due to the presence of water is explained on the basis of (1) enhanced charge transfer from the electrode to the particles and (2) greater numbers of trapped photogenerated carriers. These caniers can be trapped via reactions involving water, and the resulting species can be either reduced at potentials less negative than the conduction band edge or oxidized atpotentials less positive than the valence band edge. The large decrease in the residence time of particles at the anode due to illumination is thought to be due to a large increase in the concentration of photogenerated minority carriers (holes) in the TiO_2, which is an n- type semiconductor. The enhanced PEP effect which results from increased water content is believed to be a key factor in the diminution of the ER effect in the high-water-content particle suspensions.

144: * Kinetic Analysis of the Photocatalytic Degradation of Gas-Phase 2-Propanol under Mass Transport-Limited conditions with a TiO_2 Film Photocatalyst

Y. Ohko, A. Fujishima, and K. Hashimoto

J. Phys. Chem., B, 102(10), 1724-1729 (1998)

A kinetic study of the degradation of gas- phase 2-propanol was camed out using a TiO_2 film photocatalyst in a batch-type reactor under relatively high-intensity UV light illumination; the incident UV intensity was varied from 35 μW cm^{-2} to 60 mW cm^{-2}, and the initial 2-propanol concentration was varied from 0.1 ppmv to 100 ppmv. Although the degradation rate increased with increasing numbers of absorbed photons at lower light intensities, it gradually saturated and finally reached completely mass transport-limited conditions. We simulated the decrease in gas-phase 2-propanol concentration as a function of time under mass transport- limited conditions using the one-dimensional diffusion equation, assurning a boundary layer thickness of 1.5cm. On the basis of these results, together with previously reported results obtained under extremely low-intensity UV light illumination (36 nW cm^{-2} 45 μW cm^{-2}), we have mapped various regions on a light intensity vs initial reactant concentration plot, corresponding to pure mass transport-limited conditions and pure light intensity-limited conditions for the photocatalytic degradation of gas-phase organic compounds.

145: * Hydration-Dehydration-Induced Reversible Ordering-Disordering Transition of the Molecular Arrangement on the Surface of KCP(Br) Single Crystals

T. Kawasaki, L. Jiang, T. Iyoda, T. Araki, K. Hashimoto, and A. Fujishima

J. Phys. Chem., B, 102(11), 1989-1993 (1998)

Molecular-resolution images by atomic force microscopy (AFM) revealed a reversible ordering-disordering transition of molecular arrangernents on the (010) face of a single crystal of potassiurn tetracyanoplatinate bromide (KCP (Br)) during dehydration and dehydration treatments. The intracolumnar Pt-Pt distance along the *c*-axis in the dehydrated crystai lengthens by a factor of 30shows well-ordered arrangement like the as-grown crystal, while the intercolumnar stmcture along the orthogonal direction is not varied. Large-scale AFM images showed that the monolayer terraces reversibly slide in the c-axis direction during the dehydration-hydration treatments, reflecting the molecular dislocation along the c-axis. This surface structural change is quite consistent with well-known dehydraion effects in KCP(Br) crystals, i.e., the lattice disordering and the decreasing conductivity.

146: * Time-Dependent Behavior of Active Oxygen Species Formed on Photoirradiated TiO_2 Films in Air

K. Ishibashi, Y. Nosaka, K. Hashimoto, and A. Fujishima

J. Phys. Chem., B, 102(12), 2117-2120 (1998)

Active oxygen species formed on TiO_2 film photocatalysts in air were examined by use of a chemiluminescence method. Under relatively strong UV light irradiation, 15 mW cm^{-2}, two types of active oxygen species formed on the $Ti0_2$ surface were observed after the interception of the excitation light, i.e., one with a shorter lifetime, ca. 3 s, and another with a longer lifetime, ca. 50 s, which may correspond to superoxide (O_2^-). On the contrary, under relatively weak UV light irradiation, 1 μW cm^{-2}, only the long-lived species, O_2^-, was observed. The concentration of O_2^- on the TiO_2 surface was saturated even under weak UV illumination, while the short-lived species was not. We suggest that O_2^- is deactivated mainly by an electron transfer to surface defects or vacancy sites on the TiO_2 surface. This deactivation reaction proceeds almost independently of coexisting active species.

147: * Magnetic Properties of Mixed Ferro-Ferrimagnets Composed of Prussian Blue Analogs

S. Ohkoshi, T. Iyoda, A. Fujishima, and K. Hashimoto

Phys. Rev., B, 56(18), 11642-11652 (1997)

We have succeeded in controlling the saturation magnetization (I_S), the Weiss temperarure (θ), and the coercive field (H_C) using compounds in the seies $(Ni_x^{II}Mn_{1-x}^{II})_{1.5}[Cr^{III}CN_6]$ as model compounds. The key to this strategy is to manipulate both ferromagnetic (J>O) and antiferromagnetic (J<O) exchange interactions by incorporating the appropriate molar ratios of the transition-metai ions. Minimum values of I_S were found for x values close to 3/7 (0.429), just at the point where parallel spins (Cr^{III} and Ni^{II}) and antiparallel spins (Mr^{II}) should completely cancel out. The θ_c values increased monotonically from negative to positive with increasing x, indicating that the predominant interaction mode was shifting from antiferromagnetic to ferromagnetic. The highest coercive field was observed for a cornpound with an x value close to 3/7. The magnetization vs temperature curves below T_c exhibited various types of behavior, depending on x. For example, the curves for x=0 and x=1 exhibited monotonic increases in magnetization below T_c with decreasing T, while the curve for x=0.45 exhibiied a single maxmum, and that for x=0.38 exhibited two maxima in a field of 1000 G. Of particular interest is the fact that the compound for which x was 0.38 exhibited negative vallles of magnetization in a field of 10 G below approximately 39 K and positive values above this temperature, showing that the magnetic pole can be inverted. We analyzed these temperature dependences using molecular- field theory with three types of sublattice (Ni, Mn, Cr) sites. This phenornenon is observed because the negative magnetization due to

the Mn^{II} sublattice and the positive magnetizations due to the Ni^{II} and Cr^{III} sublattices have different temperature dependences.

148: * Autoxidation of Acetaldehyde Initiated by TiO_2 Photocatalysis under Weak UV Illumination

Y. Ohko, K. Hashimoto, and A. Fujishima

J. Phys. Chem., A, 102(15), 2699-2704 (1997)

The photocatalytic decomposition effciency of gas-phase acetaldehyde was studied using a titanium dioxide thin film under weak UV illumination. Acetic acid and carbon dioxide were detected as the main reaction products. It was round that the apparent quantum yields (QY) for acetaldehyde degradaion are determined by the normalized absorbed photon number (I_{norm}/S^{-1}), a parameter that is defined as the ratio of the number of absorbed photons to the number of adsorbed acetaldehyde molecules. This result is similar to that for 2-propanol degradation reported previously (Ohko, Y.; HashiffioLo, K.; Fujishima, A. J. Phys. Chem A 1997,10l, 8057). However, although the QY values for 2- propanol degradation reachcd a constant value (ca. 28%) for very low relaive light intensity (in the I_{norm} region less than $10^{-4}s^{-1}$), those for acetaldehyde degradation continued to increase with dereasing I_{norm} and reachcd 180ppmv, at an I_{norm} value of $3 \times 10^{-5}s^{-1}$. This discrepancy is due to the existence of radical chain reactions for the latter reaction. Compared to the maximum QY yield for 2-propanol decomposition (28%), which involves no chain-type reactions, the maximum QY for acetaldehyde conversion to acetic acid (150%) implies a radical chain-typc process with a chain length or approximately five.

149: * Photodecomposition of a Langmuir-Blodgett Film of Stearic Acid on TiO_2 Film Observed by in Atomic Force Microscopy and FT-IR

Phillip Sawunyama, Lei jiang, A. Fujishima,and K. Hashimoto

J. Phys. Chem., B, 101, 11000-11003(1998)

We have probed the TiO_2- mediated photomineralization of Langmuir-Blodgett (LB) films of stearic acid via atomic force microscopy (AFM) and FT-IR. In situ AFM images revealed that at the submicrometer level the photodecomposition process of stearic acid molecules on a polycrystalline anatase TiO_2 film is inhornogeneous, with the various reaction initiation centers or nucleation regions being randornly disiribuced throughout the phoiocatalyst surface. Furthermore, parallel FT-IR results showed that the reaction follows pseudo-first-order kinetics. To rationalize the observed randorn LB film photoetching and buckling behavior, we invoked a simple reaction model that incorporates the reactivity of the TiO_2 film and LB film disorganization phenomenon during the photodegradation process.

150: * Effect of Absorved Water on ThePhotoelectrorheology of TiO_2 Particle Suspensions

N. Sakai, Y. Komoda, T.N. Rao, D. A. Tryk, and A. Fujishima

J. Electroanal. Chem., 445, 1-6(1998)

The photoelectrorheological properties of several types of TiO_2, samples having widely varying surface water contenis were exarnined in order to understand the role of water in the photoelectrorheology of TiO_2-based fluids. The particles having low water contents showed an increase in the ER effect upon illumination, which is due to a polarization by photofenerated charges. The diminution in the photoeffect with increasing water content on the particles is attributed to the partial removal of photogenerated charges which have been trapped as a result of reactions involving water, adsorbed OH groups and oxyfen, e.g. reduction of adsorbed hydroxyl radicals and oxidation or adsorbed superoxide. The resulting photoelectrophoretic effect is believed to dominate the electrorheological force, thus reducing the photoefrect.

151: * What is Photocatalyst?

光触媒とはなにか

K. Hashimoto, and A. Fujishima

O plus E, No.211, 75-81(1997)

152: * Cordination of the Surface Properties using Fine Particles-Distribution and Cohesion in the Composite Two-Dimensional Arrays-, Function and Materials

微粒子による表面特性の制御-複合微粒子アレイのパターン分散性-

S. Matsushita, T. Miwa, and A. Fujishima

Function & Materials, 17(7),53-58 (1997)

機能材料,17(7),53-58 (1997)

153: * Photocatalytic Reactions under Week Illumination

微弱光下の光触媒反応

K. Hshimoto, K. Ishibashi, and A. Fujishima

Laser Reseach,25(6),405-410 (1997)

レーザー研究, 25(6),405-410 (1997)

154: * Electrorheology and Photoelectrochemistry

電気粘性効果と光電気化学

Y. Komoda, and A. Fujishima

Hikari kagaku, 24.32-39 (1997)

光化学, 24.32-39 (1997)

155: * Recent Topics of "The Lighe-Clean Revolution"

光触媒反応による光クリーン革命の現状

A. Fujishima

Kougyou Zairyou, 45(10),26-30 (1997)

工業材料, 45(10),26-30 (1997).

156: * The Optical Control of the Magnetic Hysteresis

磁気ヒステリシスを光で自在に制御する—次元電荷異動型高分子錯体 MnTTP-TCNE 誘導体の分子磁性を例に—

K. Nagai, T. Iyoda, A. Fujishima, and K. Hashimoto

Kotai Butsuri, 32(11),39-44 (1997)

固体物理, 32（11）,39-44（1997）

157: * Photo-Induced Hydrophilicity on the Photocatalyst Sureface and its Application

光触媒超親水化技術とその応用

A. Fujishima

Hikarigijutu contact, 35(11),626-632 (1997).

光技術コンタクト, 35(11),626-632 (1997)

158: * Diamond Electrodes - its Wide Potential Window -

電位窓が広いダイヤモンド電極

A. Fujishima

Chemistry and Chemical Industry, 51-2(2), (1998)

化学と工業, 51-2(2), (1998)

III Department of Energy Conversion Science

(エネルギー変換科学専攻)

159: Improvement of Diesel Combustion Using Pilot Injection and Reduction of Initial Fuel Injection Rate

先立ち噴射および初期噴射率抑制によるディーゼル燃焼の改善

Makoto Ikegami, Koichiro Nakatani, Koji Yamane†, Shotaro Tanaka‡
† The University of Shiga Prefecture, ‡ Yamaha Motor Co.,Ltd

Trans. JSME(B), Vol.63, No.613, pp.3158-3164, 1997

日本機械学会論文集 (B 編), 63 巻, 613 号, pp.3158-3164, 1997

The effects of pilot injection and reduced initial fuel injection rate on combustion and pollutant- and noise-emissions were experimentally studied on a high-speed direct-injection diesel engine using an injection system which might give different injection rate waveforms. The results show that the exhaust NOx concentration at middle load is lowered at a reduced rate of initial injection. For the pilot injection, the pilot fuel amount and the interval between pilot and main injections significantly influence the engine performance and exhaust emissions. At middle load, the pilot injection with a smaller amount and a longer interval may reduce NOx and engine noise. At high load, a reduced rate of initial injection lowers the exhaust NOx concentration and noise emissions, and increases smoke. But smoke is significantly reduced by increasing the average injection rate. This characteristic is remarkable at lower engine speed and little depends on a nozzle orifice diameter. For this reason, it is concluded that the most favorable is the high-pressure injection with lower pressure pilot injection. (in Japanese)

160: * Measurement of Droplet Size, Shape and Velocity in Diesel Sprays Using a Single and Double Nano-Spark Photography Method

Ali Mohammadi†, Kei Miwa†, Takuji Ishiyama, Makoto Abe†
† The University of Tokushima

JSME Int. J., Series B, Vol.41, No.1, pp.7-12, 1998.

Fundamental investigation of non-evaporating diesel spray disintegration was carried out using single and double nano-spark back-light photography of diesel sprays injected into a constant volume chamber. Droplet size, shape and velocity as well as the two-dimensional velocity vectors of the droplets have been simultaneously measured by analyzing the spray photographs, using an newly developed image processing and analyzing method. It was observed that even at the early period of injection, some droplets have a velocity much lower than the penetration velocity of the spray tip. The velocity of droplets around the spray tip is much higher than that of droplets near the nozzle orifice. At the early period of injection, droplets flew away from the spray flow around the nozzle tip. However later at the same position, droplets

were entrained into the spray flow. No droplet entrains into the spray around the spray tip at the early period of injection.

161: * Investigation of Droplets and Ambient Gas Interaction in a Diesel Spray Using a Nano-Spark Photography Method

Ali Mohammadi†, Kei Miwa†, Takuji Ishiyama, Makoto Abe‡
† The University of Tokushima, ‡ Zexel Corp.

SAE Technical paper No.981073, pp.213-223, 1998.

The disintegration process of non-evaporating diesel sprays was investigated by using single and double spark back light photography methods. An droplet image analysis method was developed to measure the in-focus droplet sizes, shapes and velocities. Furthermore, particle tracking velocimetry(PTV) method was applied to elucidate the surrounding gas movement. The results show that the area behind the spray tip is active in disintegration at the early period of injection, however the structures like branch at the spray edge produce a large number of droplets after 300 microseconds elapsed from start of injection. Velocity of droplets behind the spray tip is much higher than that in the nozzle tip region. At the early period of injection, the relative velocity of droplets and ambient gas is very high, however it decreases rapidly and becomes very close to zero from the middle of injection duration to the injection end.

162: * PIV Measurement of Gas Flows in a Jet Flame

Masahiro Shioji, Hiroshi Kawanabe, Makoto Ikegami

Proc. of The First Asia-Pacific Conference on Combustion, Osaka, Japan, pp.306-309,1997

Gas flows in a non-premixed jet flame were investigated by means of particle image velocimetry (PIV). The velocity vector was successfully estimated by calculating a two- dimensional cross-correlation coefficient between two images with a small time interval which were obtained by laser light sheeting method. Characteristics of turbulent flow in a jet flame were clarified from the distribution of fluctuating velocity and vorticity calculated from the velocity distribution. From the results, with a special attention to the pattern of vortex ring and its behavior, it is shown that such an eddy- pair pattern may be produced by an unsteady engulfing motion in the upstream of the flow. In the hot and viscous flaming region, small-scale eddies are quickly dissipated, thereby keeping the pattern of vortex rings in the downstream. Furthermore, based on the comparison of vorticity distributions in a flaming jet and a non-reacting jet, the effect of combustion on the turbulent mixing of fuel and air was discussed in more detail.

163: * Baroclinic Effect on Deformation of Diffusion Flame Front

拡散火炎面に及ぼす圧力・密度勾配の作用

Makoto Ikegami, Hiroshi Kawanabe, Masahiro Shioji

Trans. JSME(B), Vol. 63, No. 613, pp. 3131-3136, 1997

日本機械学会論文集 (B 編), 63 巻 613 号, pp.3131-3136, 1997

Numerical simulations were performed to predict fluid motions induced by interactions between density and pressure gradients. The presence of a vortex string situated in a deviated position from the jet flame axis generates two pairs of vortices near the flame front where a significant density change exists. It is predicted that the deformation and stretching of the flame front take place once the vorticity production becomes stronger than the dissipation due to viscosity. Vorticity production is caused by the baroclinic effect in the upstream position, but the generation due to gas expansion supersedes that of the baroclinic effect in the downstream position. When the pressure gradient is greater than a certain critical value, the vorticity production proceeds at a higher rate, which promotes the deformation of the flame front and accelerates the heat release. (in Japanese)

164: Metallo-Thermo-Mechanical Simulation of Laser-Quenching Process of Carbon Steel by Pulsed YAG Laser Beam

パルス YAG レーザーによる炭素鋼の焼入れの変態・熱・力学的シミュレーション

Kazuyuki Nakasaki†, Tatsuo Inoue
† Kyoto Polytecnic College

J. Society of Materials Science, Japan, Vol.46, No.3, pp.268-275, 1997

材料, 46 巻, 3 号, pp.268-275, 1997

Measurements of temperature variation and residual stress during and after laser-quenching operation are difficult due to too small area of the referred region and too short time of the operation. This motivates the importance of the numerical simulation treated in this paper. The CAE system "HEARTS" developed based on the metallo-thermo-machanics, the validity and accuracy of which had already been confirmed elsewhere, is applied to the simulation of the quenching process of a carbon steel (S45C) by pulsed YAG laser beam in order to evaluate the coupled fields of phase transformation, temperature and stresses. The results of the simulated stress distribution seem to represent the practical mode of shear stress on the quenched boundary, and the shape of the martensite transformed region is compared with the observed micrograph. (in Japanese)

165: The Japanese Sword — Heart Treatment Process Simulation Incorporating Phase Transformation

Tatsuo Inoue, Takuya Uehara, Hiroyuki Ikuta, Itsuki Miyata

Proceedings of International Confertence on Materials and Mechanics'97, Tokyo, pp.137-142, 1997

The theory of metallo-thermo-mechanics developed by the authors relevant to the analysis of coupled fields of temperature, stress/strain and metallic structures induced during phase transformation is applied to simulate the quenching process of a Japanese sword by use of the developed computer code "HEARTS". The results show the modes of martensite structure being equivalent to the shape of the blade, distortion and stresses depending on temperature distribution, which are compared with the experimental data.

166: Processing of Metal Matrix Composite by Centrifugal Casting Technique and Evaluation of the Elastic Properties

遠心鋳造法による金属基複合材料の創成とその弾性的特性の評価

Mamoru Mizuno†, Kenichiro Abe, Tatsuo Inoue
† Nagoya University

J. Society of Materials Science, Japan, Vol.46, No.8, pp.946-951, 1997

材料, 46巻, 8号, pp.946-951, 1997

Metal matrix composite with the functionally gradient properties reinforced by particles are processed by centrifugal casting technique under various casting conditions, and the mechanical properties of the material are evaluated experimentally. In the process, SiC particles are mixed with Al alloy in advance, and they are cast into a mold turning at a given constant velocity. The particles are distributed inhomogeneously into the Al alloy matrix during solidification of the matrix due to the centrifugal force caused by the difference in density between the Al matrix and SiC particle. In order to estimate the functionally gradient properties of the cast composite, the volume fraction of the particle is evaluated from microscopic observation on the cross section, and the Young's modulus is measured by a tension test. As a casting condition, the angular velocity and initial temperature of the mold are change, and the dependence of distribution of the properties on the casting condition is investigated. Then, the capability of the present casting technique to produce functionally gradient material is discussed. (in Japanese)

167: Inelastic Analysis of New Thermal Ratchetting due to Moving Temperature Front — Results of Benchmark Project(A) by JSMS

T.Igari[1)], M. Kobayashi[2)], S. Imatani, Y. Takahashi[3)], R. Take[4)], T. Inoue

1) Mitsubishi Heavy Industries, 2) Nagoya University, 3) Denryoku-Chuo-Kenkyusho, 4) Kawasaki Heavy Industries

Trans. 14th International Conference on Structural Mechanics in Reactor Technology, Lyon, Vol.9 (Division-L), pp.213-220, 1997

Results of the joint project by the Working Group of Inelastic Analysis, Committee of HighTemperature Strength, the Society of Materials Science, Japan, is summarized. The purpose of the project is to find out an appropriate inelastic constitutive equation which can simulate new thermal ratchetting of a cylinder subjected to tarveling axial temperature distribution. Experimental data of ten specimens with several traveling distances, stress levels and hold time at high temperature are prepared. The results of comparison between experiment and corresponding inelastic analysis using six types of constitutive models are shown, and the discussion on the appropriate constitutive equation is performed.

168: Inelastic Analysis of Material Ratchetting of 316FR at Varying Temperature — Results of Benchmark Project(B) by JSMS

F. Yoshida[1)], M. Kobayashi[2)], K. Tsukimori[3)], T. Uno[4)], Y. Fukuda[5)], T.Igari[6)], T. Inoue

1) Hiroshima University, 2) Nagoya University, 3) PNC, 4) Toshiba Co., 5) Hitachi Co., 6) Mitsubishi Heavy Industries

Trans. 14th International Conference on Structural Mechanics in Reactor Technology, Lyon, Vol.9 (Division-L), pp.221-228, 1997

The paper describes the results of the benchmark project of 316FR stainless steel at elevated temperature, which is the second part of the phase 4 activity of the Working Group of Inelastic Analysis, JSMS. The uniaxial stres-starin responses and the analytical prediction are discussed for three types of experiments; (i) strain-controlled ratchetting at varying temperatures, (ii) cyclic straining wuth sreess relaxation, and (iii) stress-cntrolled ratchetting with or without holding peak stress.

169: Molecular Dynamics Simulation of Materio-Thermo-Mechanical Fields in the Melting/Solidification Process

溶融・凝固過程における相変態，温度および応力の分子動力学シミュレーション

Takuya Uehara, Tatsuo Inoue

Trans. Japan Society of Mechanical Engineers (A), Vol.63, No.614, pp.2135-2141, 1997
日本機会学会論文集，A 編，63 巻，614 号，pp.2135-2141, 1997

The coupled mode of phase transformation, temperature variation and induced stress is simulated using the molecular dynamics method. A two-dimensional array of atoms with fcc structure is employed for simplicity, and a Morse-type two-body potential is introduced to evaluate the atomic force. A non-dimensional description of the fundamental equation is derived to account for the general material properties. Calculations are made for the region with temperature gradient in the x-direction, while periodic boundary condition is imposed in both directions. Characteristics of the material and parameters such as melting temperature, specific heat and thermal conductivity are first evaluated followed by steady and non-steady state heat conduction problems coupled with induced stresses. Here, emphasis is placed on the effect of the phase transformation depending on the temperature range below or above the melting point. Simulated results of temperature and stresses indicate the practical feature of macroscopic distribution, especially when compared with the solution of the heat conduction equation plotted in non-dimensional form using a Fourier number. (in Japanese)

170: Molecular Dynamics Simulation of Heat Conduction and Thermal Stress in Relation with Continuum Mechanics

Takuya Uehara, Tatsuo Inoue

Materials Science Research International, Vol.4, No.1, pp.45-52, 1998

Heat conduction phenomena and induced thermal stresses are simulated from a microscopic viewpoint by using a molecular dynamics method. Three dimensional rectangular parallelepiped model composed of 2000 atoms surrounded by periodic boundary is imposed for the simulations. Thermo-physical properties such as melting temperature, specific heat, heat conductivity and latent heat are evaluated at the first step to obtain the fundamental data for the following heat conduction simulation. The central part of the model is heated for two cases with and without melting, and the variation of temperature, potential energy and thermal stresses are simulated. These simulations are carried out with two different potential functions, Lennard-Jones and Morse type, in order to clarify the effects of the interatomic potential, which follows to qualitatively demonstrate similar tendency in spite of remarkable quantitative differences. Then the variation of temperature is compared with the numerical solution of macroscopic heat conduction equation. It is clarified that the results show good agreement with each other if they are plotted against non-dimensional time, or Fourier number. Stresses calculated by molecular dynamics method are also

compared with macroscopic thermal stresses.

171: Effect of Residual Stresses in Drawing Process on a Heat Treatment

Shoji Imatani, Hiroyuki Ikuta, Tatsuo Inoue

Physics and Mechanics of Finite Plastic and Viscoplastic Deformation, pp.35-36, 1997

Most of the engineering materials are produced through a series of forming processes of rolling, drawing and so on, and then they undergo heat treatment of quenching as well as aging as a second processing. The residual stresses are inevitably induced through the first stage of forming, and they have a predominant influence on the following heat treatment process and consequently the dimensional accuracy and the mechanical properties of the final product. In this paper a finite element analysis is carried out in order to evaluate the residual stresses due to the drawing of an axisymmetric bar. The simulation strategy and the boundary condition are carefully discussed because the real forming process involves so complicated phenomena such as friction, large deformatio and coupling between stress and temperature. The result obtained in the simulation is applied to a heat treatment code to evaluate the final residual stress of the product.

172: Simulation of Residual Stresses/Distortion and Structural Change in the Course of Stationary and Scanning Induction Hardening Processes for Steel Rings and Cylinders

Fumiaku Ikuta†, Tatsuo Inoue
† Neturen Co., Ltd.

Proceedings of the 17th Heat Treating Society Conference and Exhposition and the 1st International Induction Heat Treating Symposium, Indianapolis, pp.541-550, 1998

Structural change, residual stresses and distortion are simulated for a ring and cylinder of carbon steel under stationary and scanning incduction hardening process respectively by a CAE sysytem HEARTS. The code was developed for simulating heat treatment process based on metallo-thermo-mechanics taking into account for coupling effect of temperature, structure and strees/stain. The simulation are made as axisymetric problems with stationary and scanning internal heat sourses. Some results for materials witph different material properties and heat source supplied from incuction coil are compared with experimants on distorsion, residual stresses and fraction of metallic phases.

173: * Measurement of Stress and Magnetization by Ultrasonic Transverse Waves

Eiji Matumoto, Kotaro Miki†, Toshinobu Shibata†
† Graduate School of Engineering, Kyoto University

Journal of Electrical Engineering, Vol.48, No.8/S, pp.46-49, 1997

When the stress is applied to a isotropic magnetic material, the anisotropy is induced in the elastic or the acoustic propitious. According to the mechanical nonlinearity, the speeds of ultrasonic waves depend on the applied stress, and the polarization direction of the transverse waves on the stress-induced orthotropic anisotropy. Similarly, when the magnetic field is applied to the material, the uniaxial anisotropy is induced, which gives rise to the change of the wave speed and the polarization of the transverse wave. By use of the phenomena, it is possible to evaluate the direction and the extent of the stress or the magnetiza-tion by measuring the polarization direction and the speed change of the ultrasonic transverse waves.

174: Sensing Technique for Surface Strain Distribution with Piezoelectric Film

Shiro Biwa†, Keisuke Katsumi†, Yohei Omoto, Eiji Matsumoto, Toshinobu Shibata†
† Graduate School of Engineering, Kyoto University

Journal of Electrical Engineering, Vol.48, No.8/S, pp.50-53, 1997

A measurement technique for surface strain distributions of a structural component using sur-face-mounted piezoelectric polymer films is demonstrated. The method consists of mounting a piezoelectric film onto the structure surface, and measuring the distribution of the electric poten-tial over it induced by the deformation of the structure. The measured potentials are converted into strain components using the theoretical formula derived on the basis of linear piezoelectric-ity. The validity and the accuracy of the procedure are illustrated for (i) a plate with a penetrated circular hole and (ii) a plate with a non-penetrated back-surface slit-like groove.

175: * Measurement of Stress and Magnetization Using Ultrasonic Shear Waves Under Magnetic Field

Kotaro Miki†, Eiji Matsumoto, Toshinobu Shibata†
† Graduate School of Engineering, Kyoto University

Proceedings of the Seventh Magnetodynamics Conference, pp.52-57, 1997

Ultrasonic velocity in ferromagnetic materials depends on both stress and external magnetic field. This phenomenon, called magnetoacoustoelasticity, is one of magnetoelastic coupling. This paper presents the theoretical expression of ultrasonic velocity based on the continuum theory about magnetic materials. It is shown that velocity is expressed as a function of stress and magnetization. In this paper it is also shown that direction and strength of magnetization can be known by measuring ultrasonic velocity of shear waves for various polarization direction. And ultrasonic velocity of shear waves were measured for changing magnetic field applied parallel or perpendicular to stress under several stress levels for steel. The results showed the effectiveness of magnetoacoustoelasticity method to nondestructive stress meas-urement. (in Japanese)

176: * Behavior of Cantilever Beam Actuator Using Magnetostriction

Yoshihiro Matsuda†, Eiji Matsumoto, Toshinobu Shibata†
† Graduate School of Engineering, Kyoto University

Proceedings of the Seventh Magnetodynamics Conference, pp.68-73, 1997

Ferromagnetic materials are used as actuators by utilizing the magnetostriction during magnetization pro-cess. In this study, we analyze the behavior of a cantilever beam actuator which consists of the layers of the magnetostrictive material, permendur(Fe-49Co-2V) and the nonmagnetic material, copper. When the beam is deflected by applying the magnetic field, the layer of the magnetic material is subjected to the stress. Thus in order to obtain the exact magnetostriction and the deflection of the beam, we examine the stress dependence of the magnetostriction on the applied stress. It is shown that the calculated deflec-tion of the beam is in good agreement with the experimental result, if we take into account the stress de-pendence of the magnetostriction and the distribution of the magnetization along the axis of the beam. (in Japanese)

177: A First Algorithm for Nonlinear Acoustic Imaging

Tomas Novotny†, Eiji Matsumoto, Toshinobu Shibata†
† Graduate School of Engineering, Kyoto University

Proceedings of Measurement 97 Conference, pp.229-232, 1997

In this paper a method is introduced to numerically solve the inverse problem for frequency-domain scattering integral equation using the minimal structure constraints. Different regulariz-ing functionals are used (Tikhonov regularization, maximum entropy regularization and binary constraints) int order to compare their effects on reconstructed image. The aim is to develop memory-efficient algorithm fact enough to be performed on PC. This method does not assume weak scattering (e.g. the first Borm approximation) and allows general geometry arrangement. Several numerical examples are presented in

order to compare the performance of the method as well as the effect of the regularizing functional. We use these techniques to reconstruct a scatter-er from the synthetic data with the limited number of noisy measurements. The results show the reliability of the proposed method as well as its ability to handle the cases which the Born ap-proximation cannot be applied to.

178: Measurement of Static Strain Distribution Using Piezoelectric Polymer Film (Principle and Application to a Holed Plate)

高分子圧電フィルムを用いた静的ひずみ分布の測定（測定原理および円孔付平板に対する検討）

Keisuke Katsumi†, Shiro Biwa†, Eiji Matsumoto, Toshinobu Shibata†
† Graduate School of Engineering, Kyoto University

Transaction of Japan Society of Mechanical Engineers, Ser.A, Vol.64, No.617, pp.215-220, 1998
日本機械学会論文集 (A 編), 64 巻, 617 号, pp.215-220, 1998

The objective of the present study is to exploit the feasibility of piezoelectric polymer film sen-sors to evaluate in-plane strain distributions of structural components. In contrast to ordinary use of piezoelectric films as strain and strain-rate sensors detecting electric charges and currents po-tentials induced in the piezoelectric film mounted on the surface of a structural component in ac-count the piezoelectric constitutive law of film materials. As an illustrative example, thin films of polarized polyvinylidene fluoride (PVDF) are mounted on a holed elastic plate subjected to in-plane loading, and the induced potential distributions are measured on the film surface by an electrostatic voltmeter of non-contact type. It is demonstrated that the determined strain distribu-tions are in fair conformity with those analytically predicted. (in Japanese)

179: Comparison of Invariant Imbedding and Layer-Peeling Methods in Inverse Problem

Tomas Novotny†, Eiji Matsumoto, Toshinobu Shibata†
† Graduate School of Engineering, Kyoto University

Material Science Research International, Vol.4, No.1, pp.53-59, 1998

This paper examines an implementation of a layer-peeling method to inverse scattering problems in the time domain, which is applied here to the case of one-dimensional lossless discontinuous medium. The method is based on the fast Schur recursion applied directly to the discrete problem. The method is tested on several numerical examples in order to compare its performance to the standard invariant imbedding algorithm. The reconstructions of media from both synthetic data and measured data are presented. The layer-peeling method is shown to be considerably faster than the invariant imbedding method without the loss of precision.

180: Regularization of Inverse Problem for Wave Scattering Based on Sub-Band Decomposition by Wavelets

ウェーブレットによるサブバンド分解を利用した散乱逆問題の適切化

Takahiro Hayashi†, Shiro Biwa†, Eiji Matsumoto, Toshinobu Shibata†
† Graduate School of Engineering, Kyoto University

Transaction of Japan Society of Mechanical Engineers, Ser.A, Vol.64, No.619, pp.257-265, 1998
日本機械学会論文集 (A 編), 64 巻, 619 号, pp.257-265, 1998

In general, inverse problems related to scientific measurements are ill-posed due to lack of sufficient amount of measured data or due to measurement errors, and an inverse solution is commonly obtained by the minimization procedure for a pertinent functional with various regularization techniques. In this study, a new regularization method based on the sub-band decomposition by orthogonal discrete wavelet trans-form is proposed for inverse scattering problem. The data representing the distribution of the unknown parameters are decomposed by orthogonal wavelets into components of different spatial scale, and regu-larization parameters are chosen separately for different components. When some a priori information regarding size and location of the scatterer are available, erroneous components with smaller scale can be damped with higher penalty number while retaining essential information of the scatterers. To demon-strate the validity of the proposed method, the results of the present inverse analysis for an inverse scat-tering problem associated with the two-dimensional scalar Helmholtz wave equation linearized by Born approximation. (in Japanese)

181: Microstructural Effect on Low Cycle Fatigue Behaviour in Ti-Alloys under Biaxial Loading

Toshihiko Hoshide, Eisaku Kakiuchi, Takatoshi Hirota

Fatigue & Fracture of Engineering Materials & Structures, Vol.20, No.6, pp.941-950, 1997

Low cycle fatigue tests under axial, torsional and combined axial-torsional loading were conducted using thin-wall tubular specimens of Ti-6Al-4V titanium alloys. Two kinds of alloys with different microstructures, the $(\alpha + \beta)$ and β alloys, were investigated in fatigue tests at room temperature. When the fatigue life was correlated with the equivalent plastic strain, the life in axial loading shifted toward the lower life region compared with those in other loading modes in both alloys. Dominant surface cracks propagated in Mode I under axial and combined loading in the two alloys. Although the growth of Mode II type was predominant under torsional loading, the growth direction of the main crack coincided with the specimen axis in the $(\alpha + \beta)$ alloy, but the circumferential direction in the β alloy. The cracking morphology depended on the microstructure, especially under the torsional mode of loading, and was simulated successfully by using the proposed model for crack initiation.

182: Simulation of Microstructural Effects on Cracking Behaviour in Biaxial Fatigue

Toshihiko Hoshide

Materials Science Research International, Vol.3, No.2, pp.119-124, 1997

The aggregate model composed of elementary rectangular grains with a double slip system was applied to investigate cracking behaviour associated with microstructural factors in biaxial fatigue. The basic model proposed previously was modified by clustering elementary grains so that the modified model might be applicable to materials with various microstructures. The crack initiation life was calculated based on a dislocation pile-up model. In the analysis of crack initiation, the effective fracture suraface energy and the critical resolved shear stress were discussed from the aspect of mechanical properties of deformation. The subsequent crack growth was assumed to be governed by a competition between two growth modes; one due to crack coalescence and another due to propagation of a single crack. The cluster model was employed to analyze fatigue behaviour of Inconel 718 with a duplex grain structure and of SAE 1045 with larger inclusions. In both cases, the simulated crack distributions were similar to the experimental observations, and a good correlation was found between the analytical and the experimental fatigue lives.

183: * Evaluation of Bending Strength Affected by Specimen Geometry in Silicon Nitride

Toshihiko Hoshide, Hirokazu Sano, Hiroyuki Honda

Materials Science Research International, Vol.3, No.2, pp.112-118, 1997

Four-point bending tests of a silicon nitride were conducted using notched specimens with different notch shapes as well as smooth specimens of distinct sizes, and the effct of the specimen geometry on the bending strength was experimentally clarified. The mean strength in smooth specimens could be almost correlated with the effective volume, though the mean strength in notched specimens shifted toward the lower strength side compared with the relation for smooth specimens. From observation of fracture surface, no unique correlation of the strength with the effective volume was suggested to be ascribed to a difference in flaw morphology between smooth and notched specimens. To discuss the efficiency of the effective volume, a Monte Carlo simulation was also carried out by assuming the same distribution characteristics of cracks in a material. The simulated result revealed that the effect of the specimen geometry on the strength was explained by using the effective volume. When the flaw density was extremely low in a material, the effective volume was found to be inefficient because of a failure of the Weibull assumption.

184: * Simulation of Structural Characteristics of Ceramic Coating Film Based on Modeling of Sputtering Process

Toshihiko Hoshide, Takashi Iizuka

JSME International Journal, Series A, Vol.41, No.1, pp.25-30, 1998

Alumina coating films, which were coated on borosilicate glass by a radio-frequency (RF) magnetron sputtering method, were found to be amorphous in a previous work. It was also revealed that the microhardness of sputtered alumina film was larger with increasing RF output in the processing. There was, however, no simple model to explain experimental observations appropriately. In this work, the dynamics of rigid shperes was adopted in modeling the formation of amorphous coating film in a sputtering process, and a simulation based on the proposed model was carried out to investigate structural properties of coating film. The volume fraction of deposited particles in coating film was evaluated for various conditions in the simulation, and the dependence of film hardness on RF output was also discussed. The simulated results were found to represent experimental observations qualitatively.

185: Life Prediction by Simulation of Crack Growth in Notched Components with Different Microstructures and under Multiaxial Fatigue

Toshihiko Hoshide, Takahisa Kusuura

Fatigue & Fracture of Engineering Materials & Structures, Vol.21, No.2, pp.201-213, 1998

A modeling procedure was developed, which is applicable to crack growth in notched components subjected to multiaxial fatigue for materials with different microstructures. An algorithm for crack growth, in a microstructures that was modeled as hexagons, was established as a competition between the crack linkage growth during the crack initiation and propagation stages and the propagation of a dominant crack as a single crack. Analytical results simulated by using the developed model were compared with experimental results from fatigue tests which had been conducted using notched specimens of pure copper, carbon steel and two kinds of titanium alloy. Cracking morphology, which was experimentally observed to depend on the microstructure and the loading mode, was well simulated using the present model. The fatigue failure life of a notched specimen was statistically estimated by a Monte Carlo procedure based on the model. The simulated life with a statistical scatter-band almost coincided with the experimental data.

186: * MHD Processes Associated with Shear Reversal : An Experimental Approach from the Ultra-Low-q Regime

N. Inoue, T. Fuzita, S. Kido, S. Kondo, J. Miyazawa, J. Morikawa, Y. Murakami, H. Nakanishi, Y. Ogawa, K. Sasaki, T. Suzuki, S. Takeji, M. Watanabe, Z. Yoshida

Fusion Energy 1997, Vol.3, pp.207-212, 1997

A tokamak configuration with shear reversal is attracting interest because it may have an advantage in improving the global confinement efficiency. A concern about this class of equilibria stems from double resonant internal kink instabilities. MHD fluctations and related non-linear processes have been studied in the ultra-low-q (safety factor $q < 1$) regime with direct measurements in the shear reversal region. The MHD relaxation stabilizes kink modes by selecting (self-organaizing) appropriate pitches. The self-organaized state displays the characteristic of a "dissipative structure" in that it is accompanied by enhanced energy dissipation; the global resistance of the plasma current is substanitially enhanced. The relaxation of the magnetic energy results in heating of plasma particles.

187: Design of Volumetric Neutron Source Based on Steady State Tokamak

Y. Ogawa, N. Inoue, Z. Yoshida, T. Yamamoto, R. Hiwatari, K. Takemura, K. Tokimatu, K. Okano, Y. Asaoka, T. Yoshi

Fusion Energy 1997, Vol.3, p.677, 1997

A volumetric neutron source for testing large scale blanket components, based on a steady state tokamak device with superconducting coils, has been designed. It is found that a neutron flux of 0.8–1.0MW/m^2 is available in a medium size device (R=4.5m, a=1.0m, κ=1.8, I_P=5.6MA) under the conditions of enhancement factor H=1.6–2.2 and β_N=2.8–3.5 with NBI power of 50–80MW. The controllability of the current profile required for high plasmas up to β_N=3 with a combination of bootstrap current and neutral beam driven current (E_b=1.0MeV) at a plasma density $<n_e>=1.0\times10^{20}$m^{-3} was demonstrated. If an advanced performance scenario such as a reversed shear configuration is available, a neutron flux of 1.4MW/m^2 is achievable. To produce a reversed shear current profile stable for MHD modes, external current drive not only in the plasma central region but also in the pitch minimum region is required. NBI power of 28MW is employed in the plasma cetral region and LHW power of 6MW in the outer region of the plasma colunm. A transport calculation estimates the accumulation of helium ash to be f_{He}=4–7% with $\tau_p^*/\tau_E = 7-10$. This low helium fraction can be explained by the short particle/energy confinement time in a small device. Since tritium consumption is ~10kg/a, the installation of a breeding blanket is indispensable. The capability for tritium breeding of Li_2O/Be and Li–Pb breeders has been evaluated and it is found that a local tritium breeding ratio of 1.4 or more is feasible for Li–Pb case.

188: * Quantitative Study of Optical Guiding by Three-Dimensional Simulation

Masaaki Sobajima, Kiyoshi Yoshikawa, Masami Ohnishi, Yasushi Yamamoto, Kai Masuda, Hisayuki Toku, Takeshi Nakamura†

† SPring-8

Nucl. Instr. & Meth., A393, pp.280-283, 1997

In order to further broaden the fields of FEL application, it is necessary to generate short wavelength FELs as well as to make the bandwidth much narrower. These call for, why self-amplified spontaneous emisson, and/or long undulators are conceived. However, such methods require the precise evalution of the optical guiding effects. For this reason, we have developed a three-dimentional numerical FEL code based on ELFIN, which can treat optical guiding effects through the Fourier transformation of the laser into a number of modes in the plane perpendicular to the beam axis. Numerical results show optical guiding effects for the parameters in the FEL experiments at Free Electron Laser Institute (FELI), and the effectiveness of the long undulator as well.

189: * Simulation of Electron Backstreaming in a Microwave Thermionic Gun

Yasushi Yamamoto, Takashi Inamasu, Kai Masuda, Masaaki Sobajima, Masami Ohnishi, Kiyoshi Yoshikawa, Hisayuki Toku, Eiji Tanabe†

† AET

Nucl. Instr. & Meth., A393, pp.443-446, 1997

Electron trajectories in a 4+1/2 RF gun were caluculated by a 2-D simulation code newly developed with full Maxwell's equations with space charge effects taken into account self-consistently to evaluate RF gun performance characteristics, in particular, the effects due to backstreaming electrons. The energy spectra, and current profile of the backstreaming electrons were calculated to show appreciable concentration to the limited area of the cathode, and also that the high energy backstreaming electrons are mainly originated in the 4th cavity of the RF gun.

190: * Spontaneous Emission Spectra from a Staggered-Array Undulator

Masami Ohnishi, Sigeki Shimada, Kouji Okada, Kai Masuda, Masaaki Sobajima, Kiyoshi Yoshikawa, Yasushi Yamamoto, Hisayuki Toku

Proceedings of the 18th International Free Electron Laser Conference, Rome, Italy, pp.II101-102, 1996

The overall performance characteristics of a staggered-array undulator were studied mainly with respect to iron and aluminum disk widths, and spontaneous emission spectra through the numerical calculations. The maximum undulator field is found to be obtained for the ratio of the aluminum disk width to the undulator period of 0.45. The large tunability of the wavelength is proved to cover 6-10 μm by changing the solenoid magnetic field from 0.4T to 1.6T.

191: * Three-Dimensional Analyses of Magnetic Fields in a Staggered-Array Undulator

Kiyoshi Yoshikawa, Sigeki Shimada, Kouji Okada, Kai Masuda, Masaaki Sobajima, Jiro Kitagaki, Masami Ohnishi, Yasushi Yamamoto, Hisayuki Toku

Workshop on Single Pass, High Gain FELs Starting from Noise, Aiming at Coherent X-Rays, Garda Lake, Italy, pp.241-246, 1997

A staggered-array undulator set inside the superconducting solenoid coils is shown to provide high undulator fields together with original longitudinal magnetic fields, a small undulator period of a few centimeters, easy tunability through the solenoid coil current, as well as compact, less expensive and easy fabrication. These performance characteristics seems very favorable for the single path X-ray FEL generation, since a great number of the undulator period is essential, in general. The previous two-dimensional analyses of electron beam trajectories have shown the necessity of the transvers stabilizing effect, which led to the three-dimensional analyses with successful stabilizing effects for the staggered-array undulator of about one meter for IR FEL. For X-ray FEL generation, electron trajectories with least deviation from the z-axis is rather mandatory for the light to grow over the undulator. Three-dimensional analyses are made to show the effect of parameters on the electron trajectories.

192: * Short Pulse Electron Beam Characteristics in an RF Gun with a Photocathode

Kai Masuda, Takashi Inamasu, Masaaki Sobajima, Jiro Kitagaki, Kiyoshi Yoshikawa, Masami Ohnishi, Yasushi Yamamoto, Hisayuki Toku

Workshop on Single Pass, High Gain FELs Starting from Noise, Aiming at Coherent X-Rays, Garda Lake, Italy, pp.307-312, 1997

Electron trajectories in a $4^1/_2$-cavity RF gun were calculated by a 2-dimensional simulation code we have developed with full Maxwell's equations with space charge effects taken into account self-consistently, to evaluate short pulse electron beam characteristics for FEL application. Especially, the beam emittance evolution was evaluated and, to reduce emittance growth in the RF gun, design of focusing magnetic field was carried out by use of the 2-D simulation code.

193: * Inertial Electrostatic Confinement Fusion Neutron Source R&D and Issues

Masami Ohnishi, Yasushi Yamamoto, Mitsunori Hasegawa, Kiyoshi Yoshikawa

Transactions of the American Nuclear Society, Winter Meeting, Albuquerque, NM, Vol.77, p.503, 1997

The potential structure and its behavior are keys to the physics in understanding the principle of an IEC device. We optically identified the local electric field in the center by measuring the intensity of HeI forbidden line due to the Stark effects relative to the allowed line. We successfully applied the method to the light from a hollow cathode lamp to identify the electric field spatial distribution inside the lamp. We discussed the application of the method to our IEC plasma to clarify the measurement of potential well.

194: * Neutron Source by Inertial Electrostatic Confinement Fusion

Masami Ohnishi

J. Plasma and Fusion Research, Vol.73, pp.1080-1086, 1997

The principle, history, and present research status of an inertial electrostatic confinement (IEC) fusion are reviewed. Since the electrostatic potential formed in an IEC device is closely related to the operational principle, the experiments and theoretical works with respect to both of the electrostatic potential and the neutron generation are described in detail. Finally, the important issues to be addressed on plasma physics as well as engineering are summarized.

195: * Study on Inertial Electrostatic Confinement Fusion as Portable Neutron Source

Masami Ohnishi, Yasushi Yamamoto, Mitsunori Hasegawa, Kiyoshi Yoshikawa, G.H.Miley†

† University of Illinois

4th Int. Symp. Fusion Nuclear Technology, Meiji Kinenkan, Tokyo, p.180, 1997

The scaling of neutron generation vs. ion current would be important in evaluating the prospect of an IEC as a neutron source. We have discussed the scaling of neutron generation vs. ion current, I based on the results of both the experiments and the numerical simulations. The experiments shows the scaling of I^2, while the numerical simulation gives the stronger scaling of I^3. The regime of current in the present experiments is limited by the capability of the available power supplies. As the current increases, the potential structure is numerically shown to be more unstable. The intermittent peaking of

the density is accompanied with the unstable potential behaviors and brings about the higher density in time averaging. It may be a reason why the numerical simulation gives a stronger scaling vs. ion current. The experiments in more higher ion current regime may be required to verify the scaling estimated by the numerical simulation.

196: * Accelerator Plasma-Targrt-Based Fusion Neutron Source

G.H.Miley†, Y.Gu†, J.Demora†, Masami Ohnishi
† University of Illinois

4th Int. Symp. Fusion Nuclear Technology, Meiji Kinenkan, Tokyo, p.131, 1997

The University of Illinois inertial electrostatic confinement (IEC) device provides 10^7 2.5-MeV D-D neutrons/second, when operated with a steady-state deuterium discharge at 70kV. Being compact and light weight, the IEC potentially represents an attractive portable neutron source for activation analysis applications. The plasma discharge in the IEC is unique, using a spherical grid also serves to extract high-energy ions. Two key features of the IEC discharge physics are discussed: 1)the formation of ion "microchannels" that carry the main ion flow through grid openings, and 2) the potential well structure formed in the dense central core.

197: * Evolution of Field-Reversed Configuration by Flux Enhancement with Rotating Magnetic Field

Masami Ohnishi, Jiro Kitagaki, Yasushi Yamamoto, Kiyoshi Yoshikawa

The 17th IEEE/NPSS Symposium of Fusion Engineering, San Diego, 1997

We have numerically studied the transient behavior of the evolution of Field Reversed Configuration (FRC) plasma with rotating magnetic field. The plasma formed by a field reversed theta pinch is evolved by increasing the internal magnetic flux with a rotating magnetic field (RMF) and by regulating the axial magnetic flux. The dynamic responses of a plasma pressure, separatrix radius and length are obtained by solving the radial force balance and the energy balance under the assumption of preservation of a current profile. We study the conditions for a successful evolution on the initial plasma parameters, time variation of the RMF angular frequency and axial magnetic field. It is shown that an FRC may be evolved to the plasma with larger internal magnetic flux by applying an RMF and controlling external axial magnetic field appropriately.

198: * Preliminary Studies of Potential Well Measurement in Inertial-Electrostatic Confinement Fusion Experiments

Yasushi Yamamoto, Mitsunori Hasegawa, Masami Ohnishi, Chikara Hoshino, Kiyoshi Yoshikawa, Nobuyuki Inoue

The 17th IEEE/NPSS Symposium of Fusion Engineering, San Diego, 1997

IECF experiments with auxiliary discharges in outer region were made. Operation pressure of IECF is successfully reduced to about 0.5 Pa when auxiliary discharges are turned on. Neutron measurement shows 2×10^6/sec fusion occurred at 45 kV, 15 mA discharge. Proof of principle experiment of the potential well measurement using Stark effect shows the method works but several improvements are required.

199: * Evolution of Field Reversed Configuration Plasma with Rotating Magnetic Field

Masami Ohnishi, Jiro Kitagaki, Yasushi Yamamoto, Kiyoshi Yoshikawa

Int. Symp. of IAE, IAE, Kyoto Univ., Uji, pp.189-192, 1997

We have numerically studied that the flux enhancement of an FRC plasma by applying the rotating magnetic field with the frequency which is time varying or constant but initially asynchronous with the electron motion. It was demonstrated that the FRC plasma can be sustained by applying the rotating magnetic field with a time-varying frequency, and controlling the axial magnetic field.

200: * The Effects of Partial Pressure and Strain Rate on Water Vapor- and Hydrogen Gas-Induced Embrittlement of Co_3Ti Alloys

Takayuki Takasugi, Akihiko Kimura, Takashi Sugimoto, Hideyuki Sitoh, Toshihei Masawa

Acta mater. Vol.45, pp.4765-4773, 1997

The effects of partial pressure and strain rate on the embrittlement owing to water vapor and hydrogen gas are observed on Co-23mol%Ti and Co-21mol%Ti alloys by small punch and tensile tests at room temperature. The Co_3Ti alloys are very susceptible to environmental embrittlement owing to water vapor and hydrogen gas. Critical partial pressures below which the embrittlement does not occur are determined for both alloy compositions, both testing atmospheres and three cross-head speeds. Also, critical strain rates beyond which the embrittlement does not occur are determined in air for both alloy

compositions. The difference in the susceptibility to the environmental embrittlement between water vapor and hydrogen gas is attributed to the difference in the decomposition rate on the alloy surface. The compositional dependence of the susceptibility to the environmental embrittlement is considered to be due to the difference in the intrinsic grain boundary cohesion between two alloy compositions, i.e. to the difference in the critical hydrogen content causing intergranular cracking.

201: * Hydrogen Property in Lattice Associated with the Embrittlement of Co_3Ti Alloy

Takayuki Takasugi, Akihiko Kimura, Takashi Sugimoto, Hideyuki Sitoh, Toshihei Masawa

Intermetallics, Vol.5, pp.443-448, 1997

Some observations relating to solubility, diffusion and trap site of hydrogen were performed on Co_3Ti alloys in association with their embrittlement. Hydrogen diffusivity at room temperature was evaluated to be low, similar to that of pure Ni. The desorption curve of hydrogen reached the maximum at 430K and the corresponding activation energy was estimated to be $48kJmol^{-1}$. The fracture energy of the hydrogen-precharged Co_3Ti alloys measured by a small punch test was dependent on the hydrogen content and the alloy stoichiometry; it decreases with increasing hydrogen content and Ti content. It is suggested that the environmental embrittlement of Co_3Ti alloy requires the hydrogen transport mode not via lattice diffusion. The difference in the environmental embrittlement between the two tested alloy compositions is primarily due to the difference in the critical hydrogen content causing grain boundary fracture.

202: * Void Swelling of Japanese Candidate Martensitic Steels under FFTF/MOTA Irradiation

Akihiko Kimura, Taro Morimura, Hideki Matsui

Reports on Fusion Materials of JUPITER Program, pp.27-33, 1997

Microstructural observations of six Japanese candidate 7-9%Cr reduced activation martensitic steels were caried out after heavy neutron irradiation in order to investigate void swelling behavior of each steel. Neutron irradiations were performed in the FFTF/MOTA up to 67 dpa at temperatures between 638 and 873K. Transmission electron microscope observation revealed that voids were formed in all the steels irradiated to 67 dpa at 703K, and the highest void swelling was observed in JLM-1 which was added with 30wt.ppm of boron (0.74%), and the minimum void swelling was observed in F82H steel (0.12%). The 9%Cr martensitic steel showed the peak of void swelling at around 700K, where the void swelling gradually increased with increasing irradiation fluence to 30 dpa and increased rapidly above it. It is considered that the incubation period of void swelling of 9%Cr martensitic steels (JLM series) is about

30 dpa. The JLM- 1 steel showed the highest void swelling rate (0.025%/dpa at most). The addition of 30wt.ppm of boron enhanced void swelling, while it was suppressed by the addition of 100 wt.ppm Ti in the 9%Cr martensitic steel.

203: * Impact Testing Using 1.5mm and 1/3 Size CVN Specimens for Fusion Reactor Structural Materials

Taro Morimura, Akihiko Kimura, Hideki Matsui, Minoru Narui

Reports on Fusion Materials of JUPITER Program, pp.34-39, 1997.

The specimen size effects on ductile-brittle transition behavior were investigated for the low activation 9%Cr-2%W martensitic steels. The ductile to brittle transition of 1.5mm CVN specimens occurs so abruptly that there is almost no regime in the ductile-brittle transition curve, which enables to determine the ductile-brittle transition temperature (DBTT) more clearly. The DBTTs obtained by 1.5mm CVN specimens were usually 100K lower than those obtained by the standard size specimens. A method to determine DBTT which involves plane stress state radius at the specimen surfaces is proposed. As for the upper shelf energy, the load and deflection calibration factors were successfully incorporated to so called volume normalization.

204: * Surface Channeling of Fast Ions

Michi-hiko Mannami†, Kenji Kimura†, Kazumasa Narumi†, Masahiro Yamamoto, Shizuo Naito

† Department of Engineering Physics and Mechanics, Kyoto University

Nucl. Instr. & Meth. B, Vol.125, pp.97-101, 1997

Fast ions incident at glancing angles on single crystal surfaces are reflected from the surface, and the ion-surface interactions take place while the ions are outside of the solids. Our studies of ion-surface interactions performed at his scattering geometry are reviewed with a particular emphasis on the resonant coherent excitation (Okorokov excitation) of surface-channel MeV B ions and the energy losses of low-velocity ions which are related to the electron density distribution outside the surface.

205: * Measurements of Young's Modulus and the Modulus of Rigidity of the Solid Solution of Hydrogen in Zirconium between 300 and 1300 K

Yuh Ashida, Masahiro Yamamoto, Shizuo Naito, Mahito Mabuchi, Tomoyasu Hashino

J. Appl. Phys., Vol.82, pp.1072-1079, 1997

Young's modulus (E) and the modulus of rigidity (G) have been measured for zirconium between 300 and 1300 K and for zirconium hydrides ZrH_x ($0<x<0.9$) at 941 and 1001 K, using an apparatus capable of making *in situ* measurements of them under an ultra-high-vacuum condition. Values of E and G have been obtained from resonance frequencies for bending and torsion vibrations of a polycrystalline zirconium wire. As the temperature increases, E and G of zirconium decrease in the α phase of an hcp structure and in the β phase of a bcc structure with an abrupt decrease at the $\alpha \rightarrow \beta$ transition temperature 1135 K. As the hydrogen concentration increases, E and G of ZrH_x decrease in the α phase and increases in the β phase.

206: Structure of the Metal-Liquid Interface: Self-Consistent Combination of the First-Principles Metal Calculation and an Integral Equation Method

Masahiro Yamamoto, Masahiro Kinoshita

Chem. Phys. Lett., Vol.274, pp.513-517, 1997

This letter contributes to development of microscopic theories for the metal/liquid interface. We report results of the first attempt to combine the first-principles calculation for the metal surface and the reference hypernetted-chain method for the liquid in a fully self-consistent manner. The dipolar liquid/Pt(111) interface is considered. The electron density, liquid structure, and electrostatic potential across the interface are briefly discussed.

207: * Auger Electron Spectroscopy and Electron Energy Loss Spectroscopy Study of the Adsorption of Nitrogen on a Polycrystalline Zirconium Surface

Mitsunori Kurahashi, Masahiro Yamamoto, Mahito Mabuchi, Shizuo Naito

J. Vac. Sci. Technol. A, Vol.15, pp.2548-2552, 1997

Auger electron spectroscopy (AES) and electron energy loss spectroscopy (EELS) were used to investigate the adsorption of nitrogen gas on a polycrystalline zirconium surface at room temperature. It was

found that the adsorption of nitrogen is saturated at an exposure of ~10 L, the thickness of the nitride formed on the specimen surface is 0.4-0.5 nm at a nitrogen exposure of 100 L, and the surface has the same large electronic density of states 4-5 eV below the Fermi energy as ZrN. The measured AES and EELS spectra are consistent with the electronic structure calculated for the Zr(0001)-(1×1)-N structure.

208: Theoretical Study of Nitrogen Adsorption on Zr(0001) Surface

Masahiro Yamamoto, Mitsunori Kurahashi, Che Ting Chan†, Kai-Ming Ho‡, Shizuo Naito

† HKUST, Hong Kong, ‡ Ames Lab.-USDOE, USA

Surf. Sci., Vol.387, pp.300-311, 1997

The chemisorption of nitrogen on the zirconium (0001) surface has been investigated by first-principles total-energy and force calculations. Our results show that nitrogen adsorption at subsurface octahedral sites is energetically more favorable than at surface sites. The calculated binding energy, surface relaxation, work function and electronic structure are in good agreement with available experimental results.

209: Geometrical Material Structure of Elastoplasticity

Gerard Maugin, M. Epstein

Int. J. Plasticity, J.F.Bell's Memorial Volume, 1998

G-structures are the geometric backbone of the theory of material uniformity in continuum mechanics. Within this geometrical framework, plasticity is seen as a result of evolving distributions of inhomogeneity with driving force provided by the material Eshelby stress tensor. Consitutive principles governing the time evolution of the G-structure underlying the finite-strain theory of elastoplasticity are proposed together with a thermodynamically admissible formulation.

210: On the Crack Mechanics of Hard Ferromagnets

A. Fomethe, Gerard Maugin

Int. J. Non-Linear Mech., Vol.33, No.1, pp.85-95, 1998

This work presents the formal evaluation of the driving force that acts on a straight-through crack in

an elastic hard ferromagnet in which both ferromagnetic exchange of forces and gyroscopic magnetic-spin inertia are taken into account phenomenologically. This is achieved following two avenues, one relating the driving force to a global material force on the material manifold by exploiting the equation of balance of pseudomomentum, and the other relying upon the construction of the energy-release rate on a pure energy basis. The path-independence of the associated J-integral holds only when both material and spin inertia are neglected. The proofs use estimates of the singularity order of various fields and are first given within the fully dynamical framework of finite strains.

211: Propagation of Phase-transition Fronts and Domain Walls in Thermoelastic Ferromagnets

A. Fomethe, Gerard Maugin

Int. J. Appl. Electromagnetics and Mechanics, Vol.8, pp.143-165, 1997

The formalism of canonical balance laws and material forces, and their associated jump relations is used to establish the thermodynamical constraint of evolution on coherent phase-transition fronts in thermoelastic ferromagnetic, electric insulators. The expression of the driving force acting on the front is found in the quasi-magnetostatic framework but accounting for both magnetic ordering and magnetic-spin inertia of gyroscopic nature. Simple criteria of progress of the front are proposed on this basis. The case of ferromagnetic domain walls is viewed as a special case. This in turn allows one to establish a relationship with the theory of irreversible macroscopic magnetization by wall movement.

212: On the Structure of the Theory of Polar Elasticity

Gerard Maugin

Phil. Trans. Royal Soc. Lond. A, Vol.355, pp.1-28, 1997

This work presents a study of the formal structure of the theory of finite strain polar elasticity and thermoelasticity with special attention to the construction of canonical balance laws that concern the whole system under study and not only each seperate degree of freedom. These are the balance of energy and so-called pseudo-momentum whose (1) local form plays an essential role in the theory of smooth material inhomogeneities, (2) global form - integrated over a material region - finds a direct application in the corresponding theory of fracture and (3) associated jump equations provide a fruitful application in the theory of the progress of coherent phase transition fronts obeying the second law of thermodynamics by relating the localized surface entropy and hot heat source to the kinetics of the front and helping one devise a criterion of progress.

213: Thermomechanics of Inhomogeneous-Heterogeneous Systems

Gerard Maugin

ARI, Vol.50, pp.41-56, 1997

A unified thermomechanical framework is presented for the theory of mechanically elastic materials of which the physical description requires the consideration of additional variables of state and of their gradients. This includes the case both of additional degrees of freedom carrying their own inertia and of diffusive internal variables of state. In view of practical applicatons to fracture and the propagation of phase-transition fronts, special attention is paid to the construction and immediate consequences of the equations of balance of canonical momentum and energy at regular material points and jump discontinuities. Numerous applications concernig thermoelastic conductors, polar crystals, liquid crystals, electro-elasticity, elastic ferromagnets, and other types of solids are briefly given.

214: Nonlinear Duality between Elastic Waves and Quasi-Particles in Microstructured Solids

Gerard Maugin, Christo Christov

Proc. Estonian Acad. Sci. Phys. Math., Vol.46, pp.78-84, 1997

The point mechanics of quasi-particles associated with solitary-wave solutions of nonexactly integrable systems is briefly discussed. This is illustrated by the case of so-called Kawahara solitions that are solutions of the generalized Boussinesq equations issued from the dynamics of microstructured crystal elasticity.

215: Momentum and Pseudomomentum of Matter

Gerard Maugin

GAMM-Mitteilungen, Heft 1, pp.37-51, 1997

Physical momentum and pseudomomentum as understood by Peierls are unequivocally defined in terms of the nonlinear kinematics of continua. The many applications of the balance of pseudonmomentum to fracture and defect mechanics, the geometrical aspect of these, the canonical Hamiltonian formulation of continuum theories, dynamical small-strain elasticity and photons, the problem of the definition of electromagnetic momentum and photons, and conservation laws in soliton theory are exhibited introduc-

ing thus a true Eshelbian mechanics on material manifolds as a complement to Newtonian mechanics in physical space. This is achieved with a conceptual unity which seems to have escaped many sharp observers of the physical scene.

216: On Shock Waves and Phase-transition Fronts in Continua

Gerard Maugin

ARI, Vol.50, 1997

The canonical formalism that considers simultaneously the second law of thermodynamics and the balance of canonical momentum is used to incorporate the case of shock waves among those singularity sets whose dissipation is in fact related to the power expanded by a driving force in an irreversible motion of the singularity set. A relationship between this and the presence of a generally non-zero quasi-inhomogeneity material force at the wave front is discussed. Extensions to electromagnetic continua of various types are given and the case of shock waves is thoroughly compared to that of phase-transition fronts in the same continua. The relationship with solitonic and moving localized dissipative structures is enunciated.

IV Department of Energy Science and Technology

(エネルギー応用科学専攻)

217: * Local Chemical Bonding around Rare Earth Ions in α- and β-Si_3N_4

T. Nakayasu*, T. Yamada*, I. Tanaka, H. Adachi and S. Goto*****
*** Ube Research Laboratory, Ube Industries, Ltd., ** Department of Materials Science and Engineering, Kyoto University, *** Faculty of Engineering, Yamaguchi University**

J. Am. Ceram. Soc., **80** (1997) 2525-2532

First-principles molecular-orbital calculations of α- and β- Si_3N_4 with a trivalent lanthanide (Ln^{3+}) ion at the interstitial site are conducted using model clusters that are composed of 41-43 atoms, neglecting lattice relaxation effects. When an interstitial Ln^{3+} ion is present, strong antibonding between the Ln^{3+} ion and Si_3N_4 is found. The magnitude of the antibonding is almost the same between the α-Si_3N_4 but not so much in β-Si_3N_4. The different electronic response to the presence of the Ln^{3+} ion for the Si-N bond is concluded to be the origin of the different solubilities of interstitial Ln^{3+} ions between α- and β-SiAlONs that are reported experimentally. The contribution of the electric field that is induced by the presence of a trivalent charge at the interstitial site is examined in detail; we have found that the Si-N bond strength is not simply determined by the electric field but rather in a more complex manner.

218: * Electronic Structure of Indium Oxide by Cluster Calculations

I.Tanaka, M.Mizuno* and H.Adachi**
*** Kobe Steel, LTD, ** Department of Materials Science and Engineering, Kyoto University**

Phys. Rev. **B56** (1997), 3536-3539

We report first-principles electronic-structure calculations of In_2O_3 using the discrete variational Xα method on model clusters. The computation has been made up to the model cluster composed of 163 atoms in order to see the size effect. The In-O bond is found to be predominant in In_2 O_3, and both O-O and In-In bonds are much weaker. Antibonding interaction between O-2p with nearly filled In-4d orbitals near the top of the valence band is noticed. Valence-band structure by XPS is well reproduced by the calculation. Unoccupied In-5sp orbitals show wide spatial distribution over the third In shell. Direct interaction between In-5sp orbitals is found to be important in the excited states. When an oxygen vacancy is present, a vacancy level appears in between the band gap. The vacancy level is composed of In-5sp orbitals hybridized with O-2p orbitals, which exhibits a strong In-In bonding interaction. The occupation of the vacancy level due to the localization of electrons to the oxygen vacancy thus results in the reinforcement of the In-In bond strength. This is suggested to be the electronic mechanism for the

stability of the oxygen vacancies in the In_2O_3crystal.

219: * Atomic and Electronic Structure of V/MgO Interface

Y. Ikuhara*, Y. Sugawara, I. Tanaka and P. Pirouz*****
*** Department of Materials Science, The University of Tokyo, ** Japan Fine Ceramics Center, *** Department of Materials Science and Engineering, Case Western Reserve University**

Interface Science, **5**, (1997) 1-12

Thin films of vanadium were deposited on the (001) surface of a MgO substrate by molecular beam epitaxy (MBE) and the V/MgO interface was investigated by cross- sectional high resolution electron microscopy (HREM) and electron energy loss spectroscopy (EELS). In order to determine the location of atoms at the interface, computer simulations were performed for four possible models, and best matching between the experimental and simulated images was obtained for the model where the V atoms are located directly on top of the Mg atoms at the using the discrete-variational (DV)-Xα method for a model cluster of the interface, i.e., ($Mg_9O_9V_5$). The V-3d band was located in between the band-gap of MgO, and nearly empty Mg-3sp orbitals were found to overlap with the V-3d band. The Mg-3sp and V-3d hybridized in a bonding manner, thereby generates strong covalent bonding between V and Mg. Nearly filled O-2p orbitals were also found to hybridize with the V-3d orbitals in an antibonding manner. The bond overlap population of the V-O bond was approximately four times smaller than that of the V-Mg bond when the bond-length was the same. The near edge structure of EELS specific to the interface was obtained using a V/MgO multilayer specimen at both Mg-K and O-K edges. Comparison between the experimental and theoretical spectra by the present MO calculation clearly found the presence of hybridized orbitals of V-3d with Mg-3p.

220: * Grain Boundary Structure and Chemical Bonding State of Superplastic SiO_2-Doped TZP

Y. Ikuhara*, I. Tanaka, P. Thavorniti* and T. Sakuma*
*** Department of Materials Science, The University of Tokyo**

J. Electron Microscopy, **46** (1997) 467-472.

Superplastic SiO_2-doped TZP (tetragonal zirconia polycrystal) was fabricated by sintering at 1300oC in air. The grain boundaries were investigated by high-resolution electron microscopy (HREM), energy dispersive X-ray spectroscopy (EDS) and electron energy loss spectroscopy (EELS). It was found that no amorphous phase was present between two adjacent grains, but an amorphous pocket was formed at multiple junctions of grain boundaries. An experimental HREM image of Σ17a grain boundary was compared

with the computer-simulated image to identify the periodic channel structure along the boundary. EDS analysis revealed that yttrium and silicon were co-segregated in the vicinity of grain boundaries. The bonding state at a grain boundary was measured by EELS to reveal that O-Kedge spectrum was shifted by 4 eV toward high energy loss side. Electron energy loss near edge structure (ELNES) of O-Kedge was investigated by a first principles molecular-orbital (MO) calculation using the discrete-variational (DV)-Xα method both for ZrO_2, Y_2O_3 and SiO_2 model clusters. Comparison between the experimental and theoretical spectra by the present MO calculation found that the bonding and theoretical spectra by the present MO calculation found that the bonding state at the grain boundaries was similar to that in SiO_2 , although no silicious glassy film was present.

221: * Analysis of core-hole effects in cation L_{23} edge ELNES of MgO, α-Al_2O_3 and SiO_2 based on DV-Xα cluster calculations

K. Ogasawara*, I. Tanaka, and H. Adachi*
*** Department of Material Science and Engineering, Kyoto University**

Advances in Quantum Chemistry **29**, (1997) 441-466.

In order to clarify the effect of a core hole in the cation $L_{2,3}$-edge of electron energy -loss near-edge structures(ELNES) and X-ray absorption near-edge structures(XANES), the photoabsorption cross section(PACS) and the partial density of stats(PDOS) are calculated for MgO, α-Al_2O_3, SiO_2 (α-quartz) based on the DV-Xα cluster calculations in the absence and presence of a core hole. It is found that the PDOS is a good approximation of the PACS and the major spectral features are well reproduced by the Slater's transition state, in which one half of a core electron is excited to an unoccupied orbital. The absolute transition energy calculated by from the XANES spectra. The strongest peak that appears near the Al $L_{2,3}$-edge is found to originate from the presence of a core hole. Such an effect is less significant in MgO and α-quartz. The electronic relaxation due to the presence of a core hole was characterized by the localization of unoccupied molecular orbitals and evaluated quantitatively by calculating the localization index of these orbitals. The difference in the magnitude of core-hole effects in these oxides were well understood by the difference in the structural and chemical environment of excited atoms such as cation-cation distances and the coordination numbers.

222: * DV-Xα Study of Electronic Spectra for MoS_4^{2-} and $[(NC)CuS_2]^{2-}$ Anions

Q. Miao*, H. Adachi, I. Tanaka and X-Q. Xin***
*** Department of Chemistry, Nanjing University, China, ** Department of Material Science and Engineering, Kyoto University**

J. Phys. Chem., **A101**, (1997) 5818-5823

We have calculated theoretical UV-vis absorption spectra for tetrahedral Mo $S_4{}^{2-}$ and $[(NC)CuS_2MoS_2]^{2-}$ anions by the use of DV-Xα cluster method. The calculated spectra for both anions are in good agreement with the experiments. The results show that the first and the second band in the spectra for both anions are principally caused by the electronic tran sition s within the MoS_4 core, relating to the HOMO $1t_1$ and LUMO_s 2e and $3t_2$. The third band is sensitively affected by the structure of MoS_4 core and its environment. In the case of simple MoS_4^{2-} anion, the third band not only shifts by the Mo-S bond length but also is expected to change the structure by its environment. The third band of $[9NC0CuS_2MoS_2]^{2-}$ is changed by the interaction among Cu 3d, Mo 4d, and S 3p orbitals. We have also tried to clarify the real structure of MoS_4^{2-} anion in the actual solution, by calculating various clusters with different Mo-S distances, and have found the cluster with the bond length of 2.22 Åprovided the best fit to the experimental spectrum.

223: * Electron microscopic characterization of doped sintered α-Al_2O_3

K. Kaneko*, T. Gemming and I. Tanaka**
*** Japan Science and Technology Corporation, ** Max-Planck-Institut für Metallforschung**

Inst. Phys. Conf. Ser.,**153** (1997) 307-310.

High-resolution transmission electron microscopy (HRTEM) and analytical electron microscopy (ARM) was employed to investigate grain boundary structures, chemical compositions and chemical bondings of Zr-doped polycrystalline α- Al_2O_3. HRTEM revealed that there was no amorphous films at any grain boundary phases as well as no triple pocket was observed. From the O-K edge ELNES, no-apparent chemical shift nor changes of the shape of EELS were observed during this experiment. However, a slight modification due to structural changes became apparent after application of spatially differential ELNES method.

224: * Calculation of Grain-Boundary Bonding in Rare-Earth-Doped β-Si_3N_4

T. Nakayasu*, T. Yamada*, I. Tanaka, H. Adachi and S. Goto*****
*** Ube Research Laboratory, Ube Industries, Ltd., ** Department of Materials Scinece and Engineering, Kyoto University, *** Faculty of Engineering, Yamaguchi University**

J. Am. Ceram. Soc.,**81** (1998) 565-570.

First-principles molecular orbital calculations are performed by the discrete variational Xα method using model clusters of rare-earth-doped β- Si_3N_4 and the interface between prismatic planes of β-Si_3N_4 and intergranular glassy films. On the basis of the total overlap population of each cluster, the rare-earth ions are implied to be stable in the grain-boundary model, while they are not stable in the bulk model.

These results are consistent with experimental observations showing significant segregation of Ln^{3+} ions at the grain boundary and no solubility of Ln^{3+} into bulk β-Si_3N_4. Grain-boundary bonding is weakened with an increase of the ionic radius of the rare-earth ions, which provides a reasonable explanation for the ionic size dependence of the crack propagation behaviors as well as the growth rate of the prismatic plane in the rare-earth-doped β-Si_3N_4 during liquid-phase sintering.

225: * Chemical Bonding at the Fe/TiX (X=C,N, or O) Interfaces

M. Mizuno*, I. Tanaka and H. Adachi**
*** Material Research Laboratory, Kobe Steel, Ltd., ** Department of Materials Science and Engineeing, Kyoto University**

Acta Mater. **46**, (1998) 1637-1645

First principles molecular orbital calculations for the Fe/TiX(X=C, N or O) interfaces have been made by the use of the spin-polarized discrete-variational Xα method. At the interfaces, no significant charge transfer occurs between the Fe and TiX layers. Ionic interaction is small and covalent bonding is predominant at the interface. The interfacial bond strength is stronger when Fe atoms are located on X-atoms, that is, the Fe-on-X geometry of the Baker- Nutting orientation relationship. The Fe/TiX bond strength decreases with the rising atomic number of X. The antibonding of the Fe-O bonds at the Fe/TiO interface is noteworthy. Although the Fe/TiO interface shows the smallest lattice mismatch among three interfaces, it is expected that the chemical bonding at the interface is weakest. The interfacial bond strength by the present calculation agrees well with the potency of TiX for intragranular ferrite nucleation in steels that was recently found experimentally.

226: * Six-fold coordinated Si at grain boundaries of sintered α-Al_2O_3

K. Kaneko*, I. Tanaka and M. Yoshiya**
*** Japan Science and Technology Corporation, ** Department of Materials Science and Engineering, Kyoto University**

Appl. Phys. Lett.,**72** (1998) 191-193

High-resolution transmission electron microscopy (HRTEM) and analytical electron microscopy (AEM) have been carried out on Si-doped sintered α- Al_2O_3. HRTEM shows that there is no amorphous phase at grain boundaries. The Si-segregated boundary is found to be much more sensitive to irradiation damage than undoped Al_2O_3 grain boundaries. AEM with energy dispersive x- ray spectroscopy (EDS) shows the significant segregation of Si at grain boundaries, and AEM with electron energy-loss spectroscopy (EELS) reveals the existence of six-fold coordinated Si at the grain boundaries. The theoretical calculation s obtained by the molecular orbital method support the data obtain by EELS.

227: Steady and Unsteady Heat Transfer from a Horizontal Wire with a Wide Range of Diameter in a Pool of Subcooled He II at Pressures

Shiotsu, M., Hata, K.*, Takeuchi, Y.*, Hama, K.* and Sakurai, A.**
***Institute of Advanced Energy, Kyoto University, ****Future Energy Research Association**

Proc. of the International Cryogenic Engineering Conference/ International Cryogenic Materials Conference, Part 1, Elsevier, pp.535-538, 1997.

This paper reviews the authors' recent works on steady and transient heat transfer from horizontal wires with diameters of 0.08, 0.2, 0.5 and 0.7 mm in a pool of subcooled He II for liquid temperatures from 1.8 to 2.1 K and system pressures from 5.465 to101.3 kPa. The followings are described: 1) Steady-state CHF values and a theoretical CHF correlation based on the Gorter-Mellink equations. 2) Lifetime of Quasi-steady state existing on the extrapolation of a steady-state Kapitza conductance curve for a stepwise heat input. 3) Correlation for the lifetime of the Kapitza conductance state which can generally predicts the lifetime for a stepwise heat input with any waveform in the early stage of heat input up to the step height.

228: Transient Heat Transfer from a Silver Sheathed High-TC Superconducting Tape in Liquid Nitrogen

Shiotsu, M., Hata, K.*, Sakurai, A., Suzawa, C.***, Isojima, S.*** and Sato, K.*****
*** Institute of Advanced Energy, Kyoto University, ** Future Energy Research Association, *** Sumitomo Electric Industries Ltd.**

Proc. of the International Cryogenic Engineering Conference/ International Cryogenic Materials Conference, Part 1, Elsevier, pp.617-620, 1997

The transient heat transfer from a silver sheathed BiPbSrCaCuO tape in liquid nitrogen was measured for the exponential heat inputs, $Q_0 e^{t/\tau}$, with the period, τ, ranging from 10 ms to 10 s. Average temperature of the sheathed tape was estimated by using the result of newly developed estimation method. The critical heat flux (CHF) increases slightly with the decrease of τ from 10 s to 1 s, decreases significantly at τ around 900 ms, slightly increases for τ down to 100 ms, and increases almost proportional to τ for further decrease of τ down to 10 ms. Direct transition from non-boiling to film boiling was observed for $\tau \leq 900$ ms. The CHF at the period of 900 ms and 10 ms are about 15 % and 40 %, respectively, of the steady-state CHF.

229: Film Boiling Heat Transfer from a Vertical Cylinder in Forced Flow of Liquids Under Saturated and Subcooled Conditions at Pressures

Shiotsu, M. and Hama, K.*
***Institute of Advanced Energy**

Proc. of Eighth International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Vol. 2, pp.679-690, 1997.

Forced convection film boiling heat transfer on a vertical 3 mm-dia. and 180 mm length platinum test cylinder located in the center of the 40 mm inner diameter test channel was measured. Saturated water, and saturated and subcooled R113 were used as the test liquids that flowed upward along the cylinder in the test channel. Flow velocities ranged from 0 to 3 m/s, pressures from 102 to 490 kPa, and liquid subcoolings for R113 from 0 to 60 K. The heat transfer coefficients for a certain pressure and liquid subcooling are almost independent of flow velocity and of a vertical position on the cylinder for the flow velocities lower than about 1 m/s (the first range), and they become higher for the velocities higher than about 1 m/s (the second range). Slight dependence on a vertical position being nearly proportional to $z^{-1/4}$, where z is the height from the leading edge of the test cylinder, exists for the flow velocities in the second range. The heat transfer coefficients at each velocity in the first and second ranges are higher for higher pressure and liquid subcooling. Correlation for the forced convection film boiling heat transfer with radiation contribution on a vertical cylinder was derived by modifying an approximate analytical solution for a two-phase laminar boundary layer model to agree better with the experimental data. velocities It was confirmed that the experimental data of film boiling heat transfer coefficients in water and R113 were described by the correlation within ±20 % difference.

230: * Photographic Study on transitions from Non-Boiling and Nucleate Boiling Regimes to Film Boiling due to Increasing Heat Inputs in Liquid Nitrogen and Water

Sakurai, A.*, Shiotsu, M., Hata, K. and Fukuda, K.*****
*** Future Energy Research Association, ** Institute of Advanced Energy, Kyoto University, *** Kobe University of Mercantile Marine**

Proc. of Eighth International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Vol. 2, pp.1038-1049, 1997

The behavior of vapor bubbles and vapor film during the transition from non-boiling regime such as natural convection or transient conduction regimes to film boiling on a 1.2 mm diameter platinum horizontal cylinder in liquid nitrogen and in water due to the exponentially increasing heat inputs from a quasi-steady state to a very rapidly increasing one was examined using a high speed video camera. The water experiments were performed for the cases without and with prepressurization before each experimental run. It was confirmed by the observation of vapor behavior that the direct transitions in liquid nitrogen and in pressurized water occur due to the explosive-like heterogeneous spontaneous

nucleation(HSN) in originally flooded cavities not only in the transient conduction regime but also in the quasi-steady increasing natural convection regime without the vapor bubbles from active cavities entraining vapor. It was also confirmed the the semi-direct transition from conduction regime to film boiling with nucleate boiling due to the rapidly increasing heat inputs in water occurs due to the HSN with nucleate boiling at around the lower limit of HSN surface superheat in water even for the non-prepressure case. The lower limit of HSN surface superheat was measured as an initial boiling surface superheat caused by a quasi-steadily increasing heat input for the case with pre-pressurization before each experimental run.

231: * Effect of Surface Conditions on Transient Critical Heat Fluxes for a Horizontal Cylinder in a Pool of Water at Pressures due to Exponentially Increasing Heat Inputs

Fukuda, K.*, Shiotsu, M. and Sakurai, A.**
*** Kobe University of Mercantile Marine, ** Future Energy Research Association**

Proc. of Eighth International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Vol. 2, pp.1050-1058, 1997.

The transient critical heat fluxes, CHFs, were measured on 1.2 mm diameter horizontal cylinders with mirror finished and Emery-3 finished rough surfaces (MS, RS) in a pool of water due to exponentially increasing heat inputs, $Q_0 e^{t/\tau}$. The exponential periods, τ, were ranged from 20 s down to 2 ms, the pressures were from atmospheric up to about 2 MPa and the subcoolings were from zero to 80 K. The obtained data were compared with the corresponding data for the cylinder with commercial surface(CS) that were already reported in other paper. The trend of CHFs for the periods was generally as follows: the CHF first increases with the decrease in period up to a certain maximum CHF, then it decreases down to a minimum CHF and again increases with the decrease in period. Namely, the CHFs for the periods are separated into the first, second and third groups for longer, shorter and intermediate periods respectively. The three groups of the CHFs for the periods tested here were clearly observed for the cylinders with MS and RS though the CHFs for the shorter periods belonging to the second group were not observed for the cylinder with CS except those for the saturation condition at around atmospheric pressure. At the CHFs belonging to the second group, the direct or semi-direct transition clearly occurs from transient conduction regime to film boiling without or with the vapor bubbles for a while with instantaneous increasing of heat flux for both cylinders of MS and RS; at the CHFs, the transitions occur due to the explosive-like heterogeneous spontaneous nucleation in originally flooded cavities as already reported for cylinder with CS. It should be noted that as a typical example the minimum CHFs for the periods of 10 ms on the MS and RS cylinders at the pressure of 1 MPa for the subcooling of 40 K were about 40 % of the corresponding steady-state CHF. It was observed that the trend of CHFs for the periods belonging to the second and third groups are significantly affected by the cylinder surface conditions.

232: Experimental Studies on Power System Stability of a Superconducting Generator with High Responce Excitation

Tanzo Nitta*, Takao Okada, Yasuyuki Shirai, Takuya Kishida***, Yoshihiro Ogawa***, HIroshi Hasegawa****, Kouzou Takagi**** and Hisakazu Matsumoto****
* The University of Tokyo, ** Kansai University, *** KEPCO, **** Toshiba Corporation**

IEEE Transaction on Power Systems, Vol.12, No.2, pp.906-912, May 1997.

Superconducting generators (SCG's) have many advantages such as small size, light weight, high efficiency, improvement of power system stability in steady states and so on. SCG's with high response excitation have additional advantage of improvement of power system stability in transient states. By use of an experimental 100 kVA SCG with high response excitation whose pet name is Hesper 1, and an artificial transmission line, we carried out several experiments for power system stability. Before the experiments, we considered a block diagram for power system stability of SCG's with high response excitation, and designed automatic voltage regulators and power system stabilizer. This paper describes the above considerations and the experimental results.

233: Experimental Studies on Field Circuit of Superconducting Generator

**Tanzo Nitta*, Yasuyuki Shirai and Takuya Kishida **
*The University of Tokyo, **Kansai Electric Power Co. Inc.**

IEEE Transaction on Applied Superconductivity, Vol.7, No.2, JUNE 1997.

Because of superconducting field winding of superconducting generators (SCG's), resistance of the field circuit is extremely low and voltage drop in the circuit is almost at brushes. Therefore, machine constants concerning with the field circuit are different from those of conventional machines. In this paper, a method for obtaining the constants is proposed. By use of the method, the constants are given experimentally. In SCG's with high response excitation, which can improve transient power system stability, characteristics of high response excitation are discussed theoretically and experimentally. The experimental result is shown.

234: * Experimental Studies on Diagnosis of Operationg Conditions of Power System by use of SMES in Power System Simulator

Yasuyuki Shirai, Tanzo Nitta*, Koji Akita and Hidetoshi Nishikaito**
***The University of Tokyo, ****Kansai Electric Power Co., Inc.**

Proceedings of Advances in Power System Control, Operation & Management (APSCOM-97), Vol.2, pp.585-590, November. 1997.

A new application of SMES (Superconducting Magnet Energy Storage) for diagnosis of power systems was proposed. SMES is used for measuring and estimating operating conditions of power systems operated. SMES can generate the continuous power disturbances of arbitrary patterns to power systems without changing power system operating conditions. The small power oscillations in the power system due to the power disturbances are observed and analyzed to estimate the power system operating conditions. The availability of the proposed method for measuring natural frequencies in multi-machine power system has been being investigated. In this paper, basic experiments for measuring natural frequencies of the 5-machine longitudinal power system by use of SMES are described. The experiments are carried out using Power System Simulator and a model SMES which was designed and made for the Simulator. A few major natural frequencies of the system are measured by the proposed method. The availability of the proposed method is discussed using experimental results.

235: Solid State Deoxidation of Niobium by Calcium and Magnesium

Shengfeng Liu, Ryosuke O. Suzuki and Katsutoshi Ono

J. Alloys and Compounds, Vol.266, (1998) pp.247-254

Deoxidation of solid niobium using metallic liquid calcium or magnesium was studied. In the temperature range of 973K to 1473K, the equilibrium oxygen concentrations under the coexistence of the reductant and its oxide were analyzed. An oxygen level of a few tens of mass ppm was found when Ca and CaO coexisted, and a level of an about 100 ppm when Mg and MgO coexisted. Ca deoxidation could be applied under an inert gas atmosphere even at temperatures about 200K lower than those applied for the Ti external gettering. The thermodynamic data reported in the binary system of Nb-O in the high oxygen concentration range or at higher temperatures could not explain the measured oxygen solubilities in Nb under the coexistence of Ca-CaO or Mg-MgO.

236: Experimental Phase Equilibria in the Sr-Ca-Cu-O System Under Reduced Oxygen Atmosphere

減圧酸素雰囲気下における Sr-Ca-Cu-O 系の実験相平衡

Ryosuke O. Suzuki, Takamichi Ogawa, Daniel Risold, Ludwig J. Gauckler and* Katsutoshi Ono

*** ETH-Zurich**

Netsu Sokutei, Vol.24 No.2 (1997) pp.61-68.

熱測定, Vol.24 No.2 (1997) pp.61-68.

Phase equilibria were studied in the Sr-Ca-Cu-O system by annealing samples at 1153K in Ar-O2 gas mixtures. The stability ranges of the oxide solid solutions were observed by X-ray diffraction measurements especially at 4 compositions in 12 gas mixtures. 4 sets of invariant 4-phase equilibrium and their oxygen partial pressure, PO2, were deduced from the surrounding 3-phase equilibria. The compositions of the related phases were evaluated by combining EDX analysis and the sample compositions. These results are compared with equilibrium calculations based on thermodynamic modelling.

237: * Seebeck Effect of Fe-Al-Si Alloy and Low Temperature Thermoelectric Properties

Fe-Al-Si 合金のゼーベック効果及び低温熱源熱電変換特性

Masahiro Shohda, Masaki Kado, Takayuki Tsuji, Ryosuke O. Suzuki and Katsutoshi Ono

Fetsu-to-Hagane, vol.84 No.2 (1997) pp.154-158

鉄と鋼 vol.84 No.2 (1997) pp.154-158

The thermoelectric conversion offers unique possibility of a gigantic electric power generation utilizing low-temperature heat sources below 600K. Such sources are solar heat, terrestrial heat and exhaust waste heat from the central-station steam-electric plant. They are thermodynamically low grade but infinite and gratis. The immense production of electricity by this principle is made possible exclusively by means of the thermoelectric junction between the iron-based alloys as the conversion materials because these components of the generator can be manufactured on an efficient mass production basis. Among several possible thermoelectric junctions basically consisted of iron, the Fe-13%Al12%Si (p) - Fe12%Al (n) alloy couple has been found to exhibit a relatively high value of thermoelectric power, 71microV/K. The merit of this thermoelectric power junction with respect to the thermoelectric conversion has also been described by measuring other thermoelectric properties of these elements. (in Japanese)

238: Production of Titanium Powder by Reduction of Titanium Chloride in Molten Salt

溶融塩中でのチタン塩化物の還元による粉末チタンの製造

Tetsushi N. Deura, Tomoya Matsunaga, Ryosuke O. Suzuki and Katsutoshi Ono

Molten Salts and High Temperature Chemistry, vol.41 No.1 (1998) pp.7-16

溶融塩および高温化学, vol.41 No.1 (1998) pp.7-16

A process for production of titanium powder directly from $TiCl_4$ by Mg-reduction in molten salt is proposed that the reactants, titanium chloride and magnesium, are diluted in molten salt for the purpose of homogeneous nucleation of titanium. The relationship between the solubility of titanium chloride in the molten salt and the morphology of produced powder was investigated experimentally. The size of powder increased as the solubility of titanium chloride in molten salt increased. The mechanisms of titanium growth in the Kroll process and in the proposed process are discussed. (in Japanese)

239: Refining of tantalum by silicon deoxidation

A.Awasthi*, N.Krishnamurthy*, Y.J.Bhatt*, R.Venkataramani*, Y.Ueda and S.P.Garg*

*** Materials Processing Division, Bhabha Atomic Research Centre, Mumbai-400 085, India**

J. Alloys and Compounds 265(1998) 190-195.

The removal of residual oxygen from tantalum by pyrovacuum treatment using silicon deoxidation (as SiO(v)) was studied. The possibility of eliminating oxygen from a Ta-Si-O solid solution by preferential evaporation of SiO(v) was indicated by calculations based on the experimental or estimated values for the activities of silicon and oxygen in the solid solution as well as for the standard free energies of formation of tantalum suboxide (TaO(v)) and silicon monoxide (SiO(v)). The experimental results obtained by treating Ta-Si-O alloys of known silicon and oxygen contents at temperatures ranging from 2073 to 2273 K under $1x10^{-3}$ Pa pressure for 2 h indicated the occurrence of silicon deoxidation. In this temperature range, oxygen removal has occurred faster and to a lower residual level in Ta-O alloys containing silicon as compared to Ta-O alloys containing no silicon. When both silicon and oxygen concentrations have reached relatively lower level, viz., 1 atby SiO(v) vapourisation decreases with an increasing contribution of sacrificial deoxidation (as TaO(v)).

240: * Chemical Potentials of Oxygen for Three-phase Assemblages of $CaSiO_2(s) + Ca_2SiO_7 + CaO + SiO_2 + FeO$ Melt and $Ca_3Si_2O_7 + Ca_2SiO_4 + CaO + SiO_2 + FeO$ Melts

K. Takeuchi, E. Enaka, N. Kon-no. Y. Hoshotani, T. Orimoto and M. Iwase

Steel research, vol.68, 1997, pp.537/579

By employing an electrochemical technique involving stabilized zirconia as solid electrolyte and Mo + MoO_2 mixture as reference electrode, the equilibrium oxygen partial pressures for three-phase assemblages of $CaSiO_3(s) + Ca_3Si_2O_7(s) + CaO + SiO_2 + Fe_xO$ melt and $Ca_3Si_2O_7(s) + Ca_2SiO_4(s) + CaO + SiO_2 + Fe_xO$ melt were determined as; $\log P_{O_2}(CS + C3S2 + L)/atm = -3.22 - 13000/(T/K) \pm 0.05$ $\log P_{O_2}(C3S2 + C2S + L)/atm = -0.92 - 16400/(T/K) \pm 0.04$, respectively, where CS, C3S2 and C2S indicates $CaSiO_3(s)$, $Ca_3Si_2O_7(s)$ and $Ca_2SiO_4(s)$, respectively.

241: Basicity of Melts for the Immobilization of High-level Radioactive Waste

高レベル放射性廃棄物固化処理用融体の塩基度

K. Kawamura, Y. Miyamoto and M. Iwase

Journal of Atomic Energfy Society Japan, vol.38, no.8, pp.621-629, 1997

日本原子力学会誌、３８巻、８号、６２１－６２９、１９９７

The key to better understanding of the physico-chemical properties of melts consisting of glass and high-level nuclear waste for immobilisation is a measure of oxide anion activities. Nevertheless thermochemical activities of single ions are, in principle, not measurable. Hence, it is obliged to evaluate oxide anion activities through measurable quantities such as CO_2 solubilities and Fe_xO activities . In this paper, based upon available literature data on metallurgical slags, an overview is given on correlation between oxide anion activities and such measurable quantifies, with a particular intention to apply for high-level waste + glass melts. For high-level waste + glass melts a knowledge of Fe_xO solubility can be a relative measure of oxide anion activity. (in Japanese)

242: Recovery of gammma-Fe_2O_3 from Waste Water Generated at Hot Mechnical Rolling

熱間圧延冷却用排水からのガンマ Fe_2O_3の回収

T. Tsukada, Y. Uchida and M. Iwase

Suiyou-Kwau-Shi, vol.22, no.9, pp.537-579, 1997

水曜会誌、22 巻,9 号、pp.573-579,1997

Waste water generated at hot mechanical rolling of steel would contani gamma Fe_2O_3. This paper describes recovery of Fe_2O_3 by a two-stage heat treatment. (in Japanese)

243: Effect of MgO and BaO on Fe^{3+}/Fe^{2+} Equilibrium in a Candidate Glass for Immobilization of High Level Nuclear Waste

S. Ohashi, T. Okumura, K. Kawamura, Y. Miyamoto and M. Iwase

High Temperature Materials and Processes, vol.16, pp.169/172, 1997

For better understanding of the behaviors of MgO and BaO within glass frit PF798, which is a candidate for use in immobilization of radio active nuclear waste and consisted of $63.6SiO_2$, 16.8 B_2O_3, $4.0Al_2O_3$, 3.0ZnO, 4.4CaO and $8.2Li_2O$ in mole pct., oxidation-reduction equilibrium experiments for Fe^{3+} / Fe^{2+} couple were conducted with the melts of PF798 + MgO and PF798 + BaO at 1473 K and under a stream of pure CO_2 of 1 atm.

244: An Automatic Equipment for Determination of the FeO Activity - Laboratory and in-plant Applications

M. Iwase

Proceedings of 5th International Conference on molten slag, fluxes and salts, pp.745/751, held at Sydney, January, 5-8, 1997, ISS/AIMEus

By employing an electrochemical technique incorporating stabilized zirconia as solid electrolyte and mixture of Mo + MoO_2 as reference electrode, an automatic facility for "on-floor" determinations of the activities of FeO in steelmaking slags has been developed. With this equipment, one datum is obtainable within 5 minutes. In this paper an over view on the application of this facility is given. In addition to laboratory application, discussions are also made on in-plant applications of this system in steelmaking processes. A particular emphasis is given to (i) slag reduction practice for minimizing reoxidation of molten steel by slag, (ii) partition of manganese and sulfur in BOF, and (iii) control of chromium levels in slags for stainless steelmaking.

245: A Thermodynamic Study of Ru-Sn Binary Alloys

Ryo Kawabata*, Munetaka Myo-chin and Masanori Iwase

Metallurgical and Materials Transaction, vol.29B, 1998, pp.561/569.

An electrochemical technique incorporating stabilized-zirconia as solid electrolyte and Mo + MoO_2 mixture as the reference electrode has been applied for the determinations of the activities of Sn in

Ru-Sn alloys. At 1573 K and XSn > 0.60, the activities of Sn were very close to the ideal behavior. Nevertheless, the heat of mixing showed relatively large negative values.

246: Oxidation-Reduction Equilibrium of Fe^{3+}/ Fe^{2+} in a Candidate Glass for Immobilization of High Level Nuclear Waste

T. Okumura , K. Kawamura , Y. Miyamoto , H. Oh-uchi and M. Iwase

Glass Technology, vol.39, 1998, pp.368/374.

Oxidation-reduction equilibrium experiments for Fe^{3+} / Fe^{2+} couple were conducted with candidate glass frit PF798 for use in immobilization of high level radio active nuclear waste. This glass consists of 63.6SiO_2, 16.8 B_2O_3, 4.0Al_2O_3, 3.0ZnO, 4.4CaO and 8.2Li_2O in mole pct. The results indicated that red-ox equilibrium in this particular glass would be expressed by Fe^{2+} + (1/4)O_2 + (3/2) O^{2-} = FeO^{2-} rather than Fe^{2+} + (1/4)O_2 = Fe^{3+} + O^{2-} The results could be summarized in a formula log $(Fe^{3+})/(Fe^{2+})$ $P_{O_2}^{1/4}$ = -(1.90 ± 0.30) + (4500 ± 430) / (T/K) , being independent of the concentrations of total Fe between 1 to 4 pct by weight.

247: * Thermodynamics of Iron Oxide in Fe_xO-Dilute CaO + Al_2O_3 + Fe_xO Fluxes at 1873 K

Hiroyasu FUJIWARA, Masahiro KITOU, Takayuki MATSUI and Eiji ICHISE

Metallur. Materials Trans. B, vol.28B, (1997), No.4, pp.243-250

The distribution of iron between Fe_xO-dilute CaO + Al_2O_3 + Fe_xO fluxes and Pt + Fe alloys, as well as the redox equilibrium of iron ions in these fluxes were experimentally investigated in pressure-controlled CO_2/CO gas at 1873 K. Total iron content in flux, $(\%Fe^T)$, and the ratio of $(\%Fe^{2+})$ to $(\%Fe^T)$ in fluxes with constant $X_{CaO}/X_{Al_2O_3}$ can be related to the activity of iron, a_{Fe}, and the partial pressure of oxygen, p_{O_2} , using the equation:

$$(\%Fe^T) = \left((C_{Fe^{2+}})\, p_{O_2}^{1/2} + (C_{Fe^{3+}})\, p_{O_2}^{3/4} \right) a_{Fe}$$

$$\frac{(\%Fe^{2+})}{(\%Fe^T)} = \frac{1}{1 + (C_{Fe^{2+}}/C_{Fe^{3+}}) p_{O_2}^{1/4}}$$

where $C_{Fe^{2+}}$ and $C_{Fe^{2+}}$ are the ferrous and ferric ion capacities, respectively, defined as:

$$C_{Fe^{2+}} = \frac{(\%Fe^{2+})}{a_{Fe}} p_{O_2}^{-1/2}, C_{Fe^{3+}} = \frac{(\%Fe^{3+})}{a_{Fe}} p_{O_2}^{-3/4}$$

The present paper applies these parameters to the evaluation of the activity coefficient of Fe_xO at infinite dilution, $\gamma^{\circ}_{Fe_xO}$, relative to the liquid iron oxide in equilibrium with iron. Furthermore, the composition dependence of $\gamma^{\circ}_{Fe_xO}$ is discussed.

248: Correlation between Microfracture Type and Splitting Planes of Inada Granite and Kurihashi Granodiorite

微小クラックの分類による稲田花崗岩と栗橋花崗閃緑岩の力学的弱面について

Youqing Chen, Takashi Nishiyama, Haruyuki Kita* and Toshinori Sato**
*** Technical Research Institute, Mitsui Construction Co.,LTD, ** Tono Geoscience Center, Power Reactor and Nuclear Fuel Development Corporation**

Jour. Japan Soc. Eng. Geol., Vol. 38, No.4, pp.196-204, 1997

応用地質、第３８巻、第４号、196頁－204頁、1997

Microcrack distribution patterns on the microscopic scale and splitting planes in Inada granite and Kurihashi granodiorite were examined using a fluorescent technique and image analysis. Using the fluorescent technique , microcracks which could not be detected under natural light were visualized under ultraviolet light. Characteristics of the microcracks such as orientation and total length per unit area were measured by image analysis. Microcracks observed in the specimens were divided into three groups, intracrystalline cracks, intercrystalline cracks and grain boundary cracks . Inada granite was characterized by three weak planes intersecting perpendicularly with each other, the rift plane, grain plane and hardway plane in the order of brittleness, while Kurihashi granodiorite showed no distinctive weak plane. In the Inada granite, the rift plane was dominated by the predominant orientation of intercrystalline cracks the total length of which was relatively short, and the grain plane was coincident with the orientation of intracrystalline cracks. The grain boundary cracks showed no leading orientation. The numbers of intercrystalline cracks due to the rift plane in Kurihashi granodiorite were very small. However, Kurihashi granodiorite is estimated to contain the second rank of hidden splitting plane, because a predominent orientation of intracrystalline cracks and grain boundary cracks was found.

249: The current problems of shredder dust drived from automobiles and home electric appliances. —New system considered for dealing with shredder dust in the western-part of Japan—

シュレッダーダスト処理の現状と課題

Takashi Nishiyama and Takeshi Yamanaka*
*** Kinki Branch of Chubu Mine Safetyand Inspection Department**

Journal of the Mining and Meterials Processing Instisute of Japan, Vol.113, pp.1022-1026, 1997

資源と素材、第113巻、1022頁－1026頁、1997

It has more recently created to deal with a large amount of shredder dust generated with abandoned automobiles and home electric appliances, because of dealing landfill space nationwide and stringent regulations on leachate control. In 1992, about 1.2 million tons of the shredders containing an estimated 36 thousand tons of copper, 3.6 thousand tons of lead, 6 thousand tons of zinc and 5400Gcal, were drived from automobiles. The shredders from home eletric appliance disposal accounted for 230 thousand tons containing 22 thousand tons of copper. The tonnage of shredder dust is estimated to increase to 1.37 million tons in 2000, and to 1.56 million tons in 2005. The new project, Recycle Mine Park (RMP) is

considered to solve the problems of increasing automobile and home electric appliance scrap. RMP is processed using technology to energy and metals. Since technology to recover energy and various kinds of metals included in base metals and hazardous metals has successed in metallurgical field, the biggest problems of the project remains at establishment of reasonable, economical system. In the nothernpart of Japan, about 305 of the shredder dust mentoined above were generated. Smelters established highly skilled technique are located on the coast of the Inland Sea of Seto in the area, which support low cost of transportion. The recycing network in the westernpart of Japan excluding pretreatment is a plan which conbines the best features of a large amount of shredder dust, marine transportion and modern smelter. Pretreatment such as incineration and crack which is additional treatment for the smelter feed is proved in small scale. We hope that the unique recycing system of shredder dust composed of collection, pretreatment, marine transportation and smelter put in operation as soon as possible. The increasing cost of suitable land for landfills, the stringent regulations on leachate control, and other costs make tke system more attractive.

250: A Price Formation of Metals and Its Application for Copper

金属資源の価格形成メカニズムとその銅価格への適用

Takayoshi Shinkuma*, Hideki Fujii and Takashi Nishiyama
*** Graduate School of Human and Environmental Studies, Kyoto University**

Journal of the Mining and Material Processing Instisute of Japan, Vol.113, pp.805-810, 1997
資源と素材、第113巻、pp.805-820、1997

The instability in metal price is a very serious problem in the metal industry. There are many factors such as depletion of mineral deposits and exogenous shocks represented by wars and worldwide business fluctuations determining the phases of price increases or decreases. Resource economists have mainly focused on theoretical models which often ignore unexpected shocks on demand, while mining engineers have regarded exogenous shocks as an important factor to explain metal prices. In this study, a combined model is proposed. This model was examined by using the actual trends in copper prices between 1945 and 1993. This model predicts that the price of copper will fall in the near future.

251: * Fracture Prediction in Stretch Forming Using Finite Element Simulation Combined with Ductile Fracture Criterion

H. Takuda, K. Mori*, H. Fujimoto and N. Hatta
*** Osaka University**

Archive of Applied Mechanics, Vol.67, pp.143-150, 1997

A criterion for ductile fracture is introduced in the finite element simulation of sheet metal forming. From the calculated histories of stress and strain in each element, the fracture initiation site and the

critical stroke are predicted by means of the ductile fracture criterion. The calculations are carried out for axisymmetric stretch forming of various aluminium alloy sheets and their laminates clad by mild steel sheets. The predictions so obtained are compared with experimental observations. The results show that the combination of the finite element simulation and the ductile fracture criterion enables the prediction of forming limit in a wide range of sheet metals.

252: * Predictable Modelling of Heat Transfer Coefficient between Spraying Water and a Hot Surface above the Leidenfrost Temperature

Hitoshi Fujimoto, Natsuo Hatta, Hiroyoshi Asakawa* and Toshie Hashimoto*
*** Kyoritu Gokin**

ISIJ International, Vol.37, No.5, pp.492-497, 1997

In order to evaluate the cooling intensity of water spray impacting on a hot metallic surface above the Leidenfrost temperature, the formulation of heat transfer coefficient in the forced convection boiling region has been made as a function of the droplet size, the impinging velocity and the number density of droplets whose parameters are independent of each other. So far, many works on the mist/spray cooling process have been made, in particular, from an experimental point of view. However, the general procedure capable of evaluating heat transfer rate between a hot metallic surface and water spray has not been established yet, because there are a large number of parameters affecting the spray cooling process. Then, we have experimentally derived a new formula consisting of the above three parameters to be dominant for heat transfer rate in the spray of 293 K and the time history of the surface temperature has been measured. We have selected some kinds of full cone nozzles whose characteristics such as the average droplet diameter, the velocity and the distribution of water flux have been different from each other, and performed the cooling tests using them. Finally, the formula capable of giving best-fit to the experimental results has been proposed. The effect of the spraying characteristics on the heat transfer rate has been discussed from an experimental point of view.

253: * Prediction of Forming Limit in Bore-Expanding of Sheet Metals Using Ductile Fracture Criterion

H. Takuda, K. Mori*, H. Fujimoto and N. Hatta
*** Osaka University**

Proc. of the International Conference Advances in Materials and Processing Technologies – AMPT'97, pp.809-814, 1997

To predict the forming limit in sheet metal forming, a criterion for ductile fracture is introduced into the finite element simulation. From the histories of stress and strain in each element calculated by the finite element simulation, the fracture initiation is predicted by means of the fracture criterion. Calculations

are carried out for axisymmetric bore-expanding processes of mild steel and high strength steel sheets using flat-, hemispherical- and conical-headed punches. The comparison with experimental results show that the fracture initiation site and the critical stroke are successfully predicted by the present approach.

254: * Finite Element Analysis of Formability of a Few Kinds of Special Steel Sheets

Hirohiko Takuda, Hitoshi Fujimoto, Yoshito Kudoda, Natsuo Hatta

Steel research, Vol.68, No.9, pp.398-402, 1997

Formability of various special steel sheets in deep drawing processes is analyzed by the combination of the finite element simulation and the ductile fracture criterion. The comparison with the experimental results shows that the forming limits for various sheets are successfully obtained by the present approach, even in no appearance of localized necking. The results suggest that the application of the ductile fracture criterion allows the prediction of forming limit in a wide range of sheet steel forming processes.

255: * Experimental Study of Deformation Mechanism of a Water Droplet Impinging on Metallic Surface

Natsuo Hatta, Hitoshi Fujimoto, Kenji Kinoshita, Hirohiko Takuda

Trans. of the ASME, Journal of Fluids Engineering, Vol.119, pp.692-699, 1997

This paper is concerned with the collision dynamics of a water droplet impinging on three kinds of smooth surfaces (Inconel alloy 625, stainless-steel, and silicon) heated to avobe the Leidenfrost temperature (773 K). It has been found that the time histories of the droplet diameter, the height and the distance between the bottom of droplet and the hot surface after rebounding are almost unchangeable regardless of the kind of surface material, when the Weber number is kept so low that the droplet does not break up into some parts. However, the critical Weber number, whether or not the droplet is disintegrated into some pieces during deformation, has been confirmed to be changeable depending upon the kind of surface material. For relatively low Weber number cases, but above the critical one, the droplet breaks up into some parts after the droplet reaches a maximum diameter on the surface. As the Weber number is increased further, the droplet disintegration occurs during the spreading process. Also, the droplet disintegration mechanism has been discussed from an experimental point of view.

256: * Collision Behavior of a Water Droplet with a Hot Surface

Hitoshi Fujimoto, Natsuo Hatta, Hirohiko Takuda

Proc. of the ASME Fluids Engineering Division FED Vol.244, pp.167-172, 1997

This paper treats the deformation process of a water droplet impinging on a hot surface above the Leidenfrost temperature. Emphasis is placed on the effects of the kind of surface material and the surface temperature on the deformation process. The surface materials used are stainless-steel and silicon. The surface temperature is fixed at 673 K and at 773 K. It has been found that the time histories of droplet diameter as well as height on two kinds of surfaces are very similar in low Weber numbers such that the droplet rebounds from the surface without disintegration. However, the critical Weber number whether or not the droplet breaks up into some pieces on the surface during deformation has been confirmed to be changeable depending upon the kind of surface material. Furthermore, it has been confirmed that the effect of surface temperature on the droplet deformation process is remarkable in the later deformation period for the case of the low Weber number.

257: * Collision Dynamics of Two Droplets

Hitoshi Fujimoto, Natsuo Hatta, Hirohiko Takuda

Proc. of the ASME Fluids Engineering Division FED Vol.244, pp.173-178, 1997

This paper treats the numerical analysis of the deformation behavior of liquid after head-on collision of two droplets. The simulation process has been performed using MAC-type solusion method to solve a finite differencing approximation of the Navier-Stokes equations governing an axisymmetric incompressible fluid flow. When a water droplet collides head-on into another one with small initial Weber numbers, two droplets coalesce and remain permanently united. For larger Weber numbers, two droplets merge temporarily and subsequently separate into two or more drops. The calculated free surface configurations have been in qualitative agreement with the experimental results observed by other researchers. Also, the critical Weber number to predict coalescence/separation of liquid after head-on collision has agreed with the experimental data. The details of droplet deformation mechanism have been discussed from a qualitative as well as quantitative point of view.

258: * Formabilities of Steel/Aluminium Alloy Laminated Composite Sheets

H. Takuda, H. Fujimoto, N. Hatta

Journal of Materials Science, Vol.33, No.1, pp.91-97, 1998

The tensile properties and press formabilities of laminates experimentally produced from mild steel and various aluminium alloy sheets are examined. The tensile properties of the laminates are approximately predictable by the mixture rule of the properties of the individual sheets. The forming limits in deep drawing, as well as stretch forming due to various types of fractures of the laminated composite sheets, cannot be predicted without considering the stress and strain histories of the individual sheets during forming. Furthermore, it is found that the drawability, as well as the stretch formability, is improved by setting the mild steel sheet on the punch side for the case of aluminium alloy sheet with comparatively high ductility, and by sandwiching the aluminium alloy sheet with the mild steel sheets for the case of low ductility.

259: * Finite Element Analysis of Bore-expanding Processes with Ductile Fracture Criterion

延性破壊条件を考慮した穴拡げ加工の有限要素解析

Hirohiko Takuda, Ken-ichiro Mori*, Masashi Kaneshiro and Natsuo Hatta
*** Osaka University**

Tetsu to Hagane, Vol.84, No.3, pp.182-187, 1998

鉄と鋼, Vol.84, No.3, pp.182-187, 1998

A criterion for ductile fracture is applied to the prediction of forming limit in bore-expanding processes of sheet steels. Axisymmetric bore-expanding tests of mild steel and high strength steel sheets using conical-, hemispherical- and flat-headed punches are simulated by the rigid-plastic finite element method. From the calculated distributions and histories of stress and strain in the sheets, the fracture initiation sites and the critical strokes are predicted by means of the ductile fracture criterion. The comparison with the experimental results show that the forming limits due to various types of fracture initiations in the bore-expanding processes are successfully predicted by the present approach. (in Japanese)

260: * Numerical Analysis of Formability of a Commercially Pure Zirconium Sheet in Some Sheet Forming Processes

H. Takuda, N. Hatta

Materials Science and Engineering A, Vol.242, pp.15-21, 1998

To examine the fundamental sheet formability of zirconium, deep drawing, Erichsen and bore-expanding tests are carried out for a commercially pure zirconium sheet. These sheet forming proceses are further simulated by the rigid-plastic finite element method, and the forming limits are numerically predicted by means of a criterion for ductile fracture. The material constants in the ductile fracture criterion are determined from uniaxial and plane-strain tension tests. The results show that the drawability of the zirconium sheet is quite high, while the stretchability is low. The forming limits in deep drawing and bore-expanding processes greatly dependent on the punch profile radius and remarkably decrease with the radius. Furthermore, it is found that the fracture initiation sites and the forming limits of the zirconium sheet can be predicted fairly well by the combination of the finite element simulation and the ductile fracture criterion.

261: * Theoretical Analysis of Flow Characteristics of Multiphase Mixtures in a Vertical Pipe

揚鉱管内を上昇する混相流体の流動特性の理論的解析

Natsuo Hatta, Makoto Isobe, Hitoshi Fujimoto

Journal of the Mining and Materials Processing Institute of Japan, Vol.113, No.11, pp.833-841, 1997
資源と素材, Vol.113, No.11, pp.833-841, 1997

The purpose of the present investigation is to theoretically analyze the flow characteristics of the air-lift pump for the case where a transitional process from the solid-liquid two-phase mixture flow to the solid-gas-liquid three-phase mixture flow by injecting gas-phase into the upriser through a gas-injector is present. The system of equations governing the liquid-solid two-phase mixture flow consists of two mass conservation equations, two momentum conservation equations and an equation for two-phase volume fractions. Again, the gas-liquid-solid three-phase flow field after the position of gas injection is solved by three mass conservation equations, three momentum equations, a gas equation of state and an equation for the individual phase volume fractions. The transtions of the flow pattern of gas phase from the bubbly flow to the slug flow and from the slug flow to the churn flow are taken into account in the system of governing equations of three-phase flow. In order to verify the validity of the system of governing equations accounting for the transtion of the flow patterns, the flow characteristics calculated on the basis of the present theoretical model have been compared with experimental data by several other investigators. As a result, we have found that the present theoretical model built up in this study gives good fit to the experimental data obtained by several investigators. (in Japanese)

262: * Theoretical Modelling of Gas-Liquid Two-Phase Flow in a Vertical and Straight Pipe

Natsuo Hatta, Masaaki Omodaka, Hitoshi Fujimoto

Steel Research, Vol.69, No.3, pp.92-101, 1998

This paper treats the theoretical analysis to obtain the flow characteristics of gas-liquid two-phase mixtures in a vertical and straight pipe. The system of equations governing the gas-liquid two-phase flow field is based upon the multifluid model. The transitions of the gas flow pattern from bubbly to slug flows as well as from slag to churn flows are introduced into the system of the above governing equations. In order to confirm the validity of the present theoretical model, the flow characteristics calculated on the basis of this model have been compared with experimental data measured by changing the pipe diameter and the submergence ratio. As a result, it has been found that the present theoretical model built up in this investigation gives good fit to the measured data. We believe that the simplicity of this pump can make it possible to transport molten iron/steel between different refining processes. But, we also note that the experiments have been performed on a cold model using an air-water system.

263: * Effect of hydrolysed aluminum(III) and chromium(III) cations on the lipophilicity of talc

E. Kusaka, N. Amano* and Y. Nakahiro
*** Hitachi Zosen Co.**

International Journal of Mineral Processing, Vol. 50, No. 4, pp. 243-253, 1997.

Liquid-liquid extraction and electrokinetic studies show that both the talc particle and the isooctane droplets are affected by the presence of hydrolysable metal species of Al(III) and Cr(III). The inherent lipophilicity of talc is unchanged by the hydroxo complexes of these metal species, while positive shifts in zeta potentials of talc and isooctane take place due partly to the strong adsorption of these hydroxo complexes. In the pH range where the hydroxide precipitates, the talc particles are rendered hydrophilic between the precipitation pH and the point-of-zero charge of the metal hydroxide. This hydrophile-lipophile transition of talc in the isooctane-water system relates to heterocoagulation among talc particles, isooctane droplets and hydroxide precipitates.

264: Nuclear Spin-Lattice Relaxation in Quantum Spin Gap of 1-D s = 1 and s = 1/2 Antiferromagnets

M. Chiba, T. Kubo*, M. Hagiwara, Y. Ajiro***, T. Asano**** and T. Fukui***

*** Nara University of Education, ** The Institute of Physical and Chemical Research (RIKEN), *** Department of Physics, Kyushu University, **** Department of Applied Physics, Fukui University**

Journal of Magn. & Magn. Mater. 177-181, (1998) pp.630-631

In order to clarify the nature of the spin-gap in 1-D AF chains we have made a systematic NMR experiment on NENP $[Ni(C_2H_8N_2)_2NO_2\ (ClO_4)]$ (one of the typical s = 1 linear chain presenting the Haldane effect), $CuCl_2$ (γ-picoline)$_2$ (s = 1/2 linear chain with bond alternation) and Cu_2Cl_4 (1,4-diazacycloheptane)$_2$ (s = 1/2 zigzag chain with non-negligible second neighbor coupling). For these materials we have confirmed the existence of the spin-gap from the characteristic temperature dependence of the nuclear spin-lattice relaxation. The derived spin-gaps are consistent with those from the susceptibility and high field magnetization measurements. The field dependence of the relaxation rate, including the critical field where the spin-gap closes, is compared and discussed.

265: NMR Study ^{133}Cs in a Singlet-Ground-State System $CsFeCl_3$

M. Toda*, T. Goto*, M. Chiba and K. Adachi**

*** Graduate School of Human and Environmental Studies, Kyoto University, ** Kobe Tokiwa Junior College**

Journal of Magn. & Magn. Mater. 177-181, (1998) pp.825-826

To study spin dynamics and magnetic structure in singlet ground state system $CsFeCl_3$, we have measured the temperature dependence of nuclear spin lattice relaxation time T_1 and NMR spectrum of ^{133}Cs nuclear spin. From the experimental results of T_1^{-1} , we conclude that the softening of energy gap occurs under the magnetic field within the range of the present measurement. The experimental results of NMR spectrum left a problem in the ordered state.

266: ^{79,81}Br NMR in Triangular Lattice Antiferromagnet $CsCoBr_3$

M. Uyeda*, T. Kubo*, M. Chiba, Y. Ajiro and T. Asano*****
*** Nara University of Education, ** Department of Physics, Kyushu University, *** Department of Applied Physics, Fukui University**

Journal of Magn. & Magn. Mater. 177-181, (1998) pp.833-834

The Br NMR in a triangular lattice antiferromagnet $CsCoBr_3$ has been measured to clarify the magnetic structure of the Co^{2+} spins below T_{N3}. The three-sublattice structure for Co^{2+} spins has been deduced from the angular dependence of Br NMR frequencies.

267: * Present status of the NIJI-IV storage-ring free-electron lasers

T. Yamazaki, K. Yamada*, N.Sei*, H.Ohgaki*, S.Sugiyama*, R.Suzuki*, T.Mikado*, T.Noguchi*, M.Chiwaki*, T.Ohdaira*, M.Kawai, and M.Yokoyama****
*** Electrotechnical Laboratory, ** Kawasaki Heavy Industries Ltd.**

Nucl. Instr. & Meth., A393 (1997) pp.II-7-II-9.

NIJI-IV is the first storage ring in the world dedicated to free-electron lasers (FELs).The tunable range of the NIJI-IV FEL system is now 348-595 nm with a 6.3-m optical klystron (ETLOK-II). The net gain at around 300 nm is quite close to the threshold.Recently, measurements of the macro- and micro-temporal structures and the FEL power have been carried out at 488 nm. A preparatory experiment on the generation of high-brightness x-ray beam from the FEL-Compton backscattering, a simple active feedback system which proved to suppress the coupled-bunch instability of the stored electron beam, preparation of a compact sextupole-quadrupole-sextupole composite in order to suppress the head-tail instability, research on the degradation of optical cavity mirrors, design work of a new cavity-dump method are under way.

268: * Saturation of cavity-mirror degradation in the UV FEL

K. Yamada*, T. Yamazaki, N. Sei*, R. Suzuki*, T. Ohdaira*, T. Shimizu*, M. Kawai, M. Yokoyama**, T. Mikado*, T. Noguchi*, S. Sugiyama*, and H. Ohgaki***
*** Electrotechnical Laboratory, ** Kawasaki Heavy Industries Ltd.**

Nucl. Instr. & Meth., A393 (1997) pp.44-49.

Behavior of surface and volume degradation in dielectric multilayer mirrors, manufactured with ion beam sputtering (IBS) and electron beam evaporation (EBE), was investigated in the ultraviolet (UV)

wavelength range. It was found in the IBS mirrors that the saturation in volume degradation enabled us to use the mirrors for a long period, because the surface degradation, causing only the narrowing of the mirror bandwidth, proved not to contribute seriously to the mirror loss as far as the mirrors are used at their optimized wavelength. This will reduce the cavity-mirror degradation problem in relatively high-gain free electron laser (FEL) system by carefully selecting the laser wavelength, although the wavelength tunability in FEL is limited to a certain extent. In the EBE mirrors, only the surface-type degradation was found and the evolution of the mirror degradation was quite different from that in IBS mirrors.

269: Beam Qualify in Storage Ring NIJI-IV

N.Sei*, H.Ohgaki*, K. Yamada*, and T. Yamazaki
*** Electrotechnical Laboratory**

Nucl. Instr. & Meth., A393 (1997) pp. 38-43

Several cures to achieve a high peak current with storage ring NIJI-IV are presented. We observe a bunch lengthening and a limitation on the single bunch current. To suppress with the coupled-bunch instability, we install a longitudinal feedback system which consists of the phase detector and phase shifter. This feedback system effectively suppresses the coupled-bunch instability and shortens the electron bunch. However, we need a cures to the limitation on the single bunch current originated from a head-tail instability. Quadrupole and 6-pole magnets have been designed to be installed in a restricted space between bending magnets. Calculations on the injection orbit and dynamical aperture show that there should be a large aperture in the ring with the small bore, 45 mm. The installation of these small bore magnets will be started on coming Autumn.

270: Design of an optical cavity in the NIJI-IV for high output power

N.Sei*, T. Yamazaki, K. Yamada*, T. Mikado*, and H. Ohgaki*
*** Electrotechnical Laboratory**

Nucl. Instr. & Meth., A393 (1997) pp.59-62

We are planning a new optical cavity system which efficiently takes out intense intracavity power of a storage ring free electron laser (SRFEL) in the visible and the ultra violet (UV) regions. If a cavity mirror is started rotating at the peak of a SRFEL macro-pulse to rapidly lead a SRFEL micro-pulse to the high transmission area, we will be able to dump a part of the intracavity power sufficiently. A high-speed piezotranslator and a special mirror holder will realize this system, what is called cavity dump. The piezotranslator would make the optical cavity mirror rotate with the angular velocity of radian per one round-trip. In the case of NIJI-IV FELs, the output power of the micro-pulse would be estimated at about 7600 times around 488 nm and about 2700 times around 352 nm as strong as that in the normal

operation.

271: FEL-X Project, High brightness x rays from FEL-Compton backscattering

H.Ohgaki*, K. Yamada*, N.Sei*, T. Yamazaki, T. Noguchi*, T. Mikado*, and S. Sugiyama*

*** Electrotechnical Laboratory**

Nucl. Instr. & Meth., A393 (1997) pp.II-14-II-15

Long-wavelength FEL-based Compton backscattering X rays, FEL-X, is planned at Electrotechnical Laboratory. We expect photon yield of 107 photons/s which is as high as 103 times the present Laser-Compton backscattering facility with an intra-cavity power of only few watts, because SR-FEL has best overlap-factor to the electron beam. Photon yield from FEL-X can be comparable to or exceed that from 8 GeV ring, especially in high energy region with modest FEL power. A planar type undulator to generate a 13.8 mm FEL operating in the electron energy of 275 MeV is designed. The expected backscattered X rays have energy range of 100-800 keV by changing the gap of the undulator. Photon yield from FEL Compton backscattering has been measured in a preparatory experiment. The FEL (488 nm) photons and electron beam of 263 MeV was collided in the long straight section of the storage ring NIJI-IV. We got 2.5x105 photon/s with very small electron current of 2 mA, and this photon yield shows good agreement with an estimation with a simple scaling law.

272: FEL in quasi-isochronous storage ring STERAS

H. Ohgaki, T. Yamazaki, K. Yamada, N. Sei, H.Ohgaki*, T. Yamazaki, K. Yamada*, N.Sei*, and D. Robin**

*** Electrotechnical Laboratory, ** Lawrence Berkeley Laboratory**

Nucl. Instr. & Meth., A393 (1997) pp. II-5-II-6

Design of a Quasi-Isochronous storage ring (STERAS), that has inverted dipole to control the momentum compaction factor for the future plan of Electrotechnical Laboratory, has been improved to have large dynamical aperture. Both planar undulator with 1.5 GeV electron beam and optical klystron type undulator with 0.3 GeV electron beam are designed. Designed OK with 0.3 GeV beam condition would be better for the short wavelength FEL. However, to examine the isochronous condition, we need less than 10^{-6} of momentum compaction factor for ~200 nm FEL. FEL with long wavelength (~2mm) is suitable for the first study of the isochronous condition with 1.5 GeV electron beam. We calculate the FEL power with STERAS with the designed planar undulator. An average power of 275 mW and peak power of over 200 kW is obtained with 1 mA current of 1.5 GeV at the FEL wavelength is 200 nm. If the isochronism condition is satisfied in the FEL operation, we can obtain several hundreds kW output power in an average.

273: * Present Status of the Polarized-Photon Generation System with the Laser Compton Backscattering of the ETL Storage Ring TERAS

H. Toyokawa*, H. Ohgaki*, K. Kudo*, N. Takeda*, T. Yamazaki, T. Mikado*, S. Sugiyama*, K. Yamada*, R. Suzuki*, T. Ohdaira*, and N. Sei*

*** Electrotechnical Laboratory**

Proc. 11th Symp. on Acc. Sci. and Tech., (1997) pp.110-112

A system for generating high-energy polarized photon by exploiting the inverse laser-Compton scattering has been developed on the storage ring TERAS at the Electrotechnical Laboratory. The system is now practically used for various experiments and many interesting findings have been achieved. The system and an overview of the research activities are described in the paper.

274: Present status of the ETL Electron Accelerator Facility

電総研リニアック施設の現状

T.Mikado*, T.Yamazaki, S.Sugiyama*, K.Yamada*, H.Ohgaki*, R.Suzuki*, T.Ohdaira*, N.Sei*, H.Toyokawa*, M.Chiwaki*, and S.Okabe**

*** Electrotechnical Laboratory, ** Okabe Keisoku Kougyousho Ltd.**

Proc. 22nd Linear Acc. Meeting in Japan (1997) pp.19-21

The status of the use of electron linear accelerator TELL in these few years is described. The major research projects are also reviewed. (in Japanese)

275: Production and Application of Pulsed Slow-Positron Beam Using an Electron Linac

T. Yamazaki, R. Suzuki*, T. Ohdaira*, T. Mikado*, and Y. Kobayashi**

*** Electrotechnical Laboratory, ** National Institute of Materials and Chemical Research**

Rad. Phys. and Chem., 49 (1997) pp.651-659

Slow-positron beam is quite useful for non-destructive material research. At the Electrotechnical Laboratory (ETL), an intense slow positron beam line by exploiting an electron linac has been constructed in order to carry out various experiments on material analysis. The beam line can generate pulsed positron beams of variable energy and variable pulse period. Various capability of the intense pulsed positron beam is presented, based on the experience at the ETL, and the prospect for the future is discussed.

276: Production and Application of Pulsed Slow-Positron Beam Using an Electron Linac

T. Yamazaki, R. Suzuki*, T. Ohdaira*, T. Mikado*, and Y. Kobayashi**
*** Electrotechnical Laboratory, ** National Institute of Materials and Chemical Research**

JAERI-Conf 97-003, Recent Progress in Accelerator Beam Application (1997) pp.143-148

Slow-positron beam is quite useful for non-destructive material research. At the Electrotechnical Laboratory (ETL), an intense slow positron beam line by exploiting an electron linac has been constructed in order to carry out various experiments on material analysis. The beam line can generate pulsed positron beams of variable energy and variable pulse period. Various capability of the intense pulsed positron beam is presented, based on the experience at the ETL, and the prospect for the future is discussed.

277: An apparatus for high-resolution positron-annihilation induced Auger electron spectroscopy using a time-of-flight technique

T.Ohdaira*, R.Suzuki*, T.Mikado*, H.Ohgaki*, M.Chiwaki*, and T.Yamazaki
*** Electrotechnical Laboratory**

Appl. Surface Sci., 116 (1997) pp.177-180

The structure and performance are described of an apparatus for high-resolution positron-annihilation induced Auger electron spectroscopy installed at the Electrotechnical Laboratory. A a time-of-flight technique is adopted.

278: Auger Line shape analysis by time-of-flight positron-annihilation induced Auger-electron spectroscopy

T. Ohdaira*, R. Suzuki*, T. Mikado*, and T. Yamazaki
*** Electrotechnical Laboratory**

Material Science Forum, 255-257 (1997) pp.769-771

An analysis of the spectral line shape of LVV Auger-electrons generated from the Si(100) surface has been made with a time-of-flight PAES (positron-anihirration induced Auger-electron spectroscopy) system develped at the Electrotechnical Laboratory, which has the highest counting rate and resolution in the world. A chemical shift was successfully observed for the first time in the world with PAES.

279: * Apparatus for positron-annihilation-induced Auger electron

R. Suzuki*, T. Ohdaira*, T. Mikado*, H. Ohgaki*, M. Chiwaki*, and T. Yamazaki
*** Electrotechnical Laboratory**

Appl. Surface Sci., 100/101 (1997) p.297-300

An apparatus for positron-annihilation-induced Auger electron spectroscopy has been constructed at the intense slow positron electrons is measured with a time-of-flight technique. The combination of inhomogeneous magnetic field and pulsed positron beam enables us to measure positron-annihilation-induced Auger electron spectra with high resolution, with low background, and with high count rate (~10 min/spectrum).

280: Mechanical Property Changes and Microstructural Evolution in Neutron Irradiated Carbon / Carbon Composites

A.Kohyama

Proc. of The 4th JAPAN-CHINA Symposium on Materials for Advanced Energy Systems and Fission and Fusion Engineering, 1997

Effects of heat treatment temperature (HTT) on interfacial microstructure and interfacial mechanical properties of carbon/carbon (C/C) composites are investigated. Formation and/or growth of graphite layers adjacent to fiber- matrix interface were detected by transmission electron microscopy (TEM). Ultra micro indentation test technique was developed and was applied to C/C composites and fiber push out tests were also carried out. In case of fiber push out, the indentation curve showed a plateau which was interpreted to correspond with fiber push out. Interfacial sliding strength, evaluated from the load at the plateau, was increased with increasing HTT above 2000 K. Also, the effects of neutron irradiation on those characteristics have been investigated. The followings are the major conclusions about the neutron irradiation effects

281: Helium Effects on Irradiation-Induced Hardening of Low Activation Materials

Y.Katoh, T.Muroga*, T.Iwai and O.Motojima***
*** National Institute of Fusion Science, ** The Univ. of Tokyo**

Proc. The 4th JAPAN-CHINA Symposium on Materials for Advanced Energy Systems and Fission and Fusion Engineering, 1997

The combination of multiple beam ion irradiation using MV range accelerators and ultra low-load indentation tests is a potential technique to evaluate the mechanical property changes of solid materials

due to the radiation of energetic particles. In the first part of this work, development of experimental techniques and evaluation scheme to characterize the indentation hardness property of ion-irradiated materials, that possess perpendicularly graded hardness property within the surface layer as thin as typically one micron, is intended. For this purpose, alloys in three different classes had been irradiated and then indentation-tested. The obtained load- displacement properties were analyzed by various methods, and a few methods including one developed in this work appeared to produce reliable and highly reproducible results. In the next series of irradiation experiments, five different metals and alloys, which include a low activation ferritic steel and a vanadium alloy, were irradiation by dual-beam ions at helium-to-dpa ratios in a broad range. The indentation testing is currently underway and the results will be reported in presentation. Microstructural examination is also planned.

282: A Study of Neutron Irradiation Effects Related to the Materials Design for Force Free Helical Reactor(FFHR)

T.Muroga*, T.Noda, S,Ohnuki***, N.Yoshida****, H.Matui*****, Y.Katoh and A.Sagara***

*** National Institute of Fusion Science, ** National Research Institute for Metals, Tukuba Lab., *** Hokkaido Univ., **** Kyusyu Univ., ***** Tohoku Univ.**

Proc. The 4th JAPAN-CHINA Symposium on Materials for Advanced Energy Systems and Fission and Fusion Engineering, p34 (1996)

In the current design of FFHR,Lif-BeF_2(FliBe) is selected as a breeder/coolant material.The replacement frequency of the blanket structural materials is required to be minimal during the reactor lifetime. The irradiation conditions of the structural materials anticipated by the reactor design side are 1.5MW/m_2 and 30years (45MWa/m_2) and 400- 600 ℃ [1]. The objective of the present study is identify materials R&D issues and perform preliminary investigation.

The R&D issues for developing the FFHR blanket structural materials were examined and the preliminary investigation concerning the following three issues were carried out.

(1) Activation at neutron exposure level.(2) Compositional change by high level neutron irradiation. (3) Accumulation of high level of transmutant helium.

The radioactivity of some elements at high neutron exposure level (45MWa/m_2) were calculated considering some two-step reactions. The results showed that significant amount of long-lived radioactive nuclides were formed from Si and Ti. As for V, Cr, Fe, and W, however, the influence of the two-step reactions was shown to be negligibly small. It was also indicated that the impurity, especially Nb, Mo and Ag, should be reduced to very low level to satisfy the disposal guideline.

As to the compositional change by transmutation, the impact of W to Re/Os, V to Cr and Cu to Ni were examined. Irradiation of vanadium in HFIR was carried out as an accelerated simulation of Cr generation during irradiation. The specimens were strongly embrittled after irradiation. The change was attributed to the increase in the Cr level.

The microstructure-based methodology to suppress helium accumulation effects were investigated. Based on the study on Fe-Cr-Ni ternary doped with P and Ti, which produce high density of needle-shaped precipitates during irradiation, partitioning of helium in the matrix at high density of interface is shown to be

very effective in suppressing the helium accumulation effects on void swelling and mechanical properties.

283: Information on Second Heat of JLF-1 Steel

T.Hasegawa* and A.Kohyama
*** Nippon Steel Corporation**

Proc. The 4th JAPAN-CHINA Symposium on Materials for Advanced Energy Systems and Fission and Fusion Engineering

As the syructural material for fusion reactor, high Cr-ferritic or martensitic steels are the most promising due to their low activation and high swelling resistance. JLF-1 steel is one of the low activation martensitic steels developed in Japanese universities fusion program. The first large heat of JLF- 1 steel was made and evaluated several years ago. For further investi gation, the production of second large heat of JLF-1.

Steel has been carried out. Main objective of the second heat, which is produced as 15and 25mm-thick plates, is to investigate fracture toughness and mechanical properties under neutron irradiation or in strong magnetic field. In this paper, mechanical properties of the base plate and TIG welded joint of second heat of JLF-1 steel as well as the fabrication data are introduced. Temperature and 300 MPa at 600 ℃ with sufficient ductility. This steel has good

284: Hydrogen Action on the 316L Stainless Steel Blister with H-HE Mixture Injection

Y.Jinnan*, C.Yiren*, Z.Xinjie*, Z.Wen, C.Fengmin* and Y.Wen*
*** China Institute of Atomic Energy**

Proc. The 4th Japan-China Symposium on Materials for Advanced Energy Systems and Fission and Fusion Engineering, p.175 1996

The blistering and flaking caused by gas ions are significant surface erosion phenomena for the plasma-wall interaction in the first wall materials of fusion reactor. The 316L s.s specimens were implanted by helium, hydrogen and mixture ion beam with energy ranging between 27 keV and 38 keV to a dose of 10^{17}-8 $\times$ 10^{18} ions/cm^2 at 573 K to investigate the blistering and the hydrogen action on the blister. The results indicate that, (a) The threshold dose of blister for the helium ion in energy range 27-100 keV is higher than that for thel.0MeV helium ion irradiation, the surface effects play an important role in the blistering. (b) The specimens bombarded by the mixture beam of helium and hydrogen ion with 27keV reached the same helium dose (6.4 $\times$ 10^{17} He^+/cm^2), the diameter and density of surface bubble increase with the radio of hydrogen to helium incrasement. The more hydrogen ion, the blister more easier and serious. (c) When the kinetic energy of mixture beam decreases in the range 10-30 keV, the action of hydrogen ion for the blister appear more apparently.

285: Advanced Remote Participation Capabilities for Education and Research in Energy Science and Technology

A.Kohyama and Y.Katoh

Proceedings of UNESCO Regional Conference on Higher Education, Jul 1997.

As important roles of new technology to higher education and advanced research, distanced education and remote participation to scientific and technological researches have been recognized and are being developed. However, the concept of remote participation capabilities and their requirements and issues have been insufficiently discussed and defined. Moreover, the financial support to these activities have been quite limited.
Within the framework of International Energy Agency (IAE) remote participation to research in science and technology has been discussed. This paper provides present status of remote participation capabilities in nuclear fusion research and the future prospects as an example and addresses the importance of the same kind of activities in higher education for the 21st century. Although, the IEA activities on remote participation are voluntarily and are not supported financially, as the parts of international collaboration programs or the domestic programs on advanced technology areas, there have been a remarkable progresses in the recent years.
The major benefits of the remote participation capabilities are,
1: Provide opportunities to participate higher education and research activities utilizing the most advanced research facilities and tools under the conventional electrical networks
2: Provide facility related information and data, real time.

286: Evaluation of Low Temperature Swelling in Austenitic Stainless Steels

Y.Katoh

Effects of Radiation on Materials, ASTM STP 1325, 1997.

Major portions of structural materials of near-term fusion blankets and light water reactor core components are subject to neutron irradiation at low temperatures and low fluxes compared to those in typical void swelling studies using fast reactors. Observed swelling in austenitic stainless steels at temperatures below 673K are generally very small under typical fast reactor irradiation conditions, however, the amount of swelling might be significantly influenced by neutron flux, helium generation rate, etc. In this work, using a reaction rate theory model of swelling, the influences of such key irradiation parameters on low temperature swelling behavior in austenitic stainless steels will be demonstrated to aid the evaluation of swelling at low temperature and low neutron flux conditions.

287: The Influence of Helium Co-Implantation on Ion-Induced Hardening of Low Activation Ferritic Steel Evaluated by Micro-Indentation Technique

Y.Katoh, H.Tanigawa, T.Muroga* and T.Iwai**
*** National Institute of Fusion Science, ** The University of Tokyo**

Proc. The 8th International Conference on Fusion Reactor Materials, 1997

An experimental technique to determine the dual-ion irradiation - induced hardening of solid materials by means of micro - indentation was developed and then applied to evaluate the irradiation response of low activation martensitic steel. Micro-hardness measurements was performed on a low activation Fe-9Cr-2W

288: Evaluation of Weld Crack Susceptibility for Neutron Irradiated Stainless Steels

A.Kohyama, T.Suzuki, T.Hirose and M.Narui*
*** Tohoku Univ**

Proc. The 8th International Conference on Fusion Reactor Materials, 1997

In order to clarify the mechanisms of weld cracking, especially for heat affected zone cracking in heavily neutron irradiated stainless steels, and to establish a measure to evaluate crack susceptibility, a mini-sized Varestraint (variable restraint) test machine for hot laboratory operation was designed and fabricated. This unique PIE facility was successfully applied in the hot laboratory of IMR Oarai-Branch of Tohoku University. The maximum restraint applied was 4 % at the surface of the specimen.Specimen surface morphology and specimen microstructure were inspected by video microscope, SEM and TEM. Under the 2 % surface restraint condition, clear formation of HAZ crack was observed for the case of neutron irradiation to produce 0.5appmHe and of 2.4kJ heat input by TIG.

289: Mechanical Property Changes of Low Activation Ferritic/Martensitic Steels after Heavy Neutron Irradiation

Y.Kohno*, A.Kohyama, M.L.Hamilton, M.Narui*** and T.Hirose**
*** The University of Tokyo, ** PNNL, *** Tohoku Univ.**

Proc. The 8th International Conference on Fusion Reactor Materials, 1997

Low activation ferritic/martensitic steels are being considered for structural application in fusion DEMO reactor and the beyond, and R&D of low activation ferritic/martensitic steels have been widely

continued in these decades. In the Japan/USA (Monbusho/DOE) collaboration program, advanced Fe-XCr-2W-0.2V-Ta (X: 2.25-12) low activation ferritic/martensitic steels (JLF steels) were developed, and irradiation response in mechanical properties as well as in microstructure have been examined after heavy neutron irradiation.
Materials examined in this study were JLF steels and F82H, which was developed by JAERI. Miniaturized mechanical test specimens were irradiated in FFTF or EBR- II to doses up to 60 dpa at temperature range of 650 to 870K. Those specimens included Charpy impact specimens (1.5mm, 1/3 size), tensile specimens (S, W, SS- 3 size), pressurized tube creep specimens and disk bend specimens (3mm diameter TEM disk).
From Charpy impact test results of 1.5mm-size specimens of JLF-1 (9Cr) irradiated at around 680K, DBTT were measured to be 160, 210 and 185K following irradiation to 0, 35 and 60 dpa respectively. DBTT increased by 50 K after irradiation of 35 dpa,and then decreased by further irradiation. DBTT of F82H (8Cr) were 170K and 250K at 0 and 35 dpa respectively. Increase of DBTT in F82H seemed to be larger than in JLF-1. Change in upper shelf energy was observed to be small. As for the results of 1/3-size specimens, DBTT were almost the same as those of 1.5mm-size specimens. No significant specimen size effect was found. Results of tensile tests, irradiation creep measurements and disk bend tests will be discussed in detail.

290: * Current Status and Future R&D for Reduced-Activation Ferritic/Martensitic Steels

A.Hishinuma*, A.Kohyama, R.L.Klueh, D.S.Gelles***, W.Diez****, K.Ehrlich*****

*** Tokai Establishment,JAERI, ** Oak Ridge National Laboratory, *** Battle Pacific Northwest Laboratory, **** Consultant,EC/DGXII/Fusion Program, ***** Institute für Materialforschung I**

Proc. The 8th International Conference on Fusion Reactor Materials, 1997

Reduced-activation ferritic/martensitic steels are the first candidate alloy for the DEMOreactor and beyond, because of better thermal properties compared with the austenitic stainless steel that has been selected as a structural material of the experimental reactor like ITER. Fe-(8-9)Cr ferritic/martensitic steels are the most promising from the points of irradiation resistance, especially of the phase stability and the shift of the ductile-brittle transition temperature(DBTT) during or after irradiation.
The round robin teste under the International Energy Agency(IEA) Working Group on ferritic/martensitic steels for fusion application have been carried out, in order to coordinate the acquisition of the data needed to prove feasibility for the steels for fusion reactors, consisting of researchers from the European Union, the United States,Swizerland and Japan. In the international collaboration experiments, the large heats of the IEA-modified F82H steel and JLF-1 were produced, fabricated into plates and weld-joints, and distributed to the participants as reference materials. The main experiments on these materials, with other of ORNL9Cr-2WVTa and Eurofer will be conpleted within this century.
In addition to the assessment studies described above, development for fabrication technologies of large-heat melting and welding/joining have been studied. The utilization technology for ferromagnetic ma-

terials is also much concerned from an engineering view point, because they could cause error magnetic field and disturb the plasma control sysytem. Some of the studies on this subject have been initiated in JAERI. To enlarge the design window area, development studies of utilization technologies for quasi-brittle materials, a typical property of materials after irradiation, with the improvement studies especially for high temperature strength are scheduled.

291: Current Status of SiC/SiC Composite R&D

P.Fenici*, A.Frias Rebelo*, R.H.Jones, A.Kohyama and L.L.Snead*****
*** CER, JRC Ispra, ** Pacific Northwest National Laboratory, *** Oak Ridge National Laboratory**

Proc. The 8th International Conference on Fusion Reactor Materials, p.129, 1997

The purpose is to give an overview of the multiple activities currently underway on SiC-based Ceramic Matrix Composites for Fusion Structural Applications, either referring materials development Composites, Fibres, Matrix,interfaces)as well as addressing technological issues such as design studies and related actions comprising jining,long-tern operation performance and future testing methodologies.Since few years the activities on low activation ceramic composites in Japan,USA and Europe have been carried out in the frame of the activation ceramic composites in Japan,USA and Europe have been carried out in the frame of the IEA implementing agreement on Fusion Reactor Materials.Based on the activities presented at the first and the second IEA Workshops on "SiC/SiC Ceramic Composites for Fusion Structural Applications",held at Ispra,Italy 28-29 October 1996,and at Sendai,Japan 23-24 October 1997,and on recent results,lecture is intended to be an introduction to the more detailed expositions to be presented as Oral Contributions or as posters.
Topics to be addressed in the lecture will cover different fields as:
Motivations for SiC-based Composites in Fusion Technology;
Current Design Studies and Materials requirements;
Current status on Composites in particular Mechanical properties,physical Properties,Irradiation Behaviour,Creep Behavior;
Technological Issues such as Joining and Long-Tern operation;
Materials Development including New fibres,Matrax processing Methods and development including New fibres, Matrix processing Methods and Developments in Interfaces;
Conclusions will include also Perspective on Future Activities and International Collaborations.

292: Influence of Tantalum and Nitrogen Contents, Normalizing Condition and TMCP Process on Mechanical Properties of Low Activation 9Cr-2W-0.2V-Ta Steels for Fusion Application

T. Hasegawa*, Y. Tomita* and A. Kohyama

*** Nippon Steel Corporation**

Proc. The 8th International Conference on Fusion Reactor Materials, p.226, 1997.

Ferritic and martensitic steels are advantageous in void swelling resistance, low thermal expansion coeffcient,and high thermal conductivity compared with austenitic steels as structural materials for wall and blanket components of fusion reactors.Where important R&D issues are recognized to be irradiation induced embrittlement and irradiation creep/relaxation.

Candidate low activation ferritic and martensitic steels have been developed based on the conventional high-Cr heat-resistant steels with Mo replaced by W and Nb by Ta in order to reduce induced radioactivity. Among the candidate steels,9Cr-2W-0.2V-0.07Ta steels, which have been developed in Japanese Universities fusion program designated as JLF-1 steels, are the most promisind for their good irradiation-creep resistance and small irradiation embrittlement as well as good baseline properties.

For clarifying the reason of good creep and mechanical properties and improving the mechanical properties of the JLF-1 steels, influence of Ta ,N contents, normalizing condition and TMCP process on the mechanical properties of the 9Cr-2W-0.2V-Ta steels was investigated in contrast with conventional heat-resistant steels(9Cr-1Mo-0.2V-Nb).

The creep strength of the 9Cr-2W-0.2V-Ta steels increases with increasing amount of Ta and N contents irrespective of manufacturing processes.Concerning with manufacturing processes,the increasing of normalizing temperature or the application of TMCP processes,which corresponds to hot rolling and tempering or direct quenching and tempering processes,can improve creep strength.However,the toughness of the steels decreases with increasing creep strength. It is hypothesized that the increase of creep strength due to the increasing of normalizing temperature or the application of TMCP processes is attributed to uniform distribution of fine (Ta,V)(C,N)precipitates.

In conclusion,the 9Cr-2W-0.2V-Ta steels have equivalent creep strength and better toughness compared with 9Cr-2W-0.2Vta steels have equvalent creep strength and better toughness compared with 9Cr-1Mo-0.2V-Nb steels. The good toughness of the 9Cr-2W-0.2V-Ta steels is attributed to their fine austenite grain size.

293: Dependence of Post - Irradiation Impact Properties on the Irradiation Temperature in Reduced Activation 9Cr-2W Martensitic Steels

A. Kimura, H. Kayano*, T. Misawa, H. Matsui* and A. Kohyama**

*** Tohoku Univ., ** Muroran Industrial Univ.**

Proc. 8th International Conference on Fusion Reactor Materials, p.235, 1997.

Reduced activation martensitic steels(RAMS)have a number of attractive features as a structural material for fusion DEMO reactor. Radiation embrittlement,however,may be a critical issue for the steels which undergo a transition of fracture mode from ductile to brittle in common with the other candidates of body centered cubic metals.As shown in the previous works,the embrittlement has been considered to be primarily associated with irradiation hardening caused by lattice defects and precipitates.Since irradiation hardening of RAMS is significantly influenced by irradiation temperture,the embrittlement is considered to depend strongly onirradiation temperature.In this study,dependence of impact properties aswell as tensile properties on irradiation temperature was investigated for some Japanese RAMSs.
The materials used were the Japanese 9 % Cr-RAMSs such as JLM and JLF series steeis.Miniaturized CVN specimens(1.5x1.5x20mm^3)as well as tensile specimens (4x16x0.25mm^3)and small punch specimens(3mm ϕ x0.25mm)were irradiated in the JMTR at 90 and 300 ℃ up to doses of 0.0006,0.03 and 0.1 dpa. Some specimens were also irradiated in the FFTF/MOTA at 390(22dpa),420 ℃ (36dpa) and 460 ℃ (24dpa).
Neutron irradiation always resulted in the increase in the ductile-brittle transition temperature(DBTT). The most sever embrittlement was observed after the irradiation at 90 ℃ (0.1dpa) which resulted in the shift in the DBTT as much as 120K. The irradiation at 300 ℃ (0.03dpa) caused the DBTT shift of 20K which was smaller than the DBTT shift irradiated at 90 ℃ to a dose of 0.006dpa(55K). High dose irradiation at 390 and 460 ℃ induced rather small shift in the DBTT of 30 and 20K, respectively. Correlation between the shift in DBTT and irradiation hardening has been investigated for RAMSs, and compared with that observed in vanadium alloys.

294: Microstructural Examination of Ni-ion Irradiated Fe-Ni-Cr Alloys Followed to Microzone Deformation

M. Ando, Y. Katoh, H. Tanigawa and A. Kohyama

Proc. 8th International Conference on Fusion Reactor Materials, p.271, 1997

Examination of deformation microstructures induced by micro-indentation technique by means of transmission electron microscopy following an MV range metallic ion irradiation was performed in order to study the influence of irradiation-produced microstructural defects on plastic deformation behavior of materials. In this work, specimens of an Fe-Cr-Ni austenitic model ternary alloy before and after irradia-

tion with 4 MeV Ni ions at 723K were indentation- tested at loads as low as 9.8mN using an instrumented micro-indentation testing system. The dislocation microstructures of the specimens ' regions beneath the indents were successfully examined with a transmission electron microscopy following a cross-sectional thin film processing with a focused ion beam (FIB) processing system. This paper describes the experimental procedure developed in this study and the results from the first series of the experiments.

295: Crack Initiation and Growth Characteristics in SiC/SiC under Indentation Test

W. Zhang, T. Hinoki, Y. Katoh, A. Kohyama, T. Noda*, T. Muroga and J. Yu*****
*** National Research Institute for Metals, ** National Institute of Fusion Science, *** China Institute of Atomic Energy**

Proc. 8th International Conference on Fusion Reactor Materials, p.192, 1997.

The mechanical behavior of ceramic matrix composites (CMC) is known to be strongly influenced by fiber-matrix interfacial properties. To improve toughness of composites like SiC/SiC, a non-bonded or a weakly bonded fiber- matrix interface is an important key element. In this work, for modifying fiber-matrix interface, Hi-Nicalon fibers were coated with a carbon layer and multiple layers. The objective of this study is to investigate crack initiation and growth characteristics in SiC/SiC composites.
Materials used were 2D woven fabrics of SiC(Hi-Nicalon) reinforced CVI-SiC composites. The carbon coating and the multiple layer coating on SiC fibers were applied with a variation of coating thickness (50 $\sim$5500 nm). A scanning electron microscope with in-situ micro-indentation test capability (SEMITEC) and a micro-Vickers hardness testing equipment were utilized to apply loads. The microstructures of specimens after micro-indentation testing were examined by transmission electron microscopy (TEM) following thin film processing with a focused ion-beam (FIB) device.
The crack behavior was strongly influenced by the crack initiation site and the surrounding structures. With carbon coating of a sufficient thickness on SiC fibers, crack propagation through the fiber-matrix interface was quite scarce.Cracks tended to propagate along the matrix growth directions and usually stopped at the interface between fiber and carbon layer. This means the intrinsic catastrophic mode of failure in the brittle matrix is prohibited due to deflected crack propagation within the periphery of the fibers.

296: Applied Stress Effects Oninterstitial Type Frank Loop Evolution in Irradiatied Single Crystal Fe-Cr-Ni

H. Tanigawa, A. Kohyama, Y. Katoh and Y. Kohno*
*** The University of Tokyo**

Proc. 8th International Conference on Fusion Reactor Materials, 1997.

The first wall structural materials of fusion reactors suffer from irradiation creep caused by external applied stress, and the dimensional and mechanical property changes must be predicted to construct a fusion reactor. There have been many attempts to model irradiation creep, but the basic processes underlying those models have not been understood or proven sufficiently. The aim of this study is to obtain both phenomenological and mechanistic understanding of stress effects on early stages of microstructural evolution under irradiation. The effect of applied stress on Frank loop evolution is of special concern.
In previous studies, the dynamic effects of applied stress on interstitial type Frank loop evolution have been investigated by both ion irradiation experiments and numerical calculation, and the SIPU (Stress Induced Preferential Unfaulting) model has been proposed to explain the strong dependence of Frank loop concentration on the resolved stress normal to the 111 plane. The model has been successful in predicting the positive dependence of Frank loop concentration on a 111 plane on the resolved normal stress to a 111 plane.
In this study, the SIPU model was verified under static conditions by irradiating non-loaded specimens and later annealing under applied stress. Two types of

297: Effect of Fiber Coating on Interfacial Shear Strength of SiC/SiC by Nano-indentation Technique

T. Hinoki, A. Kohyama, S. Sato* and T. Noda**
*** Fukushima National College of Technology, ** National Research Institute for Metals**

Proc. 8th International Conference on Fusion Reactor Materials, 1997.

In order to quantitatively evaluate mechanical properties of fibers, matrices and their interfaces in fiber reinforced SiC/SiC composites, fiber push-out tests have been carried out. From the indentation load vs. displacement relations, the fiber push-out process has been discussed in comparison with the C/C composites and the loads for fiber push-in and those for fiber push-out were estimated. The trends of load-displacement curve of fiber push-out process depended on specimen thickness. The curve in the case of thick specimen had a micro step indicating fiber push-in and a larger step corresponding to fiber push-out. However just a larger step indicating fiber push-out was seen without fiber push-in process in the case of thin specimen. Interfacial shear stress was discussed and defined in both cases. The effects of fiber coatings on interfacial shear stress obtained from thin specimens were analyzed. The relationship between bending stress and interfacial shear stress of SiC(pcs)/SiC(CVI) is preliminarily postulated together with microstructural characteristics of the composites.

298: Crack Initiation and Growth Characteristics in SiC/SiC under Indentation Test

W. Zhang, T. Hinoki, Y. Katoh, A. Kohyama, T. Noda*, T. Muroga and J. Yu*****
*** National Research Institute for Metals, ** National Institute of fusion Science, *** China Institute of Atomic Energy**

Proc. 8th International Conference on Fusion Reactor Materials, 1997.

The mechanical properties of the SiC/SiC composite were affected by interfacial structure significantly. Carbon layer and multiple layers were introuced to be interphase to improve the toughness of the composite. The objective of the work is to find some suitable coatings for improving the mechanical properties by investigating the crack initiation and propagation behaviors.
Materials used were 2D woven fabrics of SiC(Hi-Nicalon) reinforced CVI-SiC composites. The carbon coating and the multiple layer coating on SiC fibers. A scanning electron microscope with in-situ micro-indentation test capability (SEMITEC) and a micro-Vickers hardness testing equipment were utilized to apply loads. The microstructures of specimens after micro-indentation testing were examined by transmission electron microscopy (TEM) following thin film processing with a focused ion-beam (FIB) device. In general, cracks initiated in matrix propagated through coating and deflected along fiber surface, also crack in fiber deflected at fiber-coating interface. This is an important mechanism for improving toughness of SiC/SiC. In push-in test, it was found that the debond load of the fibers decreased with the increment of the coating thickness. A suitable coating thickness will be defined together with microstructural optimization in the future. Crack deflection in fiber might be related with dispersed crystalline particles in fiber. At interface, crack propagated parallel to graphite and SiC basal plane.

299: The Development of Low Activation Ferritic Steels for Fusion Application

A.Kohyama, A.Hishinuma*, K.Kohno, K.Shiba*** and A.Sagara***
*** National Institute for Fusion Science, ** The University of Tokyo, *** Japan Atomic Energy Research Institute**

Sci. Rep. RITU A45, pp133-136, 1997

The development of low-activation ferritic/martensitic steels is a key to the achievement of nuclear fusion as a safe, environmentally attractive and economically competitive energy source. The Japanese and the European Fusion Materials programs have put low-activation ferritic and martensitic steels R&D at the highest priority for a demonstration reactor (DEMO) and the beyond. An international collaborative test program on low-activation ferritic/martensitic steels for fusion is in progress as an activity of the International Energy Agency (IEA) fusion materials working group to verify the feasibility of using ferritic/martensitic steels for fusion by an extensive test program covering the most relevant technical issues for the qualification of a material for a nuclear application. The development of a comprehensive data base on the representative industrially processed reduced-activation steels of type

8-9Cr- 2WVTa is underway for providing designers a preliminary set of material data for the mechanical design of components, e.g. for DEMO relevant blanket modules. The current design status of FFHR and SSTR utilizing low-activation ferritic steels is reviewed and future prospects are defined.

300: Effect of Interfacial Shear Strength on Mechanical Property of SiC/SiC

T. Hinoki, A. Kohyama, W. Zhang, H. Serizawa* and S. Sato**
*** Osaka Univ., ** Fukushima National College of Technology**

SCI. Rep. RITU A45, pp. 133-136, 1997.

In order to quantitatively evaluate mechanical properties of fibers, matrices and their interfaces in fiber reinforced SiC/SiC composites, nano-indentation tests have been carried out. Using the same technique, fiber push-out test was performed. The specimens were analyzed by means of scanning electron microscopy (SEM), before and after indentation tests. From the indentation load vs. displacement relations, the fiber pushed out process has been discussed and the initiation loads of interfacial debonding and those of interfacial sliding were defined and were discussed in comparison with the C/C composites. The load of interfacial debonding initiation was likely to increase in proportion to the fiber circumference. The initiation load of interfacial sliding increased with increment of contact area between fiber and matrix. The relation between bending strength and interfacial shear strength of SiC(pcs)/SiC(CVI) is preliminary postulated together with crack initiation and propagation characteristics and microstructural characteristics of the composites.

301: Fundamental Study of Tandem Electron Beam Welding for Nuclear Fusion and Fission Reactors

T.Suzuki, A.Kohyama and N.Abe*
*** Tohoku Univ.**

SCI. Rep. RITU A45, pp. 143-147, 1997.

As the important part of the life extension program for nuclear fission and that of the maintenance scheme of blanket of fusion reactors, repair welding technique of neutron damaged materials is recognized to be one of the most urgent subjects to be established. This work provides the potentiality and the critical issues of " Tandem electron beam welding technique " when it is applied to heavily neutron damaged materials. Where mechanical property degradation due to the displacement damaged and helium production from (n, α) reaction makes it very difficult to produce sound welded joint. This paper presents the preliminary results to see the elementary characteristics of the welded joints produced by Tandem electron beam welding technique. Not only for the stainless steel nor high-nickel alloys, also for stainless steel to high-nickel alloy welded joints were studied. The tandem electron beam welding was done at JWRI, Osaka University. By optimizing the drilling effect from the leading electron beam

and the weld defect suppression effect from the secondary electron beam, weld defect free welded joints were obtained with the excellent joint strength and ductility. The weld bead shape and penetration characteristics are also provided. The present results are quite promising to apply " Tandem electron beam welding " to heavily neutron damaged metallic structure and components.

302: A New Project on R&D of Advanced Material Systems for Conversion of Energy : CREST-ACE Program

A. Kohyama

Proceeding of The International Symposium on Advanced Energy Technology, pp.645-652, Feb 1997.

Under the title of "R & D of Environment Conscious Multi-Functional Structural Materials for Advanced Energy Systems", a new R & D activity to establish high efficiency and environmental conscious energy conversion systems, as one of the programs of Core Research for Evolutional Science and Technology (CREST), has been initiated from October 1997 to September 2002. This program cares for R & D of high performance materials and materials systems for severe environments and production of model components for energy conversion systems is carried out. The emphasis is on R & D of SiC/SiC, W/W with their system studies to establish sound material life cycles. The program outline and preliminary results on SiC/SiC are provided.

303: Hardness Evaluation of MeV-Ion Irradiated Materials by means of Very Low-Load Indentation Technique

微小押込み試験技術を用いた **MeV** イオン照射材の硬度評価

Y.Katoh, T.Muroga*, T.Iwai and O.Motojima***
*** National Institute for Fusion Science, ** The University of Tokyo**

Japan Inst. Metals, Vol.61.No3 pp.191-198 1997

日本金属学会誌、第 61 巻第 3 号 pp.191-198 1997

Characterization of the plastic deformation properties of thin damaged layers prodeuced by heavy ion beam in an MeV energy range is being attempted by means of a very low load indentation technique. This paper focuses on the development of experimental techniques and special considerations in analyzing the measured data from specimens which possess perpendicularly uneven hardness property. For this purpose, metals and alloys of different classes, namely a model austenitic alloy, pure iron and oure vanadium, were irradiated with metallic ions and subsequently subjected to instrumented indentation tests. The load-displacement property obtained from the experiment was analyzed in various schemes to extract the amount of the net hardening due to ion-irradiation. (in Japanese)

304: Production of Low Activation Steel; JLF-1, Large Heats - Current Status and Future Plan

A. Kohyama , Y. Kohno*, M. Kuroda, A. Kimura and F. Wan
*** The Univ. of Tokyo**

Proc. The 8th International Conference on Fusion Reactor Materials, p173, 1997

Based on the excellent basic properties prior to neutron irradiation and under neutron irradiation up to 100dpa, the 9Cr-2W type low activation ferritic steel, JLF-1, had been selected as one of the reference materials to the IEA low activation ferritic steels R & D activity. This paper provides the general information about the second large heat of JLF-1 steel. The basic property of thick plates (24, 12 mm in thickness) and their welded joints together with the information about microstructure are also provided

305: Femtosecond Cr:LiSAF Laser Pumped by a Single Diode Laser

Sadao Uemura* and Kenzo Miyazaki
***ETL**

Opt. Commun. Vol.138, pp.330-332 (1997).

Using a single 800-mW AlGaInP diode laser to pump a Kerr-lens mode-locked Cr:LiSAF laser, we demonstrate the generation of almost Fourier-transform limited 26-fs pulses with the spectral bandwidth of 34 nm. A novel design of the mode-locked laser cavity was used to focus tightly the pump beam of the high-power diode laser having a broad emitting area. We have pointed out that the prism edge near the folding mirrors in the laser cavity plays a role of a hard aperture for the Kerr-lens mode-locking.

306: Thermal Characteristics of a Continuous-wave Cr:LiSAF Laser

Sadao Uemura* and Kenzo Miyazaki
*** ETL**

Jpn. J. Appl. Phys. Vol.36, pp.4312-4315 (1997).

Thermal power density produced in the laser medium of a continuous-wave Cr:LiSAF laser has been investigated to make clear the laser output characteristics. For the cw Cr:LiSAF laser using axially-symmetric end pumping, the available pump power density has been found to be limited to less than 100 W/mm^3. Based on the thermal characteristics studied, an efficient laser-diode-pumped Cr:LiSAF laser has been developed.

307: All Solid-state Kerr-lens Mode-locked Cr:LiSAF Laser

Sadao Uemura* and Kenzo Miyazaki
*** ETL**

Proc. Int. Conf. on Lasers'96, (STS press, McLean, 1997) pp.360-367.

Based on the observed thermal quenching of the output power of a continuous-wave (cw) Cr:LiSAF laser, an efficient diode-pumped cw Cr:LiSAF laser has been developed. The maximum slope efficiency is 32 %, which is, to our knowledge, the highest one observed so far with cw Cr:LiSAF lasers pumped by single-broad-stripe diode lasers. We report the characteristics of a self-mode-locked Cr:LiSAF laser which is operated at reduced group-delay dispersion (GDD). The spectral change with increasing the prism insertion is found to be different from that in a Ti:sapphire laser. We observed dispersive waves generated from the mode-locked Cr:LiSAF solitary laser and estimated the GDD and third-order dispersion (TOD) of the laser cavity under the lasing condition. A large TOD is shown to limit the possible reduction of the absolute value of GDD. Using a single diode laser to pump a self-mode-locked Cr:LiSAF laser, we demonstrate the generation of Fourier-transform limited 26-fs pulses with the spectral bandwidth of 34 nm. This pulse width is, to our knowledge, the shortest in the single-diode-pumped solid-state lasers produced so far. A novel cavity design for the mode-locked laser is used to focus tightly the pump beam.

308: Flashlamp-pumped Cr:LiSAF Laser Amplifier

Hideyuki Takada*, Kenzo Miyazaki and Kenji Torizuka*
*** ETL**

IEEE J. Quantum Electron. Vol.33, pp.2282-2285 (1997)

A flash-lamp-pumped Cr:LiSAF laser amplifier has been developed that is capable of producing ultrashort pulses with a peak power of TW. A systematic experimental study of laser oscillation, its small-signal gain, and chirped-pulse amplification has been performed under the same pumping conditions. The characteristic properties and performance of the Cr:LiSAF laser amplifier are reported.

309: 5TW Ti:Sapphire Laser Chirped-pulse Amplification System

Hideyuki Takada*, Masayuki Kakehata*, Kenzo Miyazaki and Kenji Torizuka*
*** ETL**

Technical Digest, CLEO/Pacific Rim '97 (1997) pp.15-16

We have developed a Ti:Sapphire laser chirped-pulse amplification system capable of producing 240 mJ, 50 fs pulses at ~790 nm. The design and operational characteristics of the laser system are presented and discussed.

310: Laser-pulse Width Effects on the High-order Harmonic Generation

Masayuki Kakehata*, Hideyuki Takada* and Kenzo Miyazaki
*** ETL**

Technical Digest, CLEO/Pacific Rim '97 (1997) pp.68-69

We report a comparative study of high-order harmonic generation using 65-fs and 150-fs Ti:sapphire laser pulses. The highest harmonics observed with 65-fs (150-fs) laser pulses are the 127th (103rd) in He, which corresponds to harmonic wavelength of 6.25 nm.

311: Ultrashort-pulse Generation from a Diode-pumped Self-mode-locked Cr:LiSAF Laser

Sadao Uemura* and Kenzo Miyazaki
*** ETL**

Technical Digest, CLEO/Pacific Rim '97 (1997) pp.191

A diode-pumped self-mode-locked Cr:LiSAF laser generates ultrashort pulses with the bandwidth of 77.4 nm and center wavelength of 865 nm. Assuming a sech^2-shaped transform-limited pulse, the pulse duration would be 10.1 fs.

312: Possible Control of Electron Energy Distribution by a Time-Dependent Polarization-Controlled Laser Pulse

Masayuki Kakehata (ETL), Hideyuki Takada*, Kenji Torizuka*, and Kenzo Miyazaki
*** ETL**

Technical Digest, CLEO/Pacific Rim '97 (1997) pp.192-193

We propose use of a time-dependent polarization-controlled laser pulse to control electron energy distribution in an optical-field-ionized plasma. The average electron energy can be widely controlled by controlling the timing to change the polarization.

313: Critical Heat Fluxes in Pool Boiling of Subcooled Liquid Nitrogen at Elevated Pressures

Hata, K., Shiotsu, M. and Sakurai, A.*
***** Future Energy Research Association**

Proc. of the International Cryogenic Engineering Conference/ International Cryogenic Materials Conference, Part 1, Elsevier, pp.585-588, 1997.

The critical heat fluxes on a 1.2 mm diameter platinum horizontal cylinder in liquid nitrogen due to quasi-steadily increasing heat inputs were measured for the subcoolings ranging from zero to about 40 K at pressures ranging from 0.3 to 2 MPa. The critical heat flux values for saturated conditions almost agree with the corresponding values derived from the Kutateladze correlation for saturated conditions except those for the pressures higher than around 1.5 MPa. The critical heat fluxes for subcooled conditions at the pressures cannot be described by existing correlations based on hydrodynamic instability, except those near zero subcoolings at pressures lower than around 1.5 MPa. It was clarified that there exist two mechanisms for critical heat fluxes; two correlations which depend on subcoolings and pressures were suggested.

314: Natural Convection Heat transfer from Horizontal Rod Bundles in Liquid Sodium

Hata, K., Shiotsu, M., Takeuchi, Y., Hama, K., Sakurai, A.* and Sagayama, Y.**
***Future Energy Research Association, ****Tokyo Electric Power Co.**

Proc. of Eighth International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Vol. 2, pp.817-827, 1997.

Natural convection heat transfer from horizontal rod bundles in $N_{xm} \times N_{ym}$ arrays (N_{xm}, N_{ym}=5 $\sim$ 9) in liquid sodium was numerically analyzed for three types of the bundle geometry (in-line rows, staggered rows I and II). The unsteady laminar two dimensional basic equations for natural convection heat transfer were numerically solved by using the PHOENICS code considering the temperature dependence of thermophysical properties concerned. The surface heat fluxes for each cylinder were equally given for a modified Rayleigh number, R_f, ranging from 0.0637 to 63.1 ($q = 1 \times 10^4 \sim 7 \times 10^6$ W/m^2). S_x/D and S_y/D for the rod bundle which are ratio of the distance between center axes on the abscissa and the ordinate to the rod diameter were ranged from 1.6 to 2.5 on each bundle geometry. The spatial distribution of Nusselt numbers, Nu, on horizontal rods of a bundle was clarified. The average value of Nusselt number, Nu_{av}, for three types of the bundle geometry with various values of S_x/D and S_y/D were calculated to examine the effect of the array size, S/D and R_f on heat transfer. The bundle geometry for the higher Nu_{av} value under the condition of $S_x/D \times S_y/D = 4$ was examined by changing the ratio of S_x/S_y. A correlation for Nu_{av} for three types of bundle geometry above mentioned including the effects of S_x/D and S_y/D was developed. The correlation can describe the theoretical values of Nu_{av} for three types of the bundle geometry in $N_{xm} \times N_{ym}$ arrays ($N_{xm}, N_{ym} = 5 \sim 9$) for S_x/D and S_y/D ranging from 1.6 to

2.5 within 10 % difference.

315: Unsteady Laminar Forced Convection Heat transfer due to Rapid Increase in Flow Rate of Liquid Sodium in a Concentric Annulus

Takeuchi, Y., Hata, K., Shiotsu, M., Sakurai, A.* and Sagayama,Y.**
***Future Energy Research Association, **Tokyo Electric Power Co.**

Proc. of Eighth International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Vol. 2, pp.932-941, 1997.

Experiments have been made of unsteady forced convection heat transfser from a heated surface of 52 mm in length on an inner cylinder of 7.6 mm in diameter to liquid sodium flowing in a vertically oriented concentric annulus with 14.3 mm inside diameter. With constant heat flux of 1.0×10^6 W/m^2, liquid sodium flow rate was reduced ramp-wise within about 25 seconds from an initial equilibrium state, Pe=72, to Pe=6.4 and from Pe=141 to 11.5 where Pe denotes the Peclet number. A numerical model capable of describing the effect of heat conduction in the inner and outer walls of an annulus as well as in liuqid sodium was developed. The numerical results obtained by the model agree with the experimental results for the two different fow transient conditions. The numerical model proved to be valid for expressing the unsteady laminar forced convection heat transfer caused by a decrease in sodium flow rate in a concentric annular passage. The theoretical results for various flow reduction periods revealed that the time delays in heated wall temperature rise from that predicted by a model for constant flow rates were little influenced by the flow reduction periods ranging from about 25 down to 2 sec. As the surface temperatures calculated by the present model became always equal to or lower than those by the constant flow rate model over the investigated flow reduction range and periods,the constant flow rate model is a simple but effective method for safety evaluation of transient heated wall temperature rise caused by rapid decrease in flow rate.

C. Review Articles

C．総説

Chapter 3

Review Articles

I Department of Socio-Environmental Energy Science

(エネルギー社会・環境科学専攻)

1: Wood as Eco-Materials

エコマテリアルとしての木質材料

Shiro Saka

J. Soc. Mat. Sci.,Japan 47(3), 325-326, 1998

材料 47(3), 325-326, 1998

Wood as eco-materials was discussed with an emphasis on an emission of carbon dioxide from fossil resources and its fixation by forest trees. In addition, woody materials were evaluated as eco-materials on their manufacturing energy, compared with some other materials such as aluminum, concrete and steel. Furthermore, the cascade methods and antimicrobial treatment of woody materials were introduced as environmentally friendly utilization methods of biomass resources (in Japanese).

2: Application of PIXE Analysis to Atmospheric Environmental Studies

大気環境研究への PIXE 法の応用

Mikio Kasahara

Radiation, Vol.23, No.4, pp.87-96, 1997

放射線, 23 巻, 4 号, pp.87-96, 1997

Physical and chemical properties of the atmospheric aerosols is a fundamental to understand the behavior of aerosols in the atmosphere. The analysis of atmospheric aerosols is the most preferable fields of the PIXE. In this paper, the characteristics of atmospheric aerosols are reviewed at first, and the sampling method of atmospheric aerosols for the PIXE samples and the characterization of atmospheric aerosols using the PIXE analysis are discussed (in Japanese).

3: Data Inversion on the Measurement of the Size Distribution of Aerosols

エアロゾル計測におけるデータ逆変換

Susumu Tohno

Journal of Aerosol Research, Japan, Vol.12, No.4, pp.281-287, 1997

エアロゾル研究, 12 巻, 4 号, pp.281-287, 1997

Data inversion methods for instrumental measurements of the size distribution of aerosol particles were reviewed. Some theoretical aspects of the aerosol inversion problem were discussed and comparison was made between three inversion techniques currently used, that is, conventional method neglecting cross sensitvity, regularization method and non-linear iteration method for inversion of cascade impactor and diffusion battery data (in Japanese).

4: Meaningful, Realistic and Equitable?

Yoichi Kaya

Look Japan, Vol. 43, No. 504, pp. 24-25, 1998

5: Advancement of Global Warming and Japanese Strategy

Yoichi Kaya

International Affairs, No. 453, pp. 2-20, 1997

6: Forty Years of Training Program in the JAERI Nuclear Technology and Education Center

Yasunori Bessho

JAERI-Review 98-009, 1998

Positive advice and perspective are made on the future training program, namely on the future educational courses and seminars in utilization of radioisotopes and nuclear energy for domestic and for

international training at the NuTEC(Nuclear Technology and Education Center) of Japan Atomic Energy Research

7: Review on BWR Core Design

Yasunori Bessho

General Nuclear Engineering Course B of 1997, The NuTEC (Nuclear Technology and Education Center) of Japan Atomic Energy Research Institute, June 1997

BWR core technologies have been developed continuously in order to improve BWR plant reliability, capacity factor and economics. An initial core concept was developed to attain a high discharge exposure by simulating an equilibrium core with multiple types of fuel assemblies of different enrichments. The highly economical initial core has been adopted at Kashiwazaki-Kariwa unit 5 and unit 4 of TEPCO(Tokyo Electric Power Company), Shika unit 1 of Hokuriku Electric company, etc., and it has become the standard design for the initial core of BWR. This concept is also adopted in two ABWRs(Advanced Boiling Water Reactors), Kashiwazaki-Kariwa unit 6 and 7 of TEPCO.

For BWR core design, nuclear thermal-hydraulic analysis techniques with higher accuracy and reliability are developed by steadily reflecting core management results from operating BWRs. Detailed analysis programs have been completed such as fuel assembly nuclear analysis using Monte Carlo method, fuel assembly critical power evaluation using subchannel analysis and 3-D core analysis based on a nodal method, taking advantage of recent outstanding progress in computer technology. These new programs with more rigorous models are combined to form an advanced nuclear ther-mal-hydraulic analysis system to be applied to the design and development of advanced types of BWR core.

8: Present Status of High Burn-up BWR Fuel Development

Yasunori Bessho

Key Note Presentation on Manager Education Seminar, Japan Nuclear Fuel Co., Ltd., March 1998

Highly economical BWR fuels have been developed by gradually raising discharge exposure and saving uranium, aiming at the reduction of the fuel cycle cost and the amount of spent fuel. Their development have been made by the best use of techniques to increase fuel exposure. Stepwise increase of average discharge burn-up to 33, 38 and 45 GWd/t has been achieved by the development of Step-I, II and III fuels, respectively, which has resulted in the reduction of fuel cycle cost by approximately 10%, 20% and 30%, respectively.

9: Issues on High Burn-up BWR Fuel Development(1)

Yasunori Bessho

Key Note Presentation on Seminar for Managers, Nippon Nuclear Fuel Development Co., Ltd., June 1997

Following the Step-I and Step-II fuel introduction for commercial use since 1987 and 1992, respectively, with excellent results, the Step-III fuel adopted 9x9 array to achieve the 45 GWd/t with the lowest possible enrichment. The issues encountered during the nuclear-thermal hydraulic design of the high burn-up fuel, including the Step-III fuel, for example the nuclear-thermal-hydraulic stability one and the pressure drop one while improving fuel economics, are reviewed.

10: Issues on High Burn-up BWR Fuel Development(2)

Yasunori Bessho

Key Note Presentation on Seminar for Managers, Nippon Nuclear Fuel Development Co., Ltd., September 1997

The high burn-up Step-III fuel adopted 9x9 array with two large central water rods arranged in the center of the fuel bundle to obtain an appropriate distribution of moderating water. The issues encountered during the fuel mechanical design of the high burn-up fuel, including the Step-III fuel, are reviewed.

II Department of Fundamental Energy Science

(エネルギー基礎科学専攻)

11: Preparation of Ionically Conductive Thin Films Utilizing Non-equilibrium Plasma Process

非平衡プラズマプロセスを用いた電気化学機能性薄膜材料の合成

Yoshiharu Uchimoto and Takeshi Yao

溶融塩および高温化学 Vol. 40, pp. 19-30, 1997

A non-equilibrium plasma (glow-discharge plasma) is an ionized gas containing equal numbers of positive and negative charges, and large number of non-ionized neutral molecules. The glow-discharge plasma have average electron energies in the range of 1-10 eV and electron densities of 10^9-10^{12} cm^{-3}. In addition, the ratio of the electron temperature to the gas temperature is large, and can reach values of 10-1000. Due to these properties of glow discharge plasma, plasma polymerization processes have become prevalent. In this work, ionically conductive thin polymer films including lithium ion conductive thin films, cation and anion exchanger thin films, monovalent cation perm-selective membrane were prepared by the plasma polymerization process. Because of the presence of ions and electrons, plasma is a conductive fluid. Therefore the plasma could be used as a conductive fluid in an electrochemical system. In this work, vapor-phase electrolytic deposition (electrolytic deposition using a glow-discharge plasma) was proposed and applied to prepare yttria-stabilized zirconia thin films.

12: Bioaffinity Separation of Trypsin from Pancreatin Using Reverse Micelles Composed of a Nonionic Surfactant

Motonari Aachi, Makoto Harada, Akihisa Shioi, Kengo Shibata, Masaru Yamazaki and Shigeo Katoh* * (Kobe Univ.)

Advances in Bioseparation Engineering 1996-1997, Edited by The Special Study Group for "Bioseparation Engineering" under The Society of Chemical Engineers, Japan, pp. 85-90, 1998

Trypsin inhibitor was converted to hydrophobic states by covalently combining cholesteryl groups using acylation reaction and was immobilized in reverse micelles composed of a nonionic surfactant. Using this reverse micellar phase containing trypsin inhibitor as an affinity ligand, trypsin was selectively separated with high recoveries from a mixture of many kinds of contaminating proteins, i.e., pancreatin from porcine pancreas, by forward and backward extraction operations. No loss of the activity of recovered trypsin was observed through these operations when the suitable conditions were chosen.

13: Tailoring of Reverse Micelles for Protein Separation

タンパク質分離に向けての逆ミセルのテーラリング

Makoto Harada, Motonari Adachi and Akihisa Shioi

Hyomen, Vol. 35, pp. 239-245, 1997

表面、Vol. 35, 239-245, 1997

The constitution of advanced reverse micelles is important to realize ideal separation process of proteins. Reverse micelles stabilized with ionic surfactants have been commonly used for protein separations. They have, however, essential disadvantages for this purpose, i.e., denaturation and unsuitability for selective separations. Control of the electrostatic interactions between proteins and ionic surfactants makes it possible to extract proteins and to reduce denaturation of proteins significantly. This is realized by changing the composition of surfactants constituting reverse micelles, that is, the use of reverse micelles mainly composed of nonionic surfactants with minimum amount of ionic surfactants. The selective separation of a target protein can be achieved when affinity ligands, which can recognize a target protein specifically, are incorporated to reverse micelles composed of a nonionic surfactant. Highly functional systems can be realized by tailoring reverse micellar systems for the required aims.

14: Bioaffinity Separation Using Reverse Micellar System

逆ミセルを用いるバイオアフィニティ分離

Motonari Adachi

Chushutu Gijutu Shuuran, Edited by Kanto Branch of The Society of Chemical Engineers, Bunrigijyutu-Kai, and Kagakukogyosha, pp. 56-60, 1997

抽出技術集覧、化学工学会関東支部、分離技術会編、化学工業社、pp.56-60, 1997

This article describes that an ideal separation process of proteins can be realized using bioaffinity ligand immobilized in reverse micelles composed of a nonionic surfactant. Reverse micelles composed of ionic surfactant have been widely used. However, they have essential drawbacks for the separation of proteins, that is, denaturation of proteins and inadequateness for selective separations. When affinity ligands, which can recognize a target protein by biospecific interactions, are incorporated to reverse micelles composed of a nonionic surfactant, the selective separation of a target protein can be achieved. This was shown for the cases of concanavalin-alkylglucosides system, trypsin-trypsin inhibitor systems and separation of trypsin from pancreatin.

15: Characteristics and Applications of Microemulsion Structure in di-Oleyl Phosphate System

ジオレイルリン酸塩系におけるマイクロエマルション組織の特徴とその応用

Makoto Harada, Gen Nonaka, Noriaki Mizutani, Akihisa Shioi, Motonari Adachi, Katsuya Kanaoka, Kiyoshi Suzuki, Masahiro Goto and Fumiyuki Nakashio

Chemical Engineering Symposium Series 63, Fundamentals and Applications of Liquid Membrane and Materials with Molecular Recognition, Edited by The Special Study Group "Processes Using Liquid Membrane and Fluid with Molecular Recognition" under the Society of Chemical Engineering of Japan, pp.122-130,1998
化学工学シンポジウムシリーズ 63、液膜及び分子認識材料利用技術の基礎と応用、化学工学会「液膜及び分子認識液体利用プロセス」特別研究会編、pp. 122-130, 1998

Water-in-oil microemulsions are complex fluids containing nano-scale micro-structures. They attract great deals of interest from scientific and practical view points because of their potential use for reactions and separations. In spite of a number of investigations, the relation between structures and functions have not been elucidated. It is important to investigate the physicochemical properties and the structure of the complex fluids basically in order to tailor the microemulsions for technological potential use. In this review article, characteristics of microemulsion structure are discussed, especially focused on dioleyl phosphate system including the formation of nano-particles in it.

III Department of Energy Conversion Science

(エネルギー変換科学専攻)

16: The Japanese Sword — The Material, Manufacturing and Computer Simulation of Quenching Process

Tatsuo Inoue

Materials Science Research International, Vol.3, No.4, pp.193-203, 1997

Traditional methods of preparing a kind of steel called tamahagane used for the Japanese sword by tatara system and procedure of making the sword are briefly introduced with the discussions from the viewpoint of metallurgy and thermo-mechanical processing. Such traditional methods are also revealed to be consistent with the modern science and technology. The quenching process applied to the final stage of the procedure is focussed to explain how the pattern of blade, the deformation and residual stresses are induced by the computer simulation based on the theory of metallo-thermo-mechanics relevant to the coupled fields among temperature, microstructural change and stress/strain.

IV Department of Energy Science and Technology

(エネルギー応用科学専攻)

17: Recent Situation and Future of Molybdenum Mineral Resources

モリブデン資源の現状と将来

Katsutoshi Ono and Takashi Nishiyama

Energy and Resources, vol.18 No.3 (1997) pp.266-270

エネルギー・資源, vol.18 No.3 (1997) pp.266-270

Metallic molybdenum was overviewed from Mining and Metallurgical aspects. Mineralogical existence and recouces in the world were summarized, and mining and refining methods were reviewed. Although molybdenum is one of the less-common metals, its physical, electrical, chemical properties are characteristic and applied to the refractory materials, the alloying elements in the steel, and electric devices. Molybdenum compounds were also reviewed. Recycling problems were pointed from energetic and economic aspects.

18: Progress of Titanium Refining and its Future

チタン製錬技術の歩みと展望

Tetsushi N. Deura and Katsutoshi Ono

Metals and Technology, vol.67 No.9 (1997) pp.757-762

金属, vol.67 No.9 (1997) pp.757-762

Histrory of titanium refining was reviewed from its discovery to the current industrial refining processes. Hunter process with sodium reduction and Kroll process with magnesium reduction were compared from technical aspects. Some epoc making refining ideas were summarized, and their difficulties for industrial application were reviewed. Titanium chloride should be base materials for metallic titanium because of impurity removal, thermodynamic requirements, and economical operation. Future work will be forcused on the continuous refining process such as the application by molten salt chemistry.

19: The Prospect of Energy Demand in China Based on the General Trends of GDP and Energy Consumption

ＧＤＰとエネルギー消費動向から推測した中国のエネルギー需要見通し

Takashi Nishiyama and Jie Liu

Journal of Japan Society of Energy and Resources, Vol.18, No.4, pp.346-351, 1997

エネルギー・資源、第18巻、第4号、pp.346-351、1997

Short-term projections for energy consumption in China were made based on statistical data such as energy consumpution and GDP. The results were as follows: (i)The consumption of energy resouces in China has been increasing sharply with recent economic success. Energy consumption is characterized by a remarkably large share of energy from fossil fuels coming from coal. (ii)A linear relationship between per capita GDP and per capita energy consumption in the world in 1991 was found. According to an extrapolation of this trend and annual GDP growth rates of 8.6consumption in China in the future was calculated. The amount of energy consumption in China will increase from 1.2 billion tce (tonnes of coal equivalent) in 1992 to 4.2 billion tce in the year 2005, and to 6.0 billion tce in 2010. A huge amount of energy would be needed to support the Chinese society. A problem of how to supply the huge amount of energy will become serious not only in China but also in the world in the near future.

20: Trends and Prospects for Supply and Energy and Minerals

長期的視点からの資源問題の行方

Takashi Nishiyama

Journal of Japan Society of Energy and Resources, Vol.19, No.1, pp.23-28, 1998

エネルギー・資源、第19巻、第1号、pp.23-28、1998

The annual output of energy and minerals has increased dramatically over the past 100 years. In general, there are three components of growth of energy and mineral consumption, the increasing population, the rising standard of living and the advance of technology. Energy and mineral consumption increases with increasing population. The world's population continues to grow rapidly driven by very high growth rates in the developing countries, although growth rates have dropped sharply in the developed countries. However, the per capita consumption of energy in developed countries is remarkably high, while that in developing countries is low. The amount by which energy consumption increases due to population growth is low compared with the growth rate of the world's population. The per capita consumption of energy in industrialized countries is high, while that in developing countries is low. If the living standard of India or China with large populations equal to that of the U.S., a huge amount of energy would be needed to support that society. The growth rate of energy consumption will be affected most by rising standards of living. Energy from fossil fuels accounts for more than 90energy consumption. Considering the heavy dependence on fossil fuels, there is serious concern over their depletion and the destruction of the environment. In the future, the use of alternative energy resouces such as hydroelectric schemes, nuclear energy and geothermal steam, must increase because fossil fuels can not continue to bear such a large burden for very long.

D. Books

D．著書

Chapter 4

Books

1: Preventing Global Warming -Change the Economic System in the 20th Century-

地球温暖化を防ぐ — 20 世紀型経済システムの転換—

Takamitsu Sawa .
佐和　隆光

1997 / 11 / 20　published

In this book the global warming problem is discussed from the economic point of view. As the economic development necessarily requires more or less the increase of energy consumption, there exists a strong linkage between economic growth and emissions of carbon-dioxide, which causes the global warming. Therefore, the global warming should attract more economists' concerns. So far, however, quite few economists are involved in the research of economic consequences of various economic policies to combat global warming. Indeed, some people believe and advocate that introduction of the carbon tax, for instance, will seriously damage the economy, but this is not necessarily true due to several reasons mentioned in this book. Moreover, international frameworks such as emission trading, and joint implementation are fully explained and discussed. In addition, it is discussed what kinds of transformation of civilization are required to realize what is called sustainable development in the coming 21st century.

2: Medicinal Chemistry: Today and Tomorrow (Ed. by Mikio Yamazaki), "Chemical aspects of artificial gene regulatory molecules"

K. Makino .

Blackwell Science . :

1997 / /　published

This short article (p.227-231) describes our recent trial to build artificial gene regulatory molecules, oligonucleotides and peptides, which bind to the target mRNA and DNA, respectively.

3: Modern Applications of EPR/ESR (Ed. C. Z. Rudowich), "Redox behavior of 5,5-dimethyl-1-pyrroline-N-oxide (DMPO) as studied by electrochemical-ESR measurement"

K.Tajima, N. Endo, K. Kanaori, and K. Makino .

Springer . :

1998 / / published

4: Handbook on Fine Ceramics Technology

ファインセラミックス技術ハンドブック

Toshihiko Hoshide (co-editor, co-author) .
星出 敏彦 (共編, 共著)

Uchida Rokakuho Publishing Co., Ltd. . : 内田老鶴圃

1998 / 02 / 28 published

The book deals with the state of the arts on technologies of fine ceramic materials. Fundamental properties of ceramic strength are stated as follows; methodologies of fracture mechanics and statistical analyses, fracture mechanics properties, static strength, strength properties under static loading, fatigue strength and impact strength behaviours. Friction and wear characteristics of ceramic materials are also described. Some evaluation technologies as residual stress measurement, detecting method of inherent flaws and proof testing are introduced as well as standards related to ceramics in JIS. Methodology of mechnical design of ceramic components is dealt with in detail. Examples of practical design on mechanical components are mentioned about spindle for machining, bearing, mechanical seals, pneumatic guide, turbocharger, block gauge, chemical gear pump, heat exchanger, plug, and so on. Modification of ceramics, joining and coating techniques are also stated as related application technologies. Several mechanical properties of ceramics in manufacturers' catalogs are summarized in the appendix.

5: Thermodynamics

材料科学のための熱力学入門

Yasutaka Iguchi, Hiromasa Kaneko, Masanori Iwase and Itsuki Yasumatsu .
井口泰孝、金児紘征、岩瀬正則、泰松　斉

Kodansha Scientific . :　講談社サイエンティフィック

/ /　　published

This book is intended for use in an initial one-semester course in "materials" thermodynamics, although it could be used for self-study or as a supplement to a text selected for a two-semester undergraduate-graduate sequence. Each chapter is designed so that the student can learn to use thermodynamics as a problem solving tool for a broad range of materials applications. The book is written from notes developed in a course entitled "Thermodynamics of Alloys." Although this course was originally designed as an elective in mechanical engineering at the University of Nebraska-Lincoln, the broader perspective of thermodynamics of materials has emerged as a result of student contacts in earth science, mechanical, chemical and corrosion engineering, and electrical materials. For many scientists and engineers, thermodynamics may be most useful for applications where quickly obtained numerical estimates are all that is needed. Such a situation may prevail for those working in materials-related areas where the generation of thermodynamic data is not an objective in itself. The earth scientist , for example, may need to interpret the stability of mineral assemblages in a rock by using thermodynamic data available in the literature. On the other hand, metallurgists and chemists as well as mechanical, electrical, and materials engineers may be concerned with elevated temperature phase equilibria, phase transformations, and environmental reactions. For the corrosion and chemical engineer, the concept of potential (EMF) is very important in corrosion control as it relates to the Nernst Equation and associated "Pourbaix" diagrams. Fundamentals of classical thermodynamics are briefly reviewed and systematically introduced into problem solving using "thermodynamic loop" or TL analysis. This concept, derived from Kirchhoff's law, is analogous to cyclic analysis used to evaluate engine performance in mechanical systems. Virtually all material thermodynamic applications can be analyzed by TL analysis. TL analysis is a method of organization whereby the known state of a system is combined with thermodynamic properties of materials obtainable from the literature to calculate system properties in another state. TL analysis is a powerful analytical tool because it divides a problem into parts and graphically structures it in such a manner as to provide the student with a clearly depicted solution path. In addition, TL analysis eliminates some of the need for memorizing detailed formulas because it can be used to derive them. Extensive use of TL analysis is a unique feature of this book.

6: Introduction to Heat Flow

熱の流れ

Natsuo Hatta .
八田　夏夫

Morikita Shuppan . : 森北出版

1997 / 04 / 30 published

This book is designed to serve both as a text for students and as a reference for practicing engineers. The problem of heat transmission is encounterd in almost every industrial field, and because of the diversity in the field of application, there exist countless differences in detail. However, the principles underlying the problem are everywhere the same, and it is the purpose of this book to present fundamentals rather than to deal with the details of special problems. The book consists of seven chapters. The first chapter treats the phase change of materials occuring depending upon temperature. The second chapter is concerned with fundamentals of thermodynamics. The subjects of thermodynamics and heat transfer are highly complementally. Heat transfer is an extension of thermodynamics in that it considers the rate at which energy is transported. The third chapter is physical basis of heat transfer by conduction, convection and radiation and emphasizes the important role played by the requirement of energy conservation. The fourth chapter provides a detailed introduction to the conduction process. The general forms of the conduction heat equation are developed and unsteady conduction, as in the heating and cooling of solids, is considered with some numerical solution methods. The fifth chapter serves as an introduction to convection. Because of the important relation between fluid motion and forced convection, the initial parts of the chapter are devoted to fluid dynamics. The methods for computing the heat transfer rate in internal flow in a pipe and external flow over a plate are presented in detail. In sixth chapter the means by which thermal radiation is generated, the specific nature of the radiation, and the manner in which the radiation interacts with matter are described and then means for computing radiative exchange between two or more surfaces. In the last chapter we focus on convection process associated with the change in phase of a liquid.

7: FREE ELECTRON LASER AND ITS APPLICATION IN ASIA

T. Yamazaki, K. Yamada*, N. Sei*, H. Ohgaki*, S. Sugiyama*, R. Suzuki*, T.Mikado*, T.Noguchi*, M.Chiwaki*, T.Ohdaira*, M.Kawai**, and M.Yokoyama**

* Electrotechnical Laboratory

** Kawasaki Heavy Industries Ltd. .

Ionics Publishing Co., Ltd., Tokyo, pp.9-16 . :

1997 / 01 / published

The tunable region of the free-electron-laser (FEL) wavelength with the NIJI-IV system is now 348-595 nm. The net gain at around 300 nm is quite close to the threshold. Recently, the FEL pulse structure and FEL power have been measured at 488 nm. The peak and average output power with a 2.9-mA electelectron beam was observed to be 1.2 W and 39 mW, respectively, which correspond to 38-kW

intracavity power. A simple active-feedback system has been tested and it successfully suppressed the coupled-bunch instability. A combined sextupole-quadrupole-sextupole magnet system with compact sizes is now being prepared to compensate for the chromaticity and suppress the head-tail instability. As to the optical cavity, saturation of the volume degradation of mirrors has been observed. Design work of a new cavity-dump method is also under way to obtain high output power. A preparatory experiment and design work for generating high-brightness x-ray beam from FEL-Compton backscattering are under way. For the future, a quasi-isochronous storage ring STERAS and FELs with the ring are in the stage of design work.

List of Academic Staff

教官名簿

Chapter 5

List of Academic Staff

March 31, 1998

Department of Socio-Environmental Energy Science

PROFESSORS:

SHINGU, Hideo	SAWA, Takamitsu	SAKA, Shiro
MAKINO, Keisuke	YOSHIKAWA, Hidekazu	KASAHARA, Mikio
KANDA, Keiji	NISHIHARA Hideaki	KAYA, Yoichi (Visiting P)

ASSOCIATE PROFESSORS:

ISHIHARA, Keiichi	NAGATA, Yutaka	KAWAMOTO, Haruo
OOTUKI, Toru	TEZUKA, Tetsuo	TOHNO, Susumu
NAKAGOME, Yoshihiro	BESSHO, Yasunori (Visiting AP)	

INSTRUCTORS:

MIYAFUJI, Hisashi	SHIMODA, Hiroshi	YAMAMOTO, Kouhei
ONO, Koichi	FUJINE, Shigenori	TAKEUCHI, Takayuki
HAYASHI, Masatoshi		

Department of Fundamental Energy Science

PROFESSORS:

ITO, Yasuhiko	YOSHIDA, Katsukuni	YAO, Takeshi
FUJISHIMA, Akira (Visiting P)	WAKATANI, Masahiro	KONDO, Katsumi
MAEKAWA, Takashi	OBIKI, Tokuhiro	SANO, Fumimichi
OGATA, Yukio	HARADA, Makoto	OHKUBO, Taketoshi
KATAGIRI, Akira	SHIROYA, Seiji	MISHIMA, Kaichiro

ASSOCIATE PROFESSORS:

HAGIWARA, Rika
ITOH, Sumiko
TOMII, Yochi
UCHIMOTO, Yoshiharu
YOSHIDA, Zensho
HAMAGUCHI, Satoshi
NAKAMURA, Yuji
TANAKA, Hitoshi
MIZUUCHI, Tohru
HANATANI, Kiyoshi
KINOSHITA, Masahiro
MISAWA, Tsuyoshi
HIBIKI, Takashi

LECTURERS:

ADACHI, Motonari

INSTRUCTORS:

NAKASUGA, Masahiko
BESSHOU, Sakae
NAGASAKI, Kazunobu
OKADA, Hiroyuki
SAKKA Tetsuo
SHIOI, Akihisa
HARADA, Toshio
MIZUTANI, Yasuo
KOBAYASHI, Keiji
UNESAKI, Hironobu
SAITO, Yasushi

Department of Energy Conversion Science

PROFESSORS:

IKEGAMI, Makoto
SHIOJI, Masahiro
INOUE, Tatsuo
MATSUMOTO, Eiji
INOUE, Nobuyuki
YOSHIKAWA, Kiyoshi
KIMURA, Akihiko
MAUGIN, Gerard(Visiting P)

ASSOCIATE PROFESSORS:

ISHIYAMA, Takuji
IMATANI, Shoji
HOSHIDE, Toshihiko
YAMAMOTO, Yasushi
OHNISHI, Masami
NAITO, Shizuo

LECTURERS:

TAMAGAWA, Masaaki

INSTRUCTORS:

KAWANABE, Hiroshi
TSUTSUMI, Mitsuyoshi
JINBO, Kouichi
YAMAMOTO, Masahiro

Department of Energy Science and Technology

PROFESSORS:

NOZAWA, Hiroshi
SHIOTSU, Masahiro
ONO, Katsutoshi
IWASE, Masanori
NISHIYAMA, Takashi
HATTA, Natsuo
YAMAZAKI, Tetsuo
KOHYAMA, Akira
MIYAZAKI, Kenzo
IKEUCHI, Kenji(Visiting P)

ASSOCIATE PROFESSORS:

TANAKA, Isao	SHIRAI, Yasuyuki	SUZUKI, Ryosuke
FUJIWARA, Hiroyasu	KUSUDA, Hiromu	TAKUDA, Hirohiko
FUKUNAKA, Yasuhiro	CHIBA, Meiro	KATOH, Yutai

INSTRUCTORS:

UEDA, Yukitomi	Youqing Chen	FUJIMOTO, Hitoshi
KUSAKA, Eishi	YAMAMOTO, Masao	TAKEUCHI, Yuuto
HATA, Koichi		

エネルギー科学研究科教官名簿

1998/03/31 現在

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京都大学「エネルギー科学研究」第１集
の訂正のお願い

京都大学 エネルギー科学研究科 基盤整備委員会

平成９年１２月に御査収いただきました、京都大学「エネルギー科学研究」第１集の下記の記事につきまして、訂正したものを次ページ以降に綴じ込みました。誠にお手数ではございますが、差し替え (全７ページ分) をお願い申し上げます。

1. Contents : xvi ページ
2. Chapter 1: Current Research Fields 6 ページ
3. Chapter 4: Books 189 - 192 ページ

なお、本研究科では年度毎の研究実績等のデータベースを WEB 上で構築、公開しております。(URL address == http://www.energy.kyoto-u.ac.jp/syllabus/KENKYU/) 御利用いただけましたら幸いです。

b7-4	Divertor Study	ダイバータ基礎研究
b7-5	Study of Plasma Production and Heating by Electron Cyclotron Wave	電子サイクロトロン波によるプラズマ生成・加熱の研究
b7-6	Study of Plasma Heating by Neutral Beam Injection	高速中性粒子によるプラズマ加熱の研究
b8-1	Study on High Temperature Plasma Heating and Confinement	超高温プラズマの加熱・閉じ込めに関する研究
b8-2	Experimental Analysis on Vacuum Magnetic Field Structure	真空磁場配位の実験構造解析
b8-3	Development of Monte Carlo Calculation Scheme for the Simulation of Plasma Transport and Heating	プラズマの輸送と加熱のシミュレーションのための新しいモンテカルロ計算スキームの開発
b8-4	Theoretic Analysis on Charged Particle Orbit in the None-axisymmetrical Torus with Adiabatic Constants	非軸対称トーラスにおける荷電粒子軌道の断熱不変量をもちいた理論解析
b8-5	Study on the Advanced Heliotron Magnetic Field with the Control of Chaotic and Statistic Characteristics	磁力線のカオスや統計的性質の制御に基づいたヘリオトロン磁場の高性能化に関する研究
b8-6	Study on the Optimization of Ion Cyclotron Heating Antenna for Various Heating Modes	イオンサイクロトロン加熱の加熱モードによるアンテナ最適化の研究
b9-1	Infrared Photochemical Reaction of Haloalkanes	ハロアルカン類の赤外光化学反応
b9-2	Hydrogen in and on Inorganic Solid Materials	無機固体材料中の水素の挙動
b9-3	Microstructure of Porous Materials and Their Physicochemical Properties	多孔質材料の微細構造と物理化学特性
b9-4	Laser Ablation of Inorganic Solid Surfaces	固体材料表面のレーザーアブレーション

9: Electrochemical Technology (-Inovation and New Developments-)

N. Masuko, T. Osaka , Y. Ito eds. .

Kodansha & Gordon and Breach Publishers . :

1996 / / published

In recent decades the electronic industry has undergone a rapid evolution towards microscale

10: Introduction to Fluorine Chemistry(-Fundamentals and Experiments-) Inorganic, (1)Chapter 3 1.3.2 $S_2O_6F_2$ and (2)Chapter 3, 2.1 Fluorides and fluorocomplexes of silver

フッ素化学入門 (ー基礎と実験法ー) 無機化学編、(1) 第３章１．３．２ $S_2O_6F_2$, (2) 第３章２．１ 銀のフッ化物、フルオロ錯体

Rika Hagiwara .
萩原理加

Nikkan Kogyo Shimbun Co., Ltd. . : 日刊工業新聞社

1997 / 03 / 01 published

(1) Chapter3, 1.3.2 $S_2O_6F_2$
Preparation, physical and chemical properties of peroxydisulfuryl difluoride, $S_2O_6F_2$ are described. A convenient preparative method in the labolatory starting from xenon difluoride and fluorosulfonic acid are described in detail. (in Japanese)

(2) Chapter 3, 2.1 Fluorides and fluorocomplexes of silver
Preparative methods, physical and chemical properties of all the binary fluorides of silver are described in detail. Preparative, structural and chemical aspects of the complexes of silver(II) fluorocations and silver (II, III) fluoroanions are comprehensively reviewed. (in Japanese)

11: Microstructures and Functions of Matter

物質における微細構造と機能

Makoto Harada (Ed.) .
原田 誠 (編者)

The Society of Chemical Engneers Japan . : 化学工学会

1996 / 02 / 22 published

In this series, rapid communication of recent research works in chemical engineering field were compiled for the formation of self-organised microstructure and its function, by focussing on amphiphilic molecular systems, polymer and membrane systems, particulate system, inorganic reaction media, and clusters near critical point. The methodology concerned with microstructure formation by cooperative motion of molecules were also reviewed.

12: Photocatarysts for unti-pollution and sterilization

防汚・殺菌効果の光触媒 先端材料事典, 第 9 章 3 節

藤嶋 昭

. : 光機能性無機材料

1996 / / published

13: Corrosion of iron

鉄の腐食

藤嶋 昭

. : 丸善出版

1996 / / published

14: Photo Clean Revolution

光クリーン革命 酸化チタン光触媒が活躍する

藤嶋 昭、橋本和仁、渡部俊也

. : シーエムシー出版

1997 / / published

This is a guide of photocataritic TiO_2. (In Japanease)

15: Combustion in Internal Combustion Engines

内燃機関の燃焼

Makoto Ikegami .
池上　詢（共著）

.: (社) 日本伝熱学会編 (黒崎晏夫監修), エネルギー新技術体系, エヌ・ティー・エス, p105-115.

1996 / 08 / published

Fundamentals and recent progress in the combustion science and technologies of reciprocating internal combustion engines are given with special regard to fuel economy and environmental protection. For the spark-ignition engine, the in-cylinder turbulence and its effect on the flame propagation are described in depth. Also, explanations are made for the formation and destruction of air pollutants, such as unburned hydrocarbons and nitrogen oxides. For the diesel combustion, roles of spray, mixture formation, ignition delay, the subsequent rapid burning and non- premixed burning are mentioned, together with formation of pollutants such as nitrogen oxides and particulate matter. (in Japanese)

16: Metals Resources, Smelting and Recycling

金属の資源・製錬・リサイクル

西山　孝（共著：長井　寿　編著）

.: 化学工業日報社

1996 / 07 / 24 published

17: "Infrared Semiconductor Laser by Means of J x H Force Excitation of Holeds" Elec (Amazing Light, A Volume Dedicated to Charles Hard Townes on His 80th Birthday, ed. R. Y. Chiao, Springer, New York, 1996) pp.497-505.

T. Morimoto. M. Chiba and G. Kido .

Springer, New York . :

1996 / / published

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代表者　伊藤靖彦

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