

Table of Contents

Preface, Organizing Committee and Sponsors

Plenary

Physics on the Top of the Tip: Atomic Transport and Reaction in Nano-Structured Materials

- G. Schmitz, D. Baither, Z. Balogh, M.R. Chellali, G.H. Greiwe, M. Kasprzak, C. Oberdorfer, R. Schlesiger and P. Stender 3

Formation and Migration Energy of Native Defects in Silicon Carbide from First Principles: An Overview

- G. Roma, F. Bruneval, L.A. Ting, O.N. Bedoya Martínez and J.P. Crocombette 11

Diffusion Aspects in High Temperature Corrosion and in the Development of Protective Coatings

- M. Schütze 19

Grain Boundary Diffusion, Stresses and Segregation

- B.S. Bokstein 31

Chapter 1: Diffusion Fundamentals

Entropy Production and Stress–Deformation Effect on Interdiffusion

- M. Danielewski 43

Kirkendall Effect during Grain Boundary Interdiffusion in Polycrystalline Thin Films

- L. Klinger and E. Rabkin 49

Flux Driven Nucleation at Interfaces during Reactive Diffusion – New Solution of an Old Problem

- A. Gusak, G. Schmitz and N. Storozhuk 55

Determination of Diffusion Coefficients with Quantitative X-Ray Microanalysis at High - Spatial Resolution

- R. Gauvin, N. Brodusch and P. Michaud 61

A SIMS Study on Li Diffusion in Single Crystalline and Amorphous LiNbO₃

- J. Rahn, E. Hüger, E. Dörrer, B. Ruprecht, P. Heitjans and H. Schmidt 69

²⁶Al Tracer Diffusion in Nominally Undoped Single Crystalline α -Al₂O₃

- P. Fielitz, G. Borchardt, S. Ganschow and R. Bertram 75

Numerical Aspects of Electrodiffusion Problem Based on Nernst-Planck and Poisson Equations

- J. Fausek, K. Szyszkiewicz and R. Filipek 81

Chapter 2: Numerical Studies

Study of the Reactive Dynamics of Nanometric Metallic Multilayers Using Molecular Dynamics : The Al-Ni System

- A. Linde, O. Politano and F. Baras 89

Atomistic Simulation of Clustering and Annihilation of Point Defects in Molybdenum

- A. Yanilkin, Z. Insepov, G. Norman, J. Rest and V. Stegailov 95

Multiscale Modelling of Morphological Evolution of Rough Surface during Superficial, Volume and Evaporation-Condensation Diffusions

- M. Bigerelle, J. Favregeon, T. Mathia and A. Iost 101

Simulation of Metal/Oxide Interface Mobility: Effects of Mechanical Stresses on Geometrical Singularities

- V. Optasanu, L. Raceanu and T. Montesin 109

High Temperature Diffusion Processes at the Metal/Slag Interface

- A. Bogusz and P.J. Masset 115

Modeling of Fractional Diffusion on a Catalytic Particle under Different Flow Conditions	121
A.R. Carella and C.A. Dorao	
Modeling of Multi-Phase Solid State Reactions-Case of IMC Growth	127
M. Pawełkiewicz, M. Danielewski, J. Janczak-Rusch and B. Wierzba	
Fractal Dimension of Grain Boundary during Heating Comparison between Images Analyses and Monte Carlo Simulation	133
M. Bigerelle, J. Favregeon and A. Iost	
A Reactive Force Field Molecular Dynamics Simulation Study of Corrosion of Nickel	139
O. Assowe, O. Politano, V. Vignal, P. Arnoux and B. Diawara	

Chapter 3: Nanomaterials and Grain Boundaries

Structural Re-Organization Kinetics of Nanocrystalline Pt Films during <i>In Situ</i> Annealing	149
W. Gruber, S. Chakravarty, C. Baehtz and H. Schmidt	
Determination of Grain Boundary Diffusion Parameters Based on Combined Analysis of Radiotracer Technique and Mössbauer Spectroscopy Data	155
V.V. Popov	
Grain Boundary Diffusion of Silver in Copper-Iron Alloys	161
D.V. Vaganov, S. Zhevnenko and Y. Terentyev	
Grain Boundary Diffusion. Effect of Segregation or Concentration Dependence of Diffusivity	165
A. Rodin, N. Dolgopolov and S. Kryukov	
About Fe Diffusion in Cu	171
D. Prokoshkina, A. Rodin and V. Esin	
The Formation of Liquid Metal Channels Network under Grain Boundary Wetting in the Cu-Bi System	177
A.A. Novikov, A.L. Petelin, B.S. Bokstein, S.N. Zhevnenko and D.I. Orelkina	

Chapter 4: Nuclear and Alternative Energies

Surface Blistering and Flaking of Sintered Uranium Dioxide Samples under High Dose Gas Implantation and Annealing	185
G. Martin, G. Carlot, P. Desgardin, M. Vayer, C. Ramboz, T. Sauvage, P. Moretto, H. Khodja and P. Garcia	
A TEM Study of Bubbles Growth with Temperature in Xenon and Krypton Implanted Uranium Dioxide	191
A. Michel, C. Sabathier, G. Carlot, M. Cabié, S. Bouffard and P. Garcia	
Iodine Volume Diffusion Measurements in Uranium Dioxide	197
E. Pizzi, P. Garcia, G. Carlot, H. Palancher, S. Maillard, B. Pasquet, I. Roure, C. Pozo and C. Maurice	
Towards Measuring the Pu Self-Diffusion Coefficient in Polycrystalline $U_{0.55}Pu_{0.45}O_{2\pm x}$	203
S. Noyau, P. Garcia, B. Pasquet, I. Roure, F. Audubert and A. Maître	
Modelling Fission Gas Bubble Distribution in UO_2	209
R. Skorek, S. Maillard, A. Michel, G. Carlot, E. Gilabert and T. Jourdan	
Molecular Dynamics Study of Grain Boundary Diffusion of Fission Gas in Uranium Dioxide	215
K. Govers, S.E. Lemehov and M. Verwerft	
Helium Behaviour in Fe-Base Materials: Thermal Desorption and Nuclear Reaction Analyses	221
H. Lefaix-Jeuland, S. Miro and F. Legendre	
Specific Aspects of Internal Corrosion of Nuclear Clad Made of Zircaloy	227
J.B. Minne, L. Desgranges, V. Optasanu, N. Largenton, L. Raceanu and T. Montesin	
A Density Functional Study of Oxygen Mobility in Ceria-Based Materials	233
C. Frayret, A. Villesuzanne, M. Pouchard, F. Mauvy, J.M. Bassat and J.C. Grenier	
Optimisation of Metallic Interconnects for Hydrogen Production by High Temperature Water Vapour Electrolysis	239
M.R. Ardigo, V. Parry, I. Popa, S. Chevalier, W. Chandra-Ambhorn, P. Phakpeetinan and Y. Wouters	

Development of Diffusion Coatings to Optimise the High Temperature Corrosion Resistance of Fuel Cell Reformer Materials

A. Naji and M. Schütze

245

Elaboration of Uranium Monocarbide Samples for Diffusion Studies

O. Fiquet, L. Da-Silva, F. Garcia-Ferre, M. Brothier, G. Carlot, P. Garcia, G. Martin and M.F. Barthe

253

Chapter 5: Diffusion in Non Metallic Systems

Influence of Carbonation and Chemical Activity of Water on Coupled Moisture-Ion Transport in Cementitious Materials

X.M. Wang, M. Thiéry and V. Baroghel-Bouny

263

Controlling the Molecular Interactions to Improve the Diffusion Barrier of Biosourced Polymers to Organic Solutes

X.Y. Fang, O. Vitrac, S. Domenek and V. Ducruet

269

Recycling, Recovery and Improvement of Properties of Ceramic Tile Manufacturing by Adding Two Types of Glass in Clay Mixtures

H. Chemani

275

Chapter 6: Diffusion and Corrosion Processes

Diffusion in Internal Oxidation Reactions

D.J. Young

283

Determination of Diffusion Coefficients Using Thermogravimetric Measurements during High Temperature Oxidation

P. Berthod and L. Aranda

289

The Transition from Internal to External Oxidation of Ni - X Wt.% Cr at 950°C

A. Nicolas, E. Aublant, E. Feulvarch and K. Wolski

295

Corrosion Behaviour of Ti-48Al-2Nb-2Cr Alloys

B. Pelic, D. Rafaja, P.J. Masset, H.J. Seifert, L. Bortolotto, M. Schütze, G. Wolf and I. Loeh

301

Influence of Water Vapour on a Nickel-Based Alloy Oxidation

H. Buscail, R. Rolland, C. Issartel, F. Riffard, F. Rabaste and S. Perrier

309

On the Defect Structure and Transport Properties of NiS₂

Z. Grzesik, A. Poczekajło and S. Mrowec

315

Kinetics and Mechanism of High Temperature Internal Oxidation of Ni-14wt%W Alloy at 1000°C

P. Ganster, B. Pujilaksono and K. Wolski

321

Corrosion of Valve Steels in Combustion Gases of Diesel Engines under Thermal Shock Conditions

Z. Grzesik, K. Adamaszek, Z. Jurasz and S. Mrowec

327

Influence of Water Vapour on Isothermal and Thermal Cyclic Oxidation Conditions of a Nickel-Based SY625 Steel at 1100°C

R. Rolland, H. Buscail, C. Issartel, F. Riffard, F. Rabaste and S. Perrier

333

Determination of Oxygen Diffusion Coefficient in Oxidation Films of the AISI 439 Ferritic Stainless Steel

A.C.S. Sabioni, E.A. Malheiros, V. Ji and F. Jomard

339

Oxygen Diffusion Study in Oxidation Films of the AISI 304 Austenitic Stainless Steel

A.C.S. Sabioni, R.P.B. Ramos, V. Ji and F. Jomard

345

High Temperature Corrosion Behavior of Si-Containing Alloys in the Liquid Phase of Na₂SO₄ 25.7 Mass% NaCl

T. Sudiro, T. Sano, S. Kyo, O. Ishibashi, M. Nakamori and K. Kurokawa

353

Effect of Phosphoric Acid Treatment on Isothermal High Temperature Oxidation Behaviour of AISI 304 Stainless Steel at 800°C

F. Riffard, H. Buscail, F. Rabaste, C. Issartel and S. Perrier

359

Chapter 7: Diffusion in Coatings and Thin Films

Optimisation of Nickel Aluminising by CVD	367
P.J. Masset, A. Bogusz, J. Sieniawski, B. Wierzba and K. Tkacz-Śmiech	
On the Influence of a Heat Treat for an Aluminizing Progress Based on Al Microparticles Slurry for Model Ni and Ni20Cr. Experimental and Theoretical Approaches.	367
B. Rannou, M. Mollard, B. Bouchaud, J. Balmain, G. Bonnet, V. Kolarik and F. Pedraza-Diaz	373
Initial Aluminizing Steps of Pure Nickel from Al Micro-Particles	381
G. Bonnet, M. Mollard, B. Rannou, J. Balmain, F. Pedraza-Diaz, X. Montero, M. Galetz and M. Schütze	
Plasma Assisted Diffusion in Porous Materials: Experiments, Modeling and Applications	387
P. Brault, J.M. Bauchire, F. James and C. Josserand	
Assessment of the Gas Permeation through Thin Coated Polymeric Membranes; Improvement of the Gas Barrier Ability for Hydrogen Storage	393
D. Chapelle, L.P. Feng, P. Nardin and J.Y. Rauch	
Modelling of the Growth of Fe₂B Layers in AISI 1018 Steel	401
Z.N. Abdellah, M. Keddam and A. Elias	
New Materials for Hydrogen Distribution Networks: Materials Development & Technico-Economic Benchmark	407
M.H. Klopffer, P. Berne, M. Weber, S. Castagnet, G. Hochstetter and E. Espuche	

Chapter 8: Diffusion in Electronic Materials

Diffusion and Redistribution of Boron in Nickel Silicides	415
I. Blum, A. Portavoce, L. Chow, K. Hoummada and D. Mangelinck	
Reactive Diffusion of Thin Si Deposits into Ni (111)	421
B. Lalmi, C. Girardeaux, A. Portavoce, B. Aufray and J. Bernardini	
From Contact to Diffusion Controlled Growth of Nickel Silicides in Silicon Nanowires	427
A. Katsman, Y. Yaish and M. Beregovsky	
Nanometric-Size Effect upon Diffusion and Reaction in Semiconductors: Experimental and Theoretical Investigations	433
A. Portavoce, C. Girardeaux, G. Tréglia, J. Bernardini, D. Mangelinck and L. Chow	
Effect of Mn Thickness on the Mn-Ge Phase Formation during Reactions of 50 nm and 210 nm Thick Mn Films Deposited on Ge (111) Substrate	439
O. Abbes, F. Xu, A. Portavoce, C. Girardeaux, K. Hoummada and V. Le Thanh	

Chapter 9: Diffusion in Alloys and Intermetallics

Diffusion in Binary and Pseudo-Binary L1₂ Indides, Stannides, Gallides and Aluminides of Rare-Earth Elements as Studied Using Perturbed Angular Correlation of ¹¹¹In/Cd	447
R. Newhouse, J. Minish and G.S. Collins	
Diffusion in La_nCoIn_{3n+2} Phases Studied by Perturbed Angular Correlation	453
R. Newhouse and G.S. Collins	
Diffusion Mechanism in XSi₂ and X₅Si₃ (X= Nb, Mo, V) Phases	459
S. Prasad and A. Paul	
Growth Kinetics of Intermetallic Phases in Transient Liquid Phase Bonding Process (TLPB) in Al /Ni System	465
S. Tumminello and S. Sommadossi	
Nitrogen Diffusion at Low Temperature in fcc Materials Deformed by Attrition Peening	471
T. Thiriet, T. Czerwiec, D. Hertz, G. Marcos, T. Toll-Duchanoy, S. Migot, B. Brugier, M. Foucault and T. Belmonte	
SIMS Analysis of Deuterium Absorption and Diffusion in Austenitic Fe-Mn-C Steels	477
T. Dieudonné, L. Marchetti, F. Jomard, M. Wery, J. Chêne, C. Allely, P. Cugy and C.P. Scott	
Hydrogen Transport in 34CrMo4 Martensitic Steel: Influence of Microstructural Defects on H Diffusion	485
L. Moli-Sanchez, F. Martin, E. Leunis, J. Chêne and M. Wery	
Interdiffusion in Nb-Mo, Nb-Ti and Nb-Zr Systems	491
S. Prasad and A. Paul	

Diffusion Mechanism in the μ Phase in Nb-X (X= Ni, Co, Fe) Systems	497
S.S.K. Balam, R. Ravi and A. Paul	
The Solubility of Indium in Liquid Gallium Supercooled to 12 K	503
X.Y. Yin and G.S. Collins	
Diffusion Behaviour of the Grain-Growth Inhibitor Vc in Hardmetals	509
M. Brieseck, I. Hünsche, B. Caspers, G. Gille, M. Bohn and W. Lengauer	

Chapter 10: High and Micro Gravity Materials Science

Atomic-Scale Materials Processing under Strong Gravitational Field	517
T. Mashimo	
Sedimentation in Multicomponent Solids	523
B. Wierzba	
Interdiffusion in the Binary Diffusion Couples under a Strong Gravitational Field	529
Y. Ogata, K. Kondo, Y. Sakata, Y. Iguchi and T. Mashimo	
Investigation on Mechanism of Faceted Cellular Array Growth in International Space Station	533
Y. Inatomi, I. Yoshizaki, K. Sakata, T. Shimaoka, T. Sone, T. Tomobe, S. Adachi, S. Yoda and Y. Yoshimura	
Bulk Growth of InGaSb Alloy Semiconductor under Terrestrial Conditions: A Preliminary Study for Microgravity Experiments at ISS	539
M. Arivanandhan, G. Rajesh, A. Tanaka, T. Ozawa, Y. Okano, Y. Inatomi and Y. Hayakawa	
Separation in ϵ-Phase of BiPb Alloy under Mega-Gravity	545
S. Okayasu, M. Ono, T. Nishio, Y. Iguchi and T. Mashimo	
Controlling the Diffusive Field to Grow a Higher Quality Protein Crystal in Microgravity	549
H. Tanaka, K. Inaka, N. Furubayashi, M. Yamanaka, S. Takahashi, S. Sano, M. Sato, M. Shirakawa and Y. Yoshimura	
Gravitational Annealing of Colloidal Crystals	555
Y. Suzuki, J. Endoh, A. Mori, T. Yabutani and K. Tamura	
Compositionally Gradient Thin Film Deposition by Pulse Laser Ablation under High Gravity	559
T. Nishiyama, T. Kajiwara and K. Nagayama	
Numerical Analysis of the Diffusive Field around a Growing Protein Crystal in Microgravity	565
K. Inaka, H. Tanaka, S. Takahashi, S. Sano, M. Sato, M. Shirakawa and Y. Yoshimura	
Interdiffusion in InSb/Zn/InSb System	571
G. Glodán, Y. Iguchi, C. Cserháti, G. Pál, T. Mashimo and D.L. Beke	
Study of the Growth Mechanism of some Oxide Scales on Alloy 230 in High Temperature Vapor Electrolysis (HTVE) Conditions	577
S. Guillou, C. Desgranges and S. Chevalier	