SCIENCE AND TECHNOLOGY OF INTERFACES

International Symposium Honoring the Contributions of Dr. Bhakta Rath
International Symposium Honoring the Contributions of Dr. Bhakta Rath

Proceedings of a symposium sponsored by the Physical Metallurgy Committee, the Titanium Committee and the Mechanical Behavior of Materials Committee (Jt. ASM/MSCTS) of the Structural Materials Division (SMD) of TMS (The Minerals, Metals & Materials Society).


Partial funding for this publication was provided for by the Seeley W. Mudd Fund

Edited by

S. Ankem
C.S. Pande
I. Ovid’ko
S. Ranganathan

A Publication of TMS
# TABLE OF CONTENTS

Preface .......................................................................................................................................... ix

**Nanostructures and Materials**

Challenging Some Free-Energy Reduction Criteria for Grain Growth ........................................ 3  
*S. G. Srinivasan and J. W. Cahn*

Interfaces and Surfaces in Nanostructured Materials ................................................................. 15  
*G. López-Laurrabaquio, J. L. Rodríguez-López, J. M. Montejano-Carrizales and M. José-Yacaman*

Mechanical Alloying in Nanostructured Fe-Zn Binary System .................................................. 21  
*F. Zhou, Y. T. Chou and E. J. Lavernia*

Interfaces in Zr Based Nanocrystals and Combustion Synthesized Ti Aluminide ..................... 33  
*G. K. Dey*

Structure and Properties of Nanostructured Magnetic Films Prepared by Electroless and Sputter Depositions ............................................................................................................. 45  
*G. M. Chow*

**Interface Effects**

Surface Relief Effects as Evidence for Coherency of Interphase Boundaries .............................. 57  
*H. I. Aaronson*

Thermodynamics of Interfaces in Mechanically Alloyed Metals ................................................ 67  
*H. K. D. H. Bhadeshia*

Multicomponent Diffusion at Zero-Flux Planes ......................................................................... 75  
*M. E. Glicksman and A. O. Lupulescu*

Effect of Irradiation-Induced Interfaces on Thin Film Stability .................................................... 87  
*P. M. Ossi*

Interface Diffusion, Energies and Solute Segregations in Materials: A Unified Approach ........ 99  
*D. Gupta*
Mechanical Behavior

The Role of Interfaces on Mechanical Behavior of Titanium Alloys ........................................... 113
   B.W. Neuberger and S. Ankem

Reevaluation of the Environmental Effects at the Crack Tip-Metal Interfaces ......................... 131
   K. Sadananda, R.L. Holtz and A.K. Vasudevan

Hot Ductility in Titanium Alloys – A Review ............................................................................. 141
   M.A. Imam, B.K. Damkroger
   and G.R. Edwards

A New Mechanism for Superplasticity ..................................................................................... 155
   J.C.M. Li

Crystallization Behavior of a Melt-Spun Al$_{86}$Ni$_{13}$Mm$_{5}$ Alloy ............................................. 171
   S.J. Hong, H.S. Kim, C. Suryanarayana
   and B.S. Chun

Modelling of Die-Workpiece Interface During Hot Forging .................................................... 183
   K. Kannan, M. Pandheeradi, S.P. Vaze,
   S.R. Schmid and W.R.D. Wilson

Dislocation and Interfaces

Utility of the Plasmon Theory of Surface and Interfacial Energies ........................................ 197
   J.J. Gilman

The Nature of Interfacial Processes in Friction and Wear ........................................................ 207
   D. Kuhlmann-Wilsdorf

Elastic Interactions of Point Defects with Imperfect Interfaces in Coated
Semi-Infinite Solids ................................................................................................................... 219
   H.Y. Yu

An Informatics Approach to Interface Characterization:
Establishing a “Materials by Design” Paradigm ........................................................................ 231
   K. Rajan

Advanced Materials

Interfaces and Stresses in Nanostructured and High-$T_C$ Superconducting
Materials ................................................................................................................................... 245
   I. Ovid’ko

Grain Boundary Effects in High and Low $T_C$ Superconductors ............................................. 257
   C.S. Pande and R.A. Masumura
Molecular Interfaces and Their Effect on Order in Liquid Crystals

R. Shashidhar and D. Shenoy

Interface Studies in a Quasicrystalline Al-Pd-Mn Alloy

R. Divakar, V.S. Raghunathan
and S. Ranganathan

Semiconductors

Two-Step Epitaxy of Gallium Nitride on (0001) Sapphire

S. Mahajan and V. Narayanan

Epitaxial Issues and Growth Morphologies of InAlAs/InGaAs MQWs and Heterostructures on (100) and non -(100) InP Substrates

A. Christou

Synthetic Functional Oxide Nanostructures: Role of Interfaces

R. Ramesh

Role of Silicide Interfaces in Silicon Technology

F.M. d’Heurle, C. Lavoie and L. Gignac

Silicon-Germanium-Carbon Self Assembled Quantum Dot Growth and Applications in Electronic Memory Devices

D-W. Kim and S. Banerjee

Diamond Surfaces and Interfaces

J.E. Butler

Grain Boundaries

In-Situ Determination of Grain Boundary Migration During Recrystallization

D.J. Jensen, E.M. Lauridsen
and R.A. Vandermeer

Atomistic Aspects of Grain Boundary Fracture

D. Farkas and R.N. Nogueira

Coincidence Site Lattice Theory of Triple Junctions and Quadruple Points

V.Y. Gertsman

Interfacial Phenomena in Clean Steel Processing

S. Sridhar

Author Index

411

Subject Index

413
Atomic structure, composition and properties of interfaces and their effects on the performance of polycrystalline structural materials has been a topic of intensive study for many years. These studies have contributed much of our phenomenological understanding of the behavior of interfaces and have provided valuable guidelines to thermo-mechanical processing of engineering materials for property optimization. Recent advances in materials by design in the submicrometer and nanometer scales for semi- and superconducting electronics, magnetics, biomolecular systems and polymers have revealed the profound effects of interfaces on the performance of functional materials. Due to unprecedented advances in novel processing methods such as MBE, MOCVD, and PLD, among others, characterization tools such as STM, AFM, synchrotron spectroscopy and atom resolved microscopy, combined with advanced first principle computational methods ranging from density functional to improved molecular dynamics methods, researchers can now design novel materials and devices including heterostructures, quantum well devices and superlattice structures. Performance of these devices is a sensitive function of the structure and epitaxy of the interface.

The International Symposium was organized to capture the state of our knowledge on the science and technology of interfaces. The Symposium (in honor of Dr. B. B. Rath) was held during the TMS Annual meeting, Feb 17-21, 2002 at Seattle WA. This volume captures the salient papers presented at the symposium.

The symposium was sponsored by the Structural Materials Division and the Electronic, Magnetic & Photonic Materials Division of TMS and the Materials Science Critical Technology Sector of ASM International and in particular by the following committees: the Physical Metallurgy Committee (TMS), the Superconducting Materials Committee (TMS), the Titanium Committee (TMD) and the Mechanical Behavior of Materials Committee (TMS/ASM). The objective of this symposium was to present current research on advanced interface controlled materials with primary focus on advanced materials. Special attention was given to design of such interface controlled materials with their unique and highly desirable properties. The symposium was designed to assess the current status and to identify future directions of research, design and applications of the role of interfaces in nanostructured bulk solids, films and coatings as well as polycrystalline superconducting materials. Particular emphasis was placed on developing close interactions and fostering future collaborations among scientists and engineers from the USA, Western and Eastern Europe, Russia, and other Asian countries.

The organizers of this symposium were Prof. Ankem [Committee Chairman] of University of Maryland, College Park, Dr. Pande of NRL, Dr. Ovid'ko of Russian Academy of Sciences and Prof. Ranganathan of Indian Institute of Science.

The symposium was dedicated to Dr. Bhakta B. Rath for his pioneering research and for his leadership in the area of Interfaces. Many facets of his research interest in Interfaces were the subjects of various scholarly presentations at this symposium.
Dr. Bhakta B. Rath is Associate Director of Research and Head, Materials Science and Component Technology Directorate of the Naval Research Laboratory. As Head of the Directorate, he is responsible for planning, supervision, and administration of all basic and applied research in structure of matter, condensed matter physics, chemistry, electronics, materials science, plasma physics, computational physics, fluid dynamics, and bimolecular science and technology. The Directorate manages over 240 research projects conducted by a staff in excess of 900 scientists and engineers. Dr. Rath received his BS in Physics and Mathematics in India, MS in Metallurgical Engineering from Michigan Technological University, and Ph.D. from Illinois Institute of Technology. In 1961, he joined the faculty of Washington State University and held a tenured position until 1965. Between 1965 and 1972, he was on the staff of the Edgar C. Bain Laboratory for Fundamental Research of the US Steel Corporation, and from 1972 to 1976, he headed the Metal Physics Research Section of the McDonnell Douglas Research Laboratories. He joined the Naval Research Laboratory in 1976 as Head of the Physical Metallurgy Branch, and in 1982 began serving as Superintendent of the Materials Science and Technology Division. He serves on the editorial board of a number of international technical journals, and on the Board of Directors and Trustees of the American Society of Materials (ASM International), The Materials, Metals and Minerals Society (TMS), and the Federation of Materials Societies (FMS). He has been recognized with a number of awards and honors and was recently selected by the Board of Trustees of ASM and the Board of Directors of TMS to receive their prestigious award, the “2001 Distinguished Lecturer in Materials and Society” and to receive the “2001 ASM Distinguished Life Membership Award.” Dr. Rath was elected to receive the 1999 “Presidential Rank Award,” presented by The President of the United States for sustained outstanding achievements of a senior executive. Invited by the U.S. State Department, Dr. Rath has been one of the primary forces in enhancing research collaborations, developing more than 70 research projects between India and the United States in the broad field of Physical and Materials Sciences. He serves as the Executive Chair for collaboration on defense science in materials and processes between U.S. Department of Defense and the Ministries of Defense of Canada, the UK, Australia and New Zealand.

Though by no means exhaustive, the topics covered in these papers exemplify some of the most important aspects of research in the properties and structure of interfaces and are sure to provide a better understanding of this important field.

We extend our thanks to the TMS Meetings, Member Services and Publication Staff for helping in organizing this symposium and in editing and publishing this volume. Special thanks are due to the Book Publishing Coordinator Mr. Stephen J. Kendall for his support and to various authors for providing us the papers in a timely fashion and helping in making this symposium a productive and exciting one.

S. Ankem: University of Maryland, College Park
C. S. Pande: Naval Research Laboratory
I. Ovid’ko: Russian Academy of Sciences
S. Ranganathan: Indian Institute of Science
AUTHOR INDEX

A
Aaronson, H.I., 57
Ankem, S., 113

B
Banerjee, S., 341
Bhadeshia, H.K.D.H., 67
Butler, J.E., 353

C
Cahn, J.W., 3
Chou, Y.T., 21
Chow, G.M., 45
Christou, A., 297
Chun, B.S., 171

D
d’Heurle, F.M., 329
Damkroger, B.K., 141
Dey, G.K., 33
Divakar, R., 275

E
Edwards, G.R., 141

F
Farkas, D., 375

G
Gertsman, V.Y., 387
Gignac, L., 329
Gilman, J.J., 197
Glicksman, M.E., 75
Gupta, D., 99

H
Holtz, R.L., 131
Hong, S.J., 171

I
Imam, M.A., 141

J
Jensen, D.J., 361
José-Yacaman, M., 15

K
Kannan, K., 183
Kim, D-W., 341
Kim, H.S., 171
Kuhlmann-Wilsdorf, D., 207

L
Lauridsen, E.M., 361
Laavernia, E.J., 21
Lavoie, C., 329
Li, J.C.M., 155
López-Laurrabaquio, D., 15
Lupulescu, A.O., 75

M
Mahajan, S., 287
Masumura, R.A., 257
Montejano-Carrizales, J.M., 15

N
Narayanan, V., 287
Neuberger, B.W., 113
Nogueira, R.N., 375

O
Ossi, P.M., 87
Ovid’ko, I., 245

P
Pande, C.S., 257
Pandheeradi, M., 183

R
Raghunathan, V.S., 275
Rajan, K., 231
Ramesh, R., 309
Ranganathan, S., 275
Rodríguez-López, J.L., 15

S
Sadananda, K., 131
Schmid, S.R., 183
Shashidhar, R., 269
Shenoy, D., 269
Sridhar, S., 399
Srinivasan, S.G, 3
Suryanarayana, C., 171
V
Vandermeer, R.A., 361
Vasudevan, 131
Vaze, S.P., 183

Y
Yu, H.Y., 219

Z
Zhou, F., 21

W
Wilson, W.R.D., 183
SUBJECT INDEX

A
Al-Ni-Mm Alloys, 171
Ambient Temperature Creep, 113
Amorphous Alloy, 171
Avrami Equation, 361

B
Bicrystals, 3

C
Chemical Potentials, 21
Chemical Vapor Deposition, 353
Coalescence, 15-19
  Grain Boundary, 16
  Shape and Structural Changes, 15, 18
Coherency, 57
Coincident Site Lattice (CSL), 387-398
  CSL Boundaries, 388-395
Collision Cascades, 87
Confocal Scanning Laser Microscopy, 399
Critical Currents, 257
Crystallization Behavior, 171

D
Deformation Mechanisms, 113
Diamond Surface, 353
Die-Workpiece, 183
Dielectric Materials, 342-347
  Nitrided Oxide, 343-346
  Oxynitride, 343-345
  Si₃N₄, 343-344
  SiO₂, 343-345
  ZrO₂, 342, 346-347
Differential Scanning Calorimetry, 171
Differential Strength, 141
Diffusion Waves, 75
Dislocation Emission, 375
Dislocation Like Models, 219, 220, 221, 223, 228
Ductile/Brittle Response, 375

E
Elastic Interactions, 219, 220, 228
Electron Microscopy, 171
Embedded Atom, 375
Enthalpy of Bonding, 99

Entropy of Mixing, 335, 336
Environmental Effects
  Corrosion Fatigue, 137-139
  Crack Growth, 131-139
  Fatigue, 131-139
Epitaxial Issues, 297
Epitaxy, 287

F
Finite Element Analysis, 183
Free Energy, 3
Friction and Wear, 207

G
Gold Nanoparticles, 16, 18, 19
Grain Boundaries, 257, 387-398
  Grain-Boundary Dislocations, 346-348
  Grain-Boundary Engineering, 392
  Grain-Boundary Statistics, 395
Grain Boundary, 375
Grain Boundary Energy, 99
Grain Boundary Fluid, 155
Grain Boundary Sliding, 155
Grain Growth, 3
Grain Size Effects, 113
Group III-Nitrides, 287
Growth Morphologies, 297
Growth Parameters, 297
Growth Rate Distribution, 361

H
Hardness, 171
Heisenberg Theorem, 197
High Energy X-Ray, 361
High-Tc Superconductivity
  Critical Current, 251-254
  Grain Boundaries, 245, 251
Hot Ductility Dip, 141
Hot Forging, 183
HREM, 34-41

I
Imperfect Interfaces, 219, 220, 221
Interatomic Potentials, 375
Interfacial Processes, 207
Interfacial Structure, 57
Interface Coherency, 67
Interface Diffusion, 99
Interface Energies, 197
Interfaces, 34-43
Characterization, 234-236
Crystallography, 231-233
Grain Boundary Engineering, 241
Interphase Fluid, 155
Invariant Plane Strain, 57
Iron
Cast Iron
Fatigue, 138-139
Irradiation-Induced Interface, 87
K
Kinetics, 361
Kinetics of Diffusion, 75
L
Lattice Incompatibility, 14
Liquid Crystal Alignment, 269
Liquid Crystal Displays, 269
Liquid Crystals, 269
M
Mechanical Alloying, 21, 67
Microstructure, 33
Modeling, 183
Molecular Dynamics, 15, 16, 19
Molecular Dynamics Simulations, 3
Molecular Interface, 269
Multicomponent Diffusion, 75
N
Nanocomposite, 171
Nanocrystals, 34-38
Nanostructured Films
Anamalous X-Ray Scattering, 49
EXAFS, 48, 53
Magnetic Properties, 45
X-Ray Scattering, 48
Nanostructured Materials, 16
Nanostructured System, 21
Nanostructures
Deformation, 245, 249-251
Grain Boundaries, 245-251
Nanocrystalline Films, 245-249
Nematic Liquid Crystals, 269
Nucleation, 333-337
P
Particulate Solutions, 67
Plasmon Energy, 197
Plasmons, 197
Point Defects, 219-229
Primary Crystallization, 171
Q
Quadruple Points, 387, 388, 391, 392
Quantum Dot
Ge Quantum Dot, 344-345
Growth, 344-345
Image, 343
SiGe Quantum Dot, 346-348
Concentration of Ge, 346
Growth, 346
SiGeC Quantum Dot, 347-349
Doping Effect, 349
XRD Rocking Curve, 349-350
Quantum Dot Flash Memory Device
High Frequency CV, 346-347
SiO$_2$, Metal Insulator Semiconductor, 346-347
ZrO$_2$, Metal Insulator Semiconductor, 346-347
R
Recrystallization, 361
Rule-of-Mixtures Model, 171
S
Segregation-Charge Transfer, 87
Self Assembling Monolayer, 269
Silicides
CoSi$_2$, 334-336
NiSi, 337, 338
TiSi$_2$, 332, 333, 337
Slag/Steel Interface, 399
Slip Planarity, 141
Soft Interfaces, 269
Solute Partitioning, 141
Solute Segregations, 99
Stability of Beta Phase, 113
Statistics
Clustering
Fuzzy Clustering, 237
Hough Transform, 233, 234
Principal Component Analysis, 240
Informatics, 231-240
Steel, 399
  Low Alloy Steel
  Corrosion Fatigue, 138
  Crack Growth, 137
  Fatigue, 137
  Hydrogen Effect, 138
Stress Effects, 21
Surface Energy, 197
Surface Film, 207
Surface Modification, 353
Surface Relief, 57
Surface Roughness, 297
Superalloys, 183
Superconductors, 257
Superplasticity, 155

T
Textures
  Electron Back Scattered Diffraction (EBSD), 233
  Rodriguez-Frank Space, 234-238
Thermodynamics, 67
  Threading Dislocations and Their Reduction, 287
  TiAl, 34-38
  Titanium Alloy(s), 113, 141
  Tribology, 207
  Triple Junctions, 387-398
    Triple-Junction Dislocations, 397-398
    Triple-Junction Statistics, 395
Twinning, 113

W
  Work Function, 330-332

X
  X-Ray Diffraction, 171
  X-Ray Imaging, 399

Z
  Zero-Flux Planes, 75