

Advanced Materials for Applications in Extreme Environments

MATERIALS RESEARCH SOCIETY
SYMPOSIUM PROCEEDINGS VOLUME 1298

Advanced Materials for Applications in Extreme Environments

Symposium held November 29–December 3, Boston, Massachusetts, U.S.A.

EDITORS

Maria Samaras

Paul Scherrer Institute
Villigen, Switzerland

Chu Chun Fu

CEA Saclay
Saclay, France

Thak Sang Byun

Oak Ridge National Laboratory
Oak Ridge, Tennessee, U.S.A.

Marius Stan

Argonne National Laboratory
Argonne, Illinois, U.S.A.

Toru Ogawa

Japan Atomic Energy Agency
Naka, Japan

Arthur Motta

Pennsylvania State University
University Park, Pennsylvania, U.S.A.

David Simeone

CEA Saclay
Saclay, France

Roger Smith

Loughborough University
Loughborough, U.K.

Lumin Wang

University of Michigan
Ann Arbor, Michigan, U.S.A.

Xinghang Zhang

Texas A&M University
College Station, Texas, U.S.A.

Oliver Kraft

Karlsruhe Institute of Technology
Karlsruhe, Germany

Michael J. Demkowicz

Massachusetts Institute of Technology
Cambridge, Massachusetts, U.S.A.

Meimei Li

Argonne National Laboratory
Argonne, Illinois, U.S.A.



Materials Research Society
Warrendale, Pennsylvania



CAMBRIDGE UNIVERSITY PRESS

Cambridge, New York, Melbourne, Madrid, Cape Town,
Singapore, São Paulo, Delhi, Tokyo, Mexico City

Cambridge University Press
32 Avenue of the Americas, New York, NY 10013-2473, USA

www.cambridge.org

Information on this title: www.cambridge.org/9781605112756

Materials Research Society
506 Keystone Drive, Warrendale, PA 15086
<http://www.mrs.org>

© Materials Research Society 2011

This publication is in copyright. Subject to statutory exception
and to the provisions of relevant collective licensing agreements,
no reproduction of any part may take place without the written
permission of Cambridge University Press.

This book has been registered with Copyright Clearance Center, Inc.
For further information please contact the Copyright Clearance Center,
Salem, Massachusetts.

First published 2011

Printed in the United States of America

Single article reprints from this publication are available through
University Microfilms Inc., 300 North Zeeb Road, Ann Arbor, MI 48106

CODEN: MRSPDH

ISBN: 978-1-605-11275-6 Hardback

Cambridge University Press has no responsibility for the persistence or
accuracy of URLs for external or third-party Internet Web sites referred to
in this publication and does not guarantee that any content on such Web sites
is, or will remain, accurate or appropriate.

CONTENTS

Preface xi

Materials Research Society Symposium Proceedings xiii

STRUCTURAL MATERIALS AND FUELS FOR FUTURE FUSION AND FISSION TECHNOLOGIES

**Characterization of 14YWT As-Atomized, Milled, Milled
and Annealed Powders, and HIP Consolidated Alloys.3**

Nicholas J. Cunningham, Auriane Etienne,
G. Robert Odette, Erich Stergar,
Yuan Wu, and Brian D. Wirth

**Corrosion Behavior of Martensitic/Ferritic Oxide Dispersed
Strengthened Steels in Nitric Media.9**

Benoit Gwinner, Martin Auroy,
Dominique Mas, and Audrey Saint-Jevin

**Atom Probe Tomography Analysis of Ti-Y-O Clustering
During Processing of Nanoscale Oxide Particles in 14%Cr
ODS Ferritic Steels.15**

Ceri A. Williams, Paulina Unifantowicz,
Zbigniew Oksiuta, Nadine Baluc,
George D.W. Smith, and Emmanuelle A. Marquis

**Characterization of Oxide Particles in ODS Austenitic Stainless
Steel after Heavy Ion Irradiation up to High Doses.21**

Hiroshi Oka, Yosuke Yamazaki,
Hiroshi Kinoshita, Naoyuki Hashimoto,
Somei Ohnuki, Shinichiro Yamashita,
and Satoshi Ohtsuka

*** Developments of Extra-High Purity Stainless Steels
for Nuclear Corrosive Environments27**

Junpei Nakayama and Kiyoshi Kiuchi

**Crevice Corrosion Behavior of Type 316L Stainless
Steel in Gamma-ray Irradiated High-temperature Water35**

Yukio Nakahara, Chiaki Kato,
Masahiro Yamamoto, Takashi Tsukada,
Atsushi Watanabe, and Motomasa Fuse

*Invited Paper

Phase State and Physical Properties of the Mo-Ru-Ph-Pd Alloys41
Tohru Sugahara, Ken Kurosaki, Aikebaier Yusufu, Hiroaki Muta, Yuji Ohishi, Shinsuke Yamanaka, Satoshi Komamine, and Eiji Ochi	
Modeling W-V and W-Ta Alloys for Fusion Applications: Phase Stability, Short-range Order and Point Defect Properties49
M. Muzyk, D. Nguyen-Manh, K.J. Kurzydowski, N.L. Baluc, and S.L. Dudarev	
Evaluation of Adhesive Strength between Vanadium Alloys and Yttrium Oxide by Laser Shock Spallation Method55
M. Satou, H. Akamatsu, T. Nagasaka, and A. Hasegawa	
Irradiation Behavior of Precipitation Hardened Ni-base Super-alloys with EHP Grade under Multi-ion Irradiation61
Gwang-Ho Kim, Kiyoyuki Shiba, Tomotsugu Sawai, Ikuo Ioka, and Kiyoshi Kiuchi	
Magnetic Tight-Binding Simulations of Defects in Iron67
Preetma K. Soin, Andrew P. Horsfield, and Duc Nguyen-Manh	
Assessment of the Effect of Irradiation Temperature on the Mechanical Anisotropy of the Zr⁺ Ion Irradiated Zr-2.5%Nb73
Bipasha Bose and Robert J. Klassen	
Atomistic Study of Helium Bubbles in Fe: Equilibrium State79
David M. Stewart, Yury N. Osetskiy, and Roger E. Stoller	
First-Principles Investigation of Structural, Elastic and Electronic Properties of Lanthanide Titanate Oxides Ln₂TiO₅85
Hui Niu, Huiyang Gou, Rodney C. Ewing, and Jie Lian	

**Atomistic to Continuum Constitutive Modeling
of Radiation Damage on FCC Metals and Its Adaptation
for the Generation of New Materials 91**
Shree Krishna and Suvranu De

**Hierarchical Computational Approaches of the Effects
of Interstitial and Vacancy Loops on Plastic Deformation. 97**
Tomohito Tsuru, Yoshiteru Aoyagi,
and Yoshiyuki Kaji

**Density Functional Theory Calculations on Magnetic
Properties of Actinide Compounds. 103**
Eugene Heifets and Denis Gryaznov

***RADIATION DAMAGE TO CERAMIC AND INSULATING
MATERIALS FOR NUCLEAR POWER***

**Radiation Induced Cavity Formation and Gold
Precipitation at the Interfaces of a ZrO₂/SiO₂/Si
Heterostructure. 111**
Philip D. Edmondson, Chongmin Wang,
Zihua Zhu, Fereydoon Namavar,
William J. Weber, and Yanwen Zhang

*** Radiation-induced Chemical Disorder
in Covalent Materials. 117**
Manabu Ishimaru, Yanwen Zhang,
and William J. Weber

**Damage Generated by MeV-ion Beams on Titanium
Surface in Oxidizing Environment. 125**
Ngoc-Long Do, Nicolas Béreard,
Nathalie Moncoffre,
and Dominique Gorse-Pomonti

Radiation-enhanced Aqueous Dissolution of Minerals 131
Catherine A. Dukes and Raúl A. Baragiola

**Irradiation Damage in Dual Beam Irradiated
Nanostructured FeCrAl Oxide Dispersion
Strengthened Steel 141**
A. Richter, C.-L. Chen, A. Mücklich, and R. Kögler

*Invited Paper

Ion Beam Irradiation-induced Amorphization in Nano-sized $K_xLn_yTa_2O_{7-v}$ Tantalate Pyrochlore147

Fengyuan Lu, May Nyman,
Yiqiang Shen, Zhili Dong,
Gongkai Wang, Fuxiang Zhang,
Rodney Ewing, and Jie Lian

*** Radiation Damage Studies of Nuclear Ceramics Using the JANNUS-Saclay Triple-ion Beam Irradiation Platform.153**

P. Trocellier, S. Miro,
Y. Serruys, É. Bordas, H. Martin,
N. Chaâbane, S. Pellegrino,
S. Vaubailon, and J.P. Gallien

Displacement Cascade Decomposition within the Binary Collision Approximation167

Laurence Luneville, David Simeone,
Gianguido Baldinozzi,
and Dominique Gosset

Cross-sectional TEM Study of Surface Modification of Nanostructure with Gas Cluster Ion Beams.173

Noriaki Toyoda and Isao Yamada

Study of Ion Beam Mixing by X-Ray Reflectometry179

D. Simeone, D. Gosset, L. Luneville,
G. Baldinozzi, N. Moncoffre, and C. Deranlot

Defect Doping and Characterization in Oxide Single Crystals Using Femtosecond Laser.185

Shingo Kanehira, Chiwon Moon,
Eita Tochigi, Naoya Shibata, Yuichi Ikuhara,
Kiyotaka Miura, and Kazuyuki Hirao

Surface Erosion of TiO_2 Subjected to Energetic Oxygen Bombardment.191

Roger Smith and Wolfhard Möller

Krypton and Helium Irradiation Damage in Yttria-stabilised Zirconia197

M. Gilbert, C. Davoisne, M.C. Stennett,
N.C. Hyatt, N. Peng, C. Jeynes,
and W.E. Lee

*Invited Paper

Modeling Radiation-induced Alteration of the Network Structure of Alkali Borosilicate High-level Waste Glass203
Leslie Dewan, Linn W. Hobbs,
and Jean-Marc Delaye

High Temperature Thermal Analysis of Graphite and Silicon Carbide with Millimeter-wave Radiometry209
Paul P. Woskov and S.K. Sundaram

NANOSTRUCTURED MATERIALS IN HARSH ENVIRONMENTS

*** Nanostructured Engineering Alloys for Nuclear Application**217
Peter Hosemann, Erich Stergar,
Andrew T. Nelson, C. Vieh,
and Stuart A. Maloy

Coming Full Circle: The Application of Microtechnology Techniques to Evaluate Bulk Materials227
David Read and Nicholas Barbosa

Multilayer Antidiffusion Barrier Schemes for Schottky and Ohmic Contact Metallizations to InAlN/GaN HEMTs233
Eliana Kamińska, Iwona Pasternak,
Michał A. Borysiewicz, Marek Guziewicz,
Anna Piotrowska, Elżbieta Dynowska,
Rafał Jakiela, Valery Kolkovski,
and Marie-Antoinette di Forte-Poisson

Comparison of CVD and MOCVD-grown Al₂O₃ Coatings in the Performance of Cemented Carbide Cutting Tool Inserts239
Piyush Jaiswal, Abdul Sathar,
Arshiyah Shariff, Mohammed Saif,
Sukanya Dhar, and S.A. Shivashankar

Electrochemical Nanopatterning on Copper Surface Using an AFM Cantilever Tip245
Gyudo Lee, Kihwan Nam, Suho Jeong,
Huihun Jung, Bumjoon Choi,
Sang Woo Lee, Dae Sung Yoon,
Kilho Eom, and Taeyun Kwon

*Invited Paper

Responses of Carbon Onions to High Energy Heavy Ion Irradiation	251
Raed A. Alduhaileb, Kan Xie, Joshua C. Myers, Virginia M. Ayres, Benjamin W. Jacobs, Kaylee McElroy, T. Bieler, M. Crimp, Xudong Fan, Reginald M. Ronningen, Albert F. Zeller, Thomas Baumann, and Atsushi Hirata	
Effect of Seawater on Thermal Behavior of Conventional and Nanophased Carbon/Epoxy Composites	257
Mohammad K. Hossain, Kazi A. Imran, Mahesh Hosur, and Shaik Jeelani	
High Temperature Creep Strength in a Nanodispersion-strengthened Ferritic Alloy Prepared by Heavy Plastic Deformation	263
David G. Morris and Maria Antonia Muñoz-Morris	
Author Index	269
Subject Index	273

PREFACE

Symposium Q, “Structural Materials and Fuels for Future Fusion and Fission Technologies,” Symposium R, “Radiation Damage to Ceramic and Insulating Materials for Nuclear Power,” and Symposium T, “Nanostructured Materials in Harsh Environments,” were held Nov. 29–Dec. 3 at the 2010 MRS Fall Meeting in Boston, Massachusetts. This volume includes papers based upon these symposia. The underlying theme behind the papers is that of materials for next-generation technologies, especially fusion and fission energy production and the nanoscale properties of these materials when subjected to high temperature and pressure. In many cases, joint experimental and modeling programs (to minimize expensive trial-and-error techniques) are underway to understand the fundamental processes that are at the basis of the materials. This combined approach is optimal to design novel new materials that can withstand the higher operating temperature, high radiation doses, and complex thermomechanical loading required in the next-generation nuclear systems. It is especially important to understand the role of defects and flaws in small volumes as their energetics and interactions elicit the observed mechanical response.

Accelerated use and integration of nanomaterials can be enabled by the complementary combination of atomistic and multiscale simulations with integrated *in situ* instrumentation and techniques in which synthesis, testing, environmental control, and direct imaging occur simultaneously.

The articles here investigate mainly nanomaterials, ferritic martensitic steels, oxide dispersed steels (ODS), and ceramic and insulating materials. Ceramic materials are important because many have good radiation tolerance properties, and recent results also indicate that small nanoparticulate inclusions of ceramics in the ODS materials can also help mitigate the bubble growth of inert gases produced by nuclear reactions, besides improving general mechanical properties.

Materials for nuclear energy is not the only area in which the study of nanosized objects is important. The investigation of the mechanical response of nano- and microscale components that comprise other next-generation technological devices (such as nanopillars, nanotubes, nanowires, nanolayers, ultrathin films, nanoparticles, and nanocrystalline and nanotwinned materials) must be investigated in the context of their unique microstructure and its evolution.

This volume, therefore, highlights some emerging topics in novel mechanical testing techniques, *in situ* microscopy, high- and low-temperature deformation mechanisms, radiation damage investigations, and mechanical property characterization of materials, as well as recent advances in atomistic and multiscale modeling.

Thak Sang Byun
Roger Smith
Meimei Li

February 2011

MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS

- Volume 1275— Structural and Chemical Characterization of Metals, Alloys and Compounds, R. Pérez Campos, A. Contreras Cuevas, R.A. Esparza Muñoz, 2011, ISBN 978-1-60511-252-7
- Volume 1276— Advanced Structural Materials—2010, H.A. Calderon, A. Salinas Rodriguez, H. Balmori-Ramirez, 2010, ISBN 978-1-60511-253-4
- Volume 1277E—Biomaterials—2010, S.E. Rodil, A. Almaguer-Flores, K. Anselme, 2010, ISBN 978-1-60511-254-1
- Volume 1278E—Composite, Hybrid Materials and Ecomaterials, R. Bernal, C. Cruz Vazquez, L.E. Rendon Diaz Miron, V.M. Castaño, 2010, ISBN 978-1-60511-255-8
- Volume 1279— New Catalytic Materials, J.A. Wang, J. Manuel Dominguez, 2010, ISBN 978-1-60511-256-5
- Volume 1280E—Nanomaterials for Biomedical Applications, L. Zhang, T.J. Webster, A. Salinas Rodriguez, 2010, ISBN 978-1-60511-257-2
- Volume 1282— Diamond Electronics and Bioelectronics—Fundamentals to Applications IV, P. Bergonzo, J.E. Butler, C.E. Nebel, M. Nesladek, A.T.S. Wee, 2011, ISBN 978-1-60511-259-6
- Volume 1283E—Carbon-Based Electronic Devices—Processing, Performance and Reliability, M. Chhowalla, R.R. Keller, M. Meyyappan, W.J. Ready, 2011, ISBN 978-1-60511-260-2
- Volume 1284— Fundamentals of Low-Dimensional Carbon Nanomaterials, J.J. Boeckl, L. Dai, W. Lu, M.H. Rummeli, J. Warner, 2011, ISBN 978-1-60511-261-9
- Volume 1285E—Challenges in Roll-to-Roll (R2R) Fabrication for Electronics and Other Functionalities, T. Blaudeck, G. Cho, J.H. Daniel, M.R. Dokmeci, 2011, ISBN 978-1-60511-262-6
- Volume 1286E—Molecular and Hybrid Materials for Electronics and Photonics, J. Liu, 2011, ISBN 978-1-60511-263-3
- Volume 1287E—Low-Temperature-Processed Thin-Film Transistors, E. Fortunato, 2011, ISBN 978-1-60511-264-0
- Volume 1288E—Novel Fabrication Methods for Electronic Devices, P. Andrew, 2011, ISBN 978-1-60511-265-7
- Volume 1289E—Controlling Material Properties and Charge-Carrier Interactions with Quantum-Dot Coupling, 2011, ISBN 978-1-60511-266-4
- Volume 1290E—Magnetism and Correlated Electronic Structure of Nitrides—Rare-Earth and Transition Metals as Constituents and Dopants, W.R.L. Lambrecht, A. Ney, K. Smith, H.J. Trodahl, 2011, ISBN 978-1-60511-267-1
- Volume 1291E—Integrated Nonreciprocal Photonics—Materials, Phenomena and Devices, V. Fratello, M. Levy, B. Stadler, M. Vanwolleghem, 2011, ISBN 978-1-60511-268-8
- Volume 1292— Oxide Nanoelectronics, H. Hwang, J. Levy, P. Makysymovych, G. Medeiros-Ribeiro, R. Waser, 2011, ISBN 978-1-60511-269-5
- Volume 1293E—Liquid-Crystal Materials—Beyond Displays, N.L. Abbott, D.J. Broer, T. Kato, T.J. White, 2011, ISBN 978-1-60511-270-1
- Volume 1294E—Resonant Optical Antennas—Sensing and Shaping Materials, K.B. Crozier, N. Engheta, G. Ju, R. Quidant, R. Zia, 2011, ISBN 978-1-60511-271-8
- Volume 1295— Intermetallic-Based Alloys for Structural and Functional Applications, M. Palm, B. Bewlay, S. Kumar, K. Yoshimi, 2011, ISBN 978-1-60511-272-5
- Volume 1296E—New Methods in Steel Design—Steel Ab Initio, Y. Adachi, R. Dronskowski, D. Raabe, P.E.A. Turchi, 2011, ISBN 978-1-60511-273-2
- Volume 1297— Deformation Mechanisms, Microstructure Evolution and Mechanical Properties of Nanoscale Materials, J.R. Greer, D.S. Gianola, B.G. Clark, T. Zhu, A.H.W. Ngan, 2011, ISBN 978-1-60511-274-9
- Volume 1298— Advanced Materials for Applications in Extreme Environments, T.S. Byun, R. Smith, M. Li, 2011, ISBN 978-1-60511-275-6
- Volume 1299— Microelectromechanical Systems—Materials and Devices IV, M.P. de Boer, F.W. DelRio, C. Eberl, E.P. Gusev, 2011, ISBN 978-1-60511-276-3
- Volume 1300E—Bulk Metallic Glasses and their Applications, K.F. Yao, 2011, ISBN 978-1-60511-277-0

MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS

- Volume 1301— Soft Matter, Biological Materials and Biomedical Materials—Synthesis, Characterization and Applications, A.J. Nolte, K. Shiba, R. Narayan, D. Nolte, 2011, ISBN 978-1-60511-278-7
- Volume 1302E—Nanowires—Growth and Device Assembly for Novel Applications, 2011, ISBN 978-1-60511-279-4
- Volume 1303— Nanomaterials Integration for Electronics, Energy and Sensing, D. E. Perea, Y. Jung, J. B. Hannon, M. A. Reed, S. T. Picraux, 2011, ISBN 978-1-60511-280-0
- Volume 1304E—Hierarchical Materials and Composites—Combining Length Scales from Nano to Macro, J.H. Moon, G.M. Odegard, M.S.P. Shaffer, B.L. Wardle, 2011, ISBN 978-1-60511-281-7
- Volume 1305E—Group IV Semiconductor Nanostructures and Applications, L. Dal Negro, 2011, ISBN 978-1-60511-282-4
- Volume 1306E—Aerogels and Aerogel-Inspired Materials, S. Brock, G. Gould, A. Roig, D. Rolison, 2011, ISBN 978-1-60511-283-1
- Volume 1307E—Boron and Boron Compounds—From Fundamentals to Applications, M. Dudley, J.H. Edgar, M. Kuball, 2011, ISBN 978-1-60511-284-8
- Volume 1308E—Artificially Induced Crystalline Alignment in Thin Films and Nanostructures, A.T. Findikoglu, R. Huehne, T. Shimada, J.Z. Wu, 2011, ISBN 978-1-60511-285-5
- Volume 1309— Solid-State Chemistry of Inorganic Materials VIII, K-S. Choi, S.J. Clarke, P.S. Halasyamani, D.G. Mandrus, 2011, ISBN 978-1-60511-286-2
- Volume 1310E—Magneto Calorics and Magnetic Cooling, A. Fujita, K. Gschneidner Jr., O. Gutfleisch, K.G. Sandeman, A. Yan, 2011, ISBN 978-1-60511-287-9
- Volume 1311— Next-Generation Fuel Cells—New Materials and Concepts, T. He, K. Swider-Lyons, B. Park, P.A. Kohl, 2011, ISBN 978-1-60511-288-6
- Volume 1312— Polymer-Based Materials and Composites—Synthesis, Assembly, Properties and Applications, V. Bharti, M. Chipara, D. Venkataraman, 2011, ISBN 978-1-60511-289-3
- Volume 1313— Materials for Advanced Lithium Batteries, G.-A. Nazri, J-M Tarascon, D. Guyomard, A. Yamada, 2011, ISBN 978-1-60511-290-9
- Volume 1314E—Thermoelectric Materials for Solid-State Power Generation and Refrigeration, Y. Grin, G.S. Nolas, J. Sharp, T.M. Tritt, 2011, ISBN 978-1-60511-291-6
- Volume 1315— Transparent Conducting Oxides and Applications, J.J. Berry, E. Fortunato, J. Medvedeva, Y. Shigesato, 2011, ISBN 978-1-60511-292-3
- Volume 1316E—Nanofunctional Materials, Nanostructures and Nanodevices for Biomedical Applications II, R. Rao, 2011, ISBN 978-1-60511-293-0
- Volume 1317E—Interdisciplinary Approaches to Safe Nanotechnologies, C. Chaneac, S. Harper, G.V. Lowry, R.I. MacCuspie, 2011, ISBN 978-1-60511-294-7
- Volume 1318— Advances in Spectroscopy and Imaging of Surfaces and Nanostructures, J. Cumings, J. Guo, F.M. Granozio, O.V. Kolosov, 2011, ISBN 978-1-60511-295-4
- Volume 1319— Materials Issues in Art and Archaeology IX, P.B. Vandiver, C.L. Reedy, J.L. Ruvalcaba Sil, W. Li, 2011, ISBN 978-1-60511-296-1
- Volume 1320— Materials Education Development and Outreach—From K–Grad, D. Bahr, K. Jones, M. Glass, E. Allen, 2011, ISBN 978-1-60511-297-8

Prior Materials Research Society Symposium Proceedings available by contacting Materials Research Society