

MATERIALS RESEARCH SOCIETY
SYMPOSIUM PROCEEDINGS VOLUME 1369

Computational Studies of Phase Stability and Microstructure Evolution

April 25-29, 2011
San Francisco, California, USA

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571
www.proceedings.com

ISBN: 978-1-5108-0478-4

Some format issues inherent in the e-media version may also appear in this print version.

©Materials Research Society 2014

This reprint is produced with the permission of the Materials Research Society and Cambridge University Press.

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.

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

Materials Research Society
506 Keystone Drive, Warrendale, PA 15086
www.mrs.org

CODEN: MRSPDH

ISBN: 978-1-5108-0478-4

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for external or third-part 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.

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

CURRAN ASSOCIATES INC.
proceedings
.com

TABLE OF CONTENTS

Development and Application of Chen-Mobius Lattice Inversion Potential for Pd-Au Alloy	1
<i>Xianbao Duan, Zhengzheng Chen, Neeti Kapur, Xianghong Hao, Kyeongjae Cho, Bin Shan</i>	
An Experimental and Theoretical Multi-Mbar Study of Ti-6Al-4V	7
<i>Bengt E. Tegner, Simon G. MacLeod, Hyunchae Cynn, John Proctor, William J. Evans, Malcolm I. McMahon, Graeme J. Ackland</i>	
Alloying-Driven Phase Stability in Group-VB Transition Metals under Compression*, **	13
<i>Alexander Landa, Per Söderlind</i>	
MD Simulations of Compression of Nanoscale Iron Pillars	25
<i>Con J. Healy, Graeme J. Ackland</i>	
Irradiation-Driven Compositional Changes in Alloys	31
<i>Santosh Dubey, Anter El Azab, Dieter Wolf</i>	
Characterization and statistical modeling of the precipitation kinetics in the commercial aluminum alloy AA5182	37
<i>Zhenshan Liu, Volker Mohles, Olaf Engler, Günter Gottstein</i>	
Elastic Heterophase Domains in Ferroelectric Epitaxial Films	43
<i>A. L. Roytburd, J. Ouyang, B. M. Boyerinas, H. A. Bruck, J. Slutsker, A. Artemev</i>	
Ruthenium Thermodynamics in Nuclear Waste Glasses	55
<i>S. Gossé, S. Schuller, C. Guéneau, H. Boucetta</i>	
The Finite Phase-Field Method - A Numerical Diffuse Interface Approach for Microstructure Simulation with Minimized Discretization Error	62
<i>Janin Eiken</i>	
Author Index	