

The Minerals, Metals & Materials Society

Computational Thermodynamics and Phase Transformations 2007

February 25 – March 1, 2007
Orlando, Florida, USA

Printed from e-media with permission by:

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

ISBN: 978-0-87339-679-0

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

A Publication of **The Minerals, Metals & Materials Society (TMS)**

184 Thorn Hill Road
Warrendale, Pennsylvania 15086-7528
(724) 776-9000

Visit the TMS Web site at
<http://www.tms.org>

Statements of fact and opinion are the responsibility of the authors alone and do not imply an opinion on the part of the officers, staff, or members of TMS. TMS assumes no responsibility for the statements and opinions advanced by the contributors to its publications or by the speakers at its programs. Registered names and trademarks, etc., used in this publication, even without specific indication thereof, are not to be considered unprotected by the law.

No part of this book may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, microfilming, recording, or otherwise, without written permission from the publisher.

Printed in the United States of America

ISBN Number 978-0-87339-679-0

ISSN Number 109-9586

Authorization to photocopy for internal or personal use beyond the limits of Sections 107 and 108 of the U.S. Copyright Law is granted by TMS, provided that the base fee of \$7.00 per copy is paid directly to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923 USA, www.copyright.com. Prior to photocopying items for educational classroom use, please contact the Copyright Clearance Center, Inc.

For those organizations that have been granted a photocopy license by the Copyright Clearance Center, a separate system of payment has been arranged.

This consent does not extend to copying items for general distribution or for advertising or promotional purposes or to republishing items whole or in part in any work in any format.

Please direct republication or special copying permission requests to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923 USA; (978) 750-8400; www.copyright.com.

The logo for The Minerals, Metals & Materials Society (TMS) consists of the letters 'TMS' in a large, bold, black, sans-serif font. The letters are closely spaced and have a slightly irregular, hand-drawn appearance.

Copyright 2007,
The Minerals, Metals & Materials Society.
All rights reserved.

If you are interested in purchasing a copy of this book, or if you would like to receive the latest TMS publications catalog, please telephone (724) 776-9000, ext. 270, or (800) 759-4TMS.

COLLECTED PROCEEDINGS: STRUCTURE, EXTRACTION, PROCESSING, AND PROPERTIES TABLE OF CONTENTS

Computational Thermodynamics and Phase Transformations

First Principles and Atomistic Calculations of Phase and Alloy Thermodynamics I

- Lattice Stability AL-PM and AC-AL Systems: A First-Principle Study..... 1
Michael Gao, Anthony Rollett, and Michael Widom
- Clustering and Short-Range Order in Fe-Cr Alloys: A Monte Carlo Study..... 11
*Mikhail Lavrentiev, Duc Nguyen-Manh, Sergei Dudarev, Ralf Drautz,
and Peter Klaver*

Nanomaterials and Confined Systems II

- Simulation on the Phase Transformation of Silicon under Multiaxial Stress..... 17
Seongmin Jeong, and Takayuki Kitamura
- Control of Melting Using Nanoscale Coatings..... 27
Kerwyn Huang, Tairan Wang, and John Joannopoulos
- A New Polymorph of Zinc Oxide in Nanowires under Tensile Loading 37
*Ambarish Kulkarni, Min Zhou, Kanoknan Sarasmak,
and Sukit Limpijumnong*

Modeling of Phase Transformations II

- Linking Thermodynamics, Structure and Viscosity of Alumo- and Borosilicate Melts 47
Grundy, H. Liu, I.-H. Jung, S. Deckerov, and A.D. Pelton
- Precipitation Simulation of fcc Iron Precipitates in Cu-Fe Alloys 57
*María del Carmen Gutierrez-Mendez, Erika O. Avila-Davila,
Victor Lopez-Hirata, Viridiana D. Melo-Maximo, and Maribel L. Saucedo Muñoz*

Author Index

Subject Index