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978-1-107-41007-7 - Materials Research Society Symposium Proceedings: Volume 193:

Atomic Scale Calculations of Structure in Materials

Editors: Murray S. Daw and Michael A. Schlüter

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MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS VOLUME 193

Atomic Scale Calculations of Structure in Materials

Symposium held April 16-17, 1990, San Francisco, California, U.S.A.

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MATERIALS RESEARCH SOCIETY

Pittsburgh, Pennsylvania

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

Cambridge University Press

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

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org

Information on this title: www.cambridge.org/9781107410077

Materials Research Society

506 Keystone Drive, Warrendale, PA 15086

<http://www.mrs.org>

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First published 1990

First paperback edition 2012

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

CODEN: MRSPDH

ISBN 978-1-107-41007-7 Paperback

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This work was supported in part by the U.S. Army Research Office under Grant Number
DAAL03-90-G-0087. The views, opinions, and/or findings contained in this report are those of
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Preface

In recent years, our knowledge of the structure of solids has advanced considerably beyond that of understanding the bulk phases. It is now possible experimentally to resolve directly the atomic-scale structure of complex systems like interfaces, surfaces, and grain boundaries. These experimental breakthroughs have provided strong motivation for further theoretical investigations of structure. First principles calculations are capable of explaining simple reconstructions on surfaces, for example. In many cases, however, the complexity of the system demands more approximate approaches. This symposium emphasized the calculations of atomic-scale structure in the condensed phase. The structure of bulk phases as well as the structure of defects, surfaces, and grain boundaries was covered. Other areas of interest included theoretical investigation of the atomic-scale structure of clusters, overlayers and adatoms on surfaces, clean surface reconstructions, grain boundaries and interfaces, and dislocations. Excited states, compositional ordering, and magnetism were examined and structural phase transitions were addressed from atomic scale calculations. The symposium covered a broad range of theoretical techniques, from semi-empirical and many-body models to fundamental, first-principles formulations. The invited speakers highlighted theoretical advances and some also provided experimental perspective. The breadth and depth of the symposium testified to the recent rapid growth in the application of solid state theory to important materials science issues.

We would like to acknowledge the assistance of Ms. Faye Rasmussen in the preparation of the proceedings.

Murray S. Daw
Michael A. Schlüter

June 1990

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