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Microscopic Simulation of Interfacial Phenomena in Solids and Liquids

Editors: Simon R. Phillpot, Paul D. Bristowe, David G. Stroud and John R. Smith

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Microscopic Simulation of Interfacial Phenomena in Solids and Liquids

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PREFACE

This volume contains the proceedings of the symposium on "Microscopic Simulation of Interfacial Phenomena in Solids and Liquids" held at the 1997 MRS Fall Meeting. The symposium was organized to provide a forum for atomic and electronic-level calculations of interfacial properties, and published here are 53 of the papers presented.

The microscopic characterization of interfaces and surfaces has progressed significantly in recent years due to the simultaneous development of new experimental probes and new theoretical approaches. Experimentally, it is now possible to resolve the atomic structure of internal interfaces and free surfaces using techniques such as HREM and STM, and these impressive studies have been the focus of several recent MRS symposia. At the same time, the advent of parallel computers and high-performance workstations has led to more sophisticated and realistic microscopic computer simulations of materials using both classical and quantum mechanical methods. While interfacial modeling has been partly addressed in previous symposia, this meeting was the first to focus solely on the microscopic simulation of interfaces and sought to bring together researchers interested in all classes of interfaces in both solids and liquids.

The symposium was organized around six important interfacial properties:

1. *Structure of Fluid Interfaces and Surfaces*
2. *Structure of Solid Interfaces and Surfaces* (covering the atomic and electronic structure of grain boundaries, interphase boundaries, thin-film interfaces and nanostructures).
3. *Chemical Properties* (covering grain boundary segregation, surface adsorption and oxidation).
4. *Dynamical Processes* (covering phase transitions, microstructural evolution and diffusion).
5. *Magnetic and Dielectric Properties* (covering surface and interface magnetism, the effect of interfacial segregation in ferromagnetic materials, and the dielectric properties of materials).
6. *Elastic and Mechanical Properties* (covering interfacial stress, interfacial fracture, plastic deformation and combined atomistic-continuum modeling).

Although many of these properties were simulated using classical approaches, it is clear that new methodologies for performing first principles calculations are beginning to make a significant impact. One such study in this symposium deserves special mention since it was awarded a Best Poster prize by MRS: "First-Principles Study of the Interfacial Reaction and Atomic Process of Silicon Oxidation," by H. Kageshima and K. Shiraishi.

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Simon R. Phillpot
Paul D. Bristowe
David G. Stroud
John R. Smith

January 1998

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