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Multiscale Phenomena in Materials—Experiments and Modeling

Editors: I. M. Robertson, D. H. Lassila, B. Devincre and R. Phillips

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Multiscale Phenomena in Materials—Experiments and Modeling

Symposium held November 30–December 2, 1999, Boston, Massachusetts, U.S.A.

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PREFACE

Since the development of quantum mechanics, great strides have been made in understanding materials phenomena based on "first principles" associated with atomic and sub-atomic structure. Perhaps the most notable examples are in the fields of microelectronics and nuclear energy. In other fields, the connections between the fundamental nature of atomic structure and important properties are problematic because in addition to atomic structure, other structural aspects of the material at longer length scales are important. This is the case when considering the mechanical behavior of materials. Although general relationships between composition of materials and their mechanical properties have been established, a detailed understanding of the effects of the composition and microstructure based on first principles is lacking. For example, it is well known that a metal's mechanical properties such as yield strength can be grain size dependent, however, in many instances fundamental understanding of this phenomenon has been illusive.

In recent years there has been increasing interest in using what are termed "multiscale modeling" approaches to understand the effects of composition and microstructure on mechanical behavior. It is now quite common to find publications that report on related phenomena using atomistic, microscale (*dislocation dynamics*) and mesoscale/continuum computer simulations. With this enhanced interest in multiscale phenomena emerges a need for experimental work that validates and challenges the predictive capabilities of modeling and simulations.

The main purpose of this Symposium A, "Multiscale Phenomena in Materials—Experiments and Modeling," held November 30–December 2 at the 1999 MRS Fall Meeting in Boston, Massachusetts, is to bring together experimentalists and individuals working in the areas of modeling and simulations. To this end, we structured the sessions such that talks would be principally at a given length—scale and modeling and experimental subject matter was interspersed. Selected papers contributed by the symposium participants are presented with the same goal in mind. We hope that the reader will benefit from the varied nature of the papers and reflect on the many possibilities of making contact between experiments and simulations.

In addition to the papers from this symposium, selected papers from Symposium C, "Microstructural Modeling For Industrial Metals Processing," are included in the last section of this proceedings.

I.M. Robertson
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Finally, we would like to thank our respective institutions for their support of our work on this symposium:

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