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Advances in Materials Theory and Modeling—Bridging Over Multiple-Length and Time Scales

Editors: Vasily Bulatov, Luciano Colombo, Fabrizio Cleri, Laurent J. Lewis and

Normand Mousseau

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Advances in Materials Theory and Modeling—Bridging Over Multiple-Length and Time Scales

Symposium held April 16–20, 2001, San Francisco, California, U.S.A.

EDITORS:

Vasily Bulatov

Lawrence Livermore National Laboratory
Livermore, California, U.S.A.

Luciano Colombo

Cittadella Universitaria
Monserato, Italy

Fabrizio Cleri

Centro Ricerche Casaccia
Rome, Italy

Laurent J. Lewis

Université de Montreal
Montreal, Quebec, Canada

Normand Mousseau

Ohio University
Athens, Ohio, U.S.A.



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PREFACE

This proceedings volume is the record from Symposium AA, "Advances in Materials Theory and Modeling—Bridging Over Multiple-Length and Time Scales," held April 18-20 at the 2001 MRS Spring Meeting in San Francisco, California. It covers a range of topics, among which algorithmic developments and application related to our quest for simulating larger systems on longer time scales.

Computer simulations of materials are rapidly moving from the level of fundamental studies into the domain of industrial research and development tools. Several commercial packages allow the simulation of widely different properties and phenomena such as surface and defect energetics, electronic band-structure, and process modeling. However, the investigation of complex materials behavior, e.g., mechanical properties and tribology, surface catalysis, microstructure evolution under stress and temperature, depends on a continuous cross-fertilization between theory, computation, and experiment, on one side, and the development of entirely new paradigms, such as multiple length- and time-scale modeling, on the other. Through a number of invited and contributed papers, these proceedings provide an extensive review of recent advances in materials theory and modeling by: (a) addressing new frontiers for theoretical and computational research on real materials, (b) identifying the crucial areas where experimental studies have been or can be, complemented by theory and simulation, and (c) establishing a blueprint for the further development, in the coming years, of multiscale methods in computational materials science.

As was clear from the talks and posters as well as from the round-table discussion, this field is still in its infancy and a number of challenges remain to be overcome before we can perform multiscale simulations as a matter of routine. Much remains to be done to solve the problem of the interface between atomistic and finite-element or finite-difference grid, leading to real multiple-length scale simulations. Similarly, although a number of algorithms were introduced recently for boosting the simulation time scale of atomistic systems, they are not quite answering our wishes for a solid and widely applicable method. This proceedings volume sets, however, a number of promising paths which will serve as a starting point for the successful algorithms to come.

The numerous discussions at the symposium, surrounding the talks and posters and culminating at the round-table, have greatly helped clarify some outstanding issues and shed light on recent developments. We are confident that these proceedings have managed to capture some of this excitement and will serve as a reference for the numerous developments to come.

Vasily Bulatov
Luciano Colombo
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The success of this symposium was due to the efforts of a great number of people: the authors and speakers who presented their contributions at the symposium and took the time to prepare papers for these proceedings; the session chairs—E.B. Tadmor, T. Diaz de la Rubia, P. Ordejón, R.E. Miller, and R.O. Jones, who were essential in keeping the presentations on time and the debate lively; the participants at the round table—G.T. Barkema, H. Jónsson, R.E. Rudd, E.B. Tadmor, and A.F. Voter, who helped place the symposium into perspective and identify the major outstanding issues; the staff of the Materials Research Society, who, by incessant prodding over more than 18 months, made sure that all would be in time and working properly; the sponsors listed below, whose financial backing proved essential to cover the Meeting expenses. We would like to extend our most sincere appreciation to all who contributed to the success of this symposium.

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