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Multiscale Modelling of Materials

Editors: Vasily V. Bulatov, Tomas Diaz de la Rubia, Rob Phillips, Efthimios Kaxiras
and Nasr Ghoniem

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Multiscale Modelling of Materials

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PREFACE

An emerging theme in computational materials science is that of multiscale modelling. While the definition of “multiscale modelling” itself is developing as new ideas and applications appear, a broad interpretation of this field includes efforts to exploit insights arising either from distinct methodologies, or from the attempt to incorporate multiple mechanisms into the same modelling paradigm. Though multiple scale models are not new (their origins can be traced to early attempts to explain macroscopic phenomena on the basis of molecular interactions within a physical system, or between a system and its boundaries), the topic has recently taken on a new sense of urgency. This is in large part due to the recognition that brute force computational approaches often fall short of allowing for direct simulation of both the characteristic structures and temporal processes found in real materials. As a result, a number of hybrid approaches are now finding favor in which ideas borrowed from distinct disciplines or modelling paradigms are unified to produce more powerful techniques.

Symposium J, “Multiscale Modelling of Materials,” at the 1998 MRS Fall Meeting in Boston, Massachusetts, attempted to serve as a forum for taking stock of recent developments in multiscale modelling. The symposium was characterized by high attendance, lively discussion, a series of successful invited talks, and important contributed talks and posters. In addition, this symposium participated in three separate joint sessions with other symposia:

- (i) Symposium K, “Computation of Rates of Activated Processes”

This joint session was engendered in part on the recognition that multiscale efforts are needed not only in order to treat the multiple length scales that arise in materials, but also to treat the multitude of time scales arising in many processes. Indeed, much of the discussion in this joint session was aimed at determining how to connect the exceedingly short time scales characterizing atomic motion to the time scales of interest in physical phenomena, ranging from seconds upward.

- (ii) Symposium M, “Fracture and Ductile vs. Brittle Behavior—Theory, Modelling and Experiment”

Developments that were widely discussed in this symposium were primarily methodological, and concerned the general question of how best to exploit atomic-scale calculations without having to resort to such calculations throughout the medium of interest. A common theme in these models is the use of continuum ideas in one region, and atomic-scale calculations only in the vicinity of what one might loosely call the “process zone.” A number of different schemes were presented in which the continuum regions were treated with finite element descriptions, while the regions of full atomic resolution were treated using conventional atomistic arguments. The key difficulty that must be faced in these types of methods is the “handshaking” between the different regions.

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(iii) Symposium N, "Microstructural Processes in Irradiated Materials"

A joint session with Symposium N focused on the application of molecular dynamics, kinetic Monte Carlo and rate theory methods to describing microstructure changes in irradiated materials. Presentations ranged from descriptions of the atomistic process of defect production in irradiated materials (a picosecond and nanometer-scale problem) to rate equation-based simulations of damage accumulation and microstructure evolution in irradiated steels (a macroscopic length and time-scale problem). Furthermore, several talks described the coupling of these simulation methods to provide a unified simulation approach across all relevant length and time scales. Applications to embrittlement of reactor pressure vessel steels provided an excellent example of how multiscale modelling can be used to model and understand problems of actual industrial interest in real materials.

One of the specific problem areas in which multiscale modelling has seen increasing success is the investigation of thin-film growth and processing. These ideas were illustrated in this symposium via a variety of models involving a few key elements, the first being a microscopic parameterization of the key atomic-scale processes that take place during the growth process. Once these processes have been parameterized, a kinetic Monte Carlo (KMC) scheme can be implemented in order to simulate the process of interest, in which all relevant microscopic processes are taken into account with appropriate rates. Finally, KMC results can be incorporated into large-scale theoretical models, which serve to describe the film morphology at macroscopic scales. In addition to the modelling of growth processes, a number of efforts addressed different classes of defects in materials including point defects, surfaces and grain boundaries. The role of defects as a key structural component in materials is well known. The fact that such defects are often associated with length scales intermediate between atomic and microstructural features makes them a continuing challenge in the context of materials modelling.

This symposium illustrated the important role of multiscale modelling as a key component in the current efforts to construct a viable field of computational materials science. A number of important problems and challenges remain to be addressed, some major unresolved themes being the seamless coupling of different regions described by disparate methodologies, and the issue of multiple time scales. Nevertheless, the symposium showed that a legitimate foundation for future work has been laid.

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