Why Another New Journal?

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Last year when I received a survey from the Institute of Physics (IOP) about the need for another journal in materials science, I tossed the questionnaire into the trash—but not without some hesitation. The hesitation occurred because I felt an obligation to tell the people at IOP that we already have a proliferation of journals. The survey ended in the trash because I didn't have the time to read what they were proposing, let alone another new journal. Little did I know that a few months later I would receive a phone call from IOP asking me to attend a meeting in New York to discuss what they found from those who did answer their survey—a crying need for a journal covering computational materials science and engineering. What happened in the interim to convince me of the need for such a journal?

First and foremost in affecting my opinion was a DOE-sponsored workshop on Computational Issues in the Mechanical Behavior of Metals and Intermetallics, organized by Richard Hoagland of Washington State University, Alan Needleman of Brown University, and myself. A report about the workshop, held at the end of September 1991, will soon appear in *Materials Science and Engineering.* We convened the workshop because new atomistic and continuum methods, aided by the emergence of more powerful computational facilities, are making the prediction of mechanical material behavior a reality. The attendees were chosen to represent the broad spectrum of computations—i.e., atomistics, dislocations/interfaces, microstructure, and continuum elasticity and plasticity—necessary to make mechanical behavior prediction possible. Over the course of the three-day workshop, we discovered some crucial information:

- None of us alone or with our current collaborators could impact the field of mechanical property prediction.
- It will take joint collaboration between scientists and engineers working at all spatial levels to make the dream of mechanical property prediction come true.

Once the right mix of people started talking, the above conclusions became clear. Consider atomistics, for example. Currently we can perform highly reliable, semi-empirical, molecular dynamics simulations of about a million atoms for about a nanosecond. These calculations can yield important quantitative information about mechanisms, e.g., of dislocation interactions with precipitates or of the fracture process, but they are a far cry from the real world problems which involve processes of 10^{23} atoms over times that could span years. These calculations can be made useful, however, by combining them with microscopic or continuum models based on the mechanisms observed in computer simulations. The combined model has the potential of predictive capability. Continuum models by themselves, however, are not predictive. They require input of phenomenological parameters or materials properties that traditionally are extracted from experiment, but also may be obtained from atomistic simulations. How can we facilitate this necessary collaboration? Perhaps we can make a start by creating a common publication arena.

During the workshop it was also discovered that materials scientists, physicists, chemists, and mechanics experts generally don't talk across disciplines with one another, don't publish in the same journals, and don't frequent the same meetings. A notable exception has been the Materials Research Society, which fosters interactions among the materials, physics, and chemistry communities at its Fall and Spring Meetings. More commonly, each group of scientists and engineers is unaware of the computations and simulations of the other groups. In fact, they may not realize that their research could provide the key link to reality that another group needs. It seemed clear that in order to impact mechanical properties calculations, it was important to get all of these people talking. Could a specialized journal provide the exposure that would spark collaborative research? By providing a forum for computational materials science at all levels, I felt that such a journal could foster the communication that is clearly absent.

If this problem exists in the area of mechanical properties, it is likely to exist across all of materials science and engineering. I spent the last year at DOE's Office of Basic Energy Sciences where a hot topic of conversation was the new presidential initiative, the Advanced Materials and Processing Program (AMPP) (see *MRS Bulletin* **XVII** (3) 1992, p. 18). Processing calculations are commonly performed at an engineering level, predicting quantities such as temperature or stress state. How do the ultimate material properties relate to the process parameters? This is the million dollar question. Are the materials scientists who can potentially calculate materials properties aware of the work of engineers who do process modelling? I think not. Again, the same problem—there is no interconnection between the microstructural modellers and the process modellers.

As this problem coalesced as a major concern at the workshop, proposals were made to:

- Foster development of two-way communication links and joint programs between scientists and engineers in the materials, physics, chemistry, and mechanics disciplines.
- Elicit recognition, in both the technical and funding arenas, that obtaining useful results in computational materials science requires synergistic contributions from scientists and engineers working on phenomena occurring at all spatial levels, from atomistic to continuum.

Consistent with these goals, the establishment of a new journal has become a significant step in improving communication.

Another concern, however, is the increasing size of journals in which computations frequently appear. Again, take atomistics, the area with which I am most familiar. My colleagues and I frequently publish our research in *Physical Review B.* This journal has grown so much in size that each year now has a five digit page count. Over five feet of library shelf space is taken up by the 1991 issue! Only a small number of articles in each issue are of interest to me, but the time needed simply to go through the table of contents is prohibitive. Certainly an expert in continuum mechanics or microstructure evolution does not have the time to follow the atomistics literature in *Physical Review.* Couple that with the number of other journals in which similar research is published, e.g. *Surface Science, Philosophical Magazine, Acta Metallurgica et Materalia, Journal of Physics,* and it is clear why there is a communication failure. The need is for a very focused journal whose entire contents is of intimate interest to its readers, a journal that contains research papers covering all of com-

putational materials science and engineering.

I have received almost unanimous enthusiasm about the announcement of our new journal, *Modelling and Simulation in Materials Science and Engineering*. Particularly satisfying is the response from the continuum mechanics community. Several members of this community have said their materials-related work is not appreciated by the mechanics community and is not read by the materials community since it appears in mechanics journals. This new journal will cover the whole range of methods and applications of modelling and simulation in materials science and engineering. It will serve the emerging multidisciplinary materials community through original contributions to modelling methods and applications. The contents will provide an important link between theory and experiment, covering properties, structure and behavior of all classes of materials at all scales from the atomic to the macroscopic.

The first issue of *Modelling and Simulation in Materials Science and Engineering* will be published in October, and quarterly thereafter. The first issue has just been sent to the publisher, and many of the papers for the second issue have already been accepted.

Acknowledgments

This work was supported by U.S. DOE Contract DE-AC04-76DP00789.

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