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Simulations of structural materials

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INTRODUCTION

The possibility of developing structural materials by computer simulation is now within our reach, largely due to recent advances in modeling techniques and computational capabilities. This achievement can be of great value to industrial applications: a simulation prior to fabrication of a prototype part can guide the engineer in material selection and designation of process parameters. Subsequent simulations in conjunction with test data can speed the development process of various product components.

A confluence of two trends makes the present time ripe for focusing on the enhancement of material-simulation capabilities. Firstly, the need for such capabilities in industrial applications is steadily increasing. A case in point is the desire of the American automobile industry to introduce more light-weight materials into its vehicles in order to improve fuel economy and lower emissions. This necessitates the development of new composite structural materials and wear coatings. Experience shows that simulation can decrease the cost, as well as shorten the time required for development processes. Competition in the marketplace has made both time and cost savings critical. Secondly, substantial progress has been made in our materials-modeling algorithms and software. Our current capabilities suggest that we are close to having the ability to produce a variety of simulation-software packages for the development of structural materials.

For the field of atomistic calculations, extensive discussions among the Workshop participants identified the following three goals toward successful modeling of structural materials:

(i) produce reliable and accurate programs for applications in structural-materials problems;
(ii) create the means and mechanisms for an information exchange in computational methods, results and needed applications;

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(iii) improve existing computational tools and develop new methodologies and concepts that will enable connections within multiscale physics.

Specific suggestions for reaching these goals are discussed in detail in the Findings and Recommendations section.

Industrial needs

New, lighter-weight, relatively inexpensive structural materials are important to a number of American industries, including aerospace, shipping, and automotive. This need is perhaps most pressing currently in the automotive industry, from which we draw representative examples.

Limited knowledge of correlations among microstructure, processing variables, and macroscopic materials characteristics has restricted metal-matrix composite (MMC) usage in automobiles [1], although MMCs are being researched in U.S. automotive laboratories. Also corrosion is a serious obstacle for (light-weight) magnesium introduction. There is substantial research on coatings in the U.S. auto industry for corrosion resistance. Wear resistance of magnesium and aluminum is poor compared to steels, and so wear-resistant coatings are being developed as well.

In the research and development of light-weight alloys, coatings, and MMCs, there are currently very limited simulation capabilities available. This is unfortunate, because high development costs and long development times would make it more difficult for U.S. auto companies to remain competitive. Furthermore, it would delay fuel-economy improvements and reduction of CO_2 emissions.

The advantage of materials simulations to the U.S. auto industry in terms of lowered development costs and development times have been demonstrated in other areas. Computer die designs for sheet metal forming are just beginning to show substantial benefits. This die design step was, before computer simulation, the source of one of the longest lead-time requirements in model changeovers for the auto industry. A second area where computer simulation has substantially lowered both costs and development time is in crash tests. Crash tests are rather expensive to carry out, in part because of the relatively extensive instrumentation required, and this makes computer simulation attractive.

Recent developments in simulation capabilities

Perhaps a central issue in structural-materials simulation is the correct prediction of critical stresses associated with crack propagation in materials. While there has been considerable progress recently in structural-materials simulation capabilities [2], currently a reliable method for prediction of such critical stresses is not available.

On the one hand, we do have reliable, accurate atomic-scale computations [3]. It is now possible to solve the (quantum-mechanical) Schrödinger equation for, e.g., dislocations in Si, phase transformations in perovskites, growth modes on covalent crystals, and interfaces involving ceramics, metal alloys, and impurities [3]. The accuracy of these computations is sufficient to make them capable of predicting quantitatively the behavior of complex systems. These atomistic-scale computations are already yielding reliable, fundamental materials information.

However, these computations are currently limited to about 100 atoms per unit cell, far too small to describe a crack tip, for instance. New methods which scale linearly with the

number of atoms per cell should significantly increase the capabilities of these methods. The expected increase in computer speeds in the next five years of perhaps a factor of 50 will also significantly enhance the capabilities of the methods. With these improvements, one might expect atomistic-scale computations to begin to connect to the microscopic-scale structures on the order of 1000 Å.

In parallel to the expansion of the scale in atomistic computations, continuum-scale and finite-element modelers are attempting to include finer length-scale effects in their computations [2]. As the length-scale capabilities of atomistic- and finite-element/continuum-scale modelers approach each other, one might expect increased information exchange between the two regimes with the benefit of enhanced reliability. Ultimately, one might hope for a robust, mathematical connection between the length-scale regimes. In the interim, parameters computed in the atomistic/microscopic regime should be increasingly available for usage in continuum equations.

FINDINGS AND RECOMMENDATIONS

In order to achieve the goals mentioned above for modeling structural materials we propose the following four initiatives:

(1) The 'Materials-Physics Exchange'

Several Workshop participants mentioned that research groups in many academic institutions and government and industrial labs are hampered by lack of access to computational tools. These research groups are faced with three equally impractical options: (i) buy software packages from commercial companies, but at a price that they can ill-afford; (ii) obtain codes through collaboration with experts, but lack of contacts or other circumstances make this interaction very difficult; and (iii) develop their own codes directly from the physics literature, at a great cost in human resources. The existence of a 'Materials-Physics Exchange' would solve these problems and allow researchers to concentrate on interesting applications rather than wasting time and effort to duplicate existing codes.

The 'Materials-Physics Exchange' could be housed either at an academic institution or a national lab, and would make *existing* computer codes available to researchers interested in materials modeling. This is envisioned as an analog to the 'Quantum-Chemistry Exchange', which is run by the Chemistry Department of Iowa State University (Ames, IA), and has made it possible for chemists to share computer codes for a minimal fee (circa $100 per code). The only obligation of the users is to give proper acknowledgement of the code in publications that result from its use (each individual code states the particular method of acknowledgement that its authors request). The codes could be distributed through a site on the World Wide Web or by mailing of disks.

It is envisioned that the codes would be provided to the users as research tools, which implies no further support after distribution, and no particular effort on the authors' part to make the code user-friendly. For these reasons, the codes would be only useful to experts. Nevertheless, the availability of codes in this manner would be very beneficial to many users, as the experience of the chemistry community indicates. Further experience in this matter comes from researchers in the U.K., where wide availability of codes has made it possible to produce a large volume of interesting results.

(2) The 'Consortium for Code Evaluation and Validation'

This entity is envisioned as a collaboration between researchers in academic institutions and government and industrial labs, whose goal would be to produce comprehensive tests, evaluations and comparisons of codes that are in use. These activities would accomplish the following goals:

(i) determine the most efficient codes that are applicable for specific physical systems, among competing methodologies;

(ii) compile lists of useful quantities, such as, for example, formation and migration energies of point defects in semiconductors, metals and intermetallic compounds. These would be the definitive theoretical values, obtained with the latest and most accurate methods available. These lists would be continuously enlarged and updated with results from the literature, or from calculations carried out within the Consortium;

(iii) compare existing empirical and semi-empirical methods against the results of definitive first-principles calculations. This would provide a guide to the community as to which empirical or semi-empirical method is the most reliable for a particular application;

(iv) act as a clearinghouse for computing values of parameters that are useful for industrial applications. Once a particular problem has been identified as an important one (through interaction with industrial researchers), and the feasibility of the calculation is assessed, the Consortium would be in a position to suggest the best way of solving the problem. The calculations might be carried out either within the Consortium or by contacting research groups that can handle the task in an efficient and accurate manner.

All these activities are now carried out in a rather unorganized manner by a multitude of research groups throughout the world. The results of the calculations are scattered in the scientific literature and are often hard to access. At the same time, several *different* results may exist in the literature for the same physical quantity. For instance, early calculations of point-defect activation energies in semiconductors gave results substantially different from more recent calculations. This has to do mostly with increases in computational power, which allowed for more-accurate and better-converged calculations. Calculations from several groups have recently converged on the definitive answers for these quantities. However, no authoritative comparison has been made to older results, which are better known and still quoted by nonpractitioners. This leads to confusion and can have the effect that the computational methodologies themselves are viewed with mistrust. The situation would be considerably improved by the Consortium activities outlined above. These activities would require a significant number of researchers (principal investigators, postdocs and graduate students), that need to be supported over a long period. The initial stage to set up the Consortium would require a higher level of support, which could be scaled down after its activities have been well organized. An approximate time scale for the initial stage is five years.

It is expected that any results and computational tools produced by the Consortium would be available freely to the scientific community. The computational tools would again be developed to the level at which experts could use them effectively, with no particular attention to user interface. The codes would also be available to software companies interested in turning them into software packages with the proper user interface, as well as graphical and other enhancements, which could then be marketed as finished products for use by intelligent nonexperts. The relation of the Consortium to software companies should be synergistic, enhancing the prospects that the product of the Consortium activities will be a widely used computational tool, either in its 'raw' form, or as a commercial software package.

The suggested mode of operation of the Consortium may give rise to certain legal issues of code ownership and rights over its use. These issues would have to be resolved before any code is released. There is significant expertise on how to deal with these issues, for instance in the U.K. scientific community, where such government-supported Consortia have operated for a number of years with strong ties to industry. This expertise should be tapped to the extent possible.

(3) Development of new algorithms and methods

At present there exist a number of interesting ideas on how to enhance the power of ab initio and empirical approaches. Many of these ideas are in the testing-and-development stage, and they deserve full support. While it is not clear which of these ideas will eventually prove to be reliable and robust enough to be applied widely to materials modeling, it is certain that some of these ideas will be at the heart of computational approaches of the future. We will briefly describe some of these exciting ideas for illustration.

In the field of electronic-structure calculations, several new approaches have been proposed that attempt to achieve O(N) scaling (i.e., computational cost that scales linearly with the size of the system N). This should highly enhance computational efficiency over current approaches that typically exhibit $O(N^3)$ or comparable scaling. These approaches in principle apply to both ab initio and semi-empirical methods, but so far have been implemented mostly in the latter context.

In the area of ab initio calculations, several new schemes have been proposed in the literature, that attempt to provide a more flexible approach to the solution of the single-particle Schrödinger equations arising from density-functional theory. These involve real-space formulations with homogeneous or adaptive grids, multigrids, wavelets, etc.

In the case of semi-empirical approaches, and in particular the tight-binding approximation, further developments are necessary to improve their reliability, transferability and accuracy. Such developments could involve the use of non-orthogonal bases, the extension to three-center integrals, the use of extended atomic-orbital bases, and a better description of parameter scaling with distance. The reliability of empirical interatomic potentials may also be enhanced by further investigation.

Finally, there exists a need for improvement of algorithms that can determine stable configurations in systems with very large numbers of degrees of freedom. Traditional algorithms such as conjugate gradient and simulated annealing may prove inefficient in very complex systems. The recent use of genetic algorithms to optimize the structure of large numbers of carbon atoms is an example of interesting new directions. The problem is even more severe when saddle-point configurations are sought in a very large configuration space.

In all the above examples further exploratory work is needed. Perhaps the most efficient way to pursue this type of work is in the traditional mode of single principal investigators, in charge of small groups of post-docs and graduate students.

(4) Links within multiscale physics

The results of electronic-structure and atomistic calculations are essential in developing insight into microscopic processes. These results are often capable of addressing important materials issues, including bulk and surface diffusion, chemical effects in interface adhesion, bulk phase transitions, etc. However, in many materials problems, it is desirable to make links between the

microscopic phenomena and macroscopic variables. At present, the links between such domains of multiscale physics are made through passing of parameters. For instance, activation energies, and in some cases free energies, can be calculated for certain microscopic mechanisms responsible for long-range mass transport. While this has often been a fruitful method, a more integrated approach between the atomistic and longer scales (both temporal and spatial) would potentially constitute a more powerful tool for materials modeling.

Efforts for a more integrated approach between various length and time scales for materials modeling are in nascent form. Much needs to be developed in this direction, including possibly new concepts and methodologies. These activities are of exploratory nature, which makes it difficult to provide specific recommendations for their future direction. In terms of general recommendations, it is suggested that:

(i) specific areas and problems should be identified where an integrated approach may provide breakthroughs in materials modeling. The idea of multiscale integration does not necessarily apply to every conceivable problem, and in fact may be ineffective in several areas. Identification of the proper areas for future work on multiscale integration is an essential first step toward this goal. Possible examples where integration may prove useful are dislocation dynamics and rheological problems in polymer melts;

(ii) small groups of investigators from diverse backgrounds should be brought together to work closely on specific problems for multiscale integration of materials modeling. The groups should be well-focused and diverse enough to include specialists from the various areas necessary for the integration (e.g. atomistic calculations and continuum elasticity). It is expected that such close collaborations will succeed in developing some of the basic methodologies and certain new concepts that can serve as examples for wider application of the integrated approach.

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