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Is Computational Materials Science Overrated?

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Computational materials science is one of the fastest growing disciplines in materials science. With an ever-growing number of papers in this area– there are journals devoted entirely to the subject – and with the number of scientists involved in materials modeling increasing rapidly, the time is right to examine what impact computational materials science has had on the materials community. How one defines that impact depends on what questions are asked. One could examine what role computational modeling has played in the development of new materials or, perhaps more importantly, what breakthroughs in our fundamental understanding of materials behavior can be attributed to computational modeling. However, given the hyperbole that sometimes is associated with computational modeling, a more provocative way to phrase the question might be: "Is computational materials science overrated?"

As practitioners of computational materials science, we would like to answer with a robust and confident "No." To be honest, however, the answer is probably more of a humble and slightly embarrassed "Yes."

Too often the expectations about what modeling can deliver exceed the actual product. It is interesting, however, that these inflated expectations often belong more to non-practitioners than to those of us who do this work on a regular basis. If one asks someone in the computational "trenches" about the tools available to them today, one would (we think) get the very rational

response that, while our tools hold great promise, they still need substantial development. That these tools are deficient is not surprising – computational materials science is a field only a few decades old. Thus, we feel we need to focus as much on the promise of the field as on its current status, where, for such a young field, there have been many striking successes that range over many phenomena encompassing many length and time scales. We will discuss a few representative examples of these successes here, while apologizing to our colleagues who we do not mention. We will also mention some of the limitations to the methods we have available.

Perhaps the most fundamental type of computational materials science is the calculation of the electronic structure of solids. Such computations have clearly had great successes in the prediction of materials structure and properties. Lattice constants can be predicted for many crystalline materials to within a few percent of the experimental values. Recent calculations of elastic constants[1] yield results in very close agreement with experiment, yet are far easier to determine. Developments in many-body theory now allow for the prediction of band-gaps in simple semiconductors.[2] A most striking example is the work from Marvin Cohen's group on the prediction of the pressure dependent properties of silicon, including the existence of a superconducting state, and a reasonable value for the transition temperature.[3] What makes this work so compelling is that it constitutes the prediction of complex, many-body macroscopic response using fundamental computational materials science. Indeed, in our opinion, the notion that one can begin with the atomic number of an atom and end up with a quantitative prediction of lattice and elastic constants and even the superconducting transition temperature is truly amazing. If computational materials science is overated, it is certainly, in some part, due to past successes.

However, based on such successes, electronic-structure calculations are, many times, presented as being more exact than they actually are. There are many approximations inherent in these calculations (after all, LDA does mean “local density approximation”), and it is easy to obtain misleading and, quite possibly, incorrect results. Further, the approximations restrict the range of applicability, and a technique which is suitable for silicon may fail dramatically for a magnetic oxide. Perhaps the most serious limitation to these approaches is the small system sizes that can be studied. Development of parallel computing is improving these prospects somewhat, though the ability to calculate systems with more than a few thousand atoms is some ways off.

Moving up in scale brings us to atomistic simulations. Given where we were just a few years ago, the progress in performing atomistic simulations has grown tremendously. Of course, much of that progress is due to faster and more easily available computers and software. An important success for atomistics has been to couple the simulations with experiment to extend the capabilities of both. An excellent example is how comparison of atomic scale structures with HRTEM images can lead to a much better understanding of grain boundary structures.[4] Without the simulation results, one

would not be able to interpret fully the high-resolution images. Another successful application of atomistic simulations has been in the study of the properties of individual defects, such as grain boundaries or dislocations, where defect structure/property relations have been mapped out for a number of classes of materials.[5] The use of atomistic simulations has also led to dramatic successes in the study of thin film growth. Very simple atomic scale simulations can be used to understand the kinetics describing attachment and detachment of atoms from islands.[6] More complicated models can be used to predict dopant profiles for ion implantation in Si.[7]

The limitations of atomistic simulations include the descriptions of the interatomic forces, the size of the systems to be studied, and the inherently small time scales. While some progress has been made in the development of robust interatomic potentials, these are often rather inaccurate and thus calculations based on them are only approximations to a real material. Thus, it is often better to use atomistics to study phenomenology rather than to make predictions of the properties of specific materials. The examples given above were generally of this kind. System size is a great limitation for some applications. For example, a cubic micron of copper contains approximately 10^{11} atoms. Calculations with that many atoms exceed the computational capabilities of even the biggest computers of today by at least two orders of magnitude. In our opinion, the most difficult limitation of atomistics is the time scale. In molecular dynamics, all atomic motions are included. Thus, the fundamental time step must be small enough to capture the very fast atomic vibrations, which limits the time step to the order of 10^{-15} seconds. A million time steps or so are thus needed to model a nanosecond of time – a severe computational constraint. Further, the study of a larger number of atoms implies that one must study phenomena over larger time scales. Recent work has indicated that there are ways to increase the time scale for certain classes of activated processes.[8] Though promising, the impact of these methods is as yet unclear.

In much of materials science, it is the interaction of groups of defects that define the materials response. For example, plastic deformation requires the movement of many dislocations. Atomistics, while useful for individual defects, cannot cover the length and time scales needed for such simulations. A promising approach to study deformation phenomena is called dislocation dynamics, in which the dislocations are treated as the fundamental entities of the simulations. The forces on the dislocations are calculated and the equations of motion are solved over time, much as in molecular dynamics. Much quite impressive work has been done in this area, including the development of fully three-dimensional simulations.[9] However, while having some partial success stories, for example developing an understanding of dislocation interactions in strained epilayers,[10] dislocation dynamics simulations have not had a significant impact on the modeling of the properties of real materials.

Why have dislocation dynamics simulations not produced demonstrable success stories? There are a number of technical limitations to the methods as now used, a discussion of which is beyond the scope of this article. Improvements to the methods will certainly be incorporated in these methods over time. However, the real difficulties lie not within computational materials science itself, but rather with the link between experiment and theory. In almost all of the success stories in computational materials modeling, the experiments with which the simulations are compared are relatively straightforward both to do and to interpret – in essence, the theory for the macroscopic phenomenon is well developed. For example, superconductivity can be measured with a few wires hooked to the sample. Mechanical properties, however, are not easy to describe in terms of fundamental processes. We simply do not know how to reduce the many degrees of freedom of the dislocations to the relatively few parameters needed to describe the macroscopic experiments.

It is in this capacity that computational materials science offers the most promise. Simulations may be used to explore the interactions of defects with a level of detail simply unavailable to current experiment. These details can then be used to construct the necessary theories. Where the true promise of computational materials science lies, then, is in establishing the meeting between the experiment and theory of these complex phenomena. Experiments are being performed on smaller and smaller scales, while calculations are being extended to larger and larger scales. When the two finally meet, there will be an explosion in our level of understanding.

There are many other types of modeling that have had important successes and we certainly cannot describe them all here. As one example, grain growth modeling, done with a rather large variety of methods, has nailed down the rate equation of coarsening.[11] In the same field, the effect of particle pinning continues to be rather controversial, but simulations are leading the way to a deeper understanding of this important phenomena.[12] On a larger scale, computational materials simulations have re-invigorated the study of the effects of texture because they enabled us to make useful predictions across the entire range of experiments.[13] Such successes are found in many other fields as well, from polymer science, to composites, to manufacturing. In almost all cases, however, the modeling provides a guide to a better understanding of the materials science and does not yield a definitive prediction of the behavior of specific materials. It is only by coupling the modeling with experiment can progress truly be made.

An important component in the future of computational materials science is the incredible increase in computer speed over the past two decades. These increase have occurred both in the desktop computers that we all have available as well as in the high-end of computing, where the largest machines today perform trillions of operations per second, a ten-thousand-fold increase over the fastest computers at the beginning of this decade. The opportunities afforded by these new capabilities are enormous, from the extension of each of the modeling methods at their individual

scales to the ability to connect phenomena at many scales within a single calculation. An important example of the latter is the recent work on coupling atomistic simulations within finite-element calculations.[14] By incorporating more complete descriptions of the sub scale science within a simulation, we may be able to avoid many of the approximations needed today.

We are optimistic about the future of computational materials science. The tools we have today are certainly not uniformly of high quality, but the improvements over the past few years have been significant. However, we wish to interject a cautionary note to the overall optimistic tone of this article. Whether computational modeling grows into an important part of materials science depends greatly on who owns the field. If it is not owned by the materials community then it will likely lead to too much "discovery" of what is already known and to many irrelevant or redundant calculations and the field may well wither and die. To be a successful enterprise, computational modeling must be embraced as a new discipline of materials science. For that to happen, university materials departments must develop a curriculum to train this new kind of materials scientist. The training must include not only materials science, but also the fundamentals of mathematics and computational science needed to perform first-rate simulations. These latter subjects are rarely available to students in materials science today, but must be if computational materials science is to grow to a point where the answer to the question posed in the title of this article is a resounding "No."

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