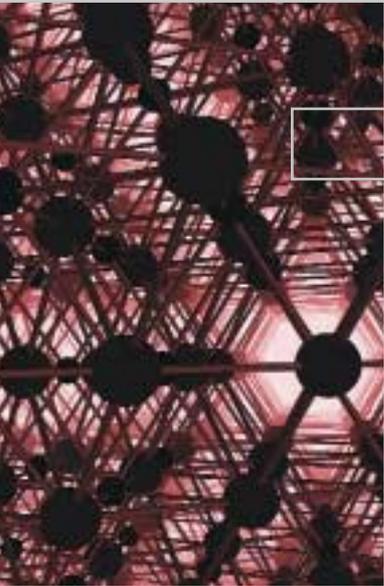


By Victor D. Chase

Meeting Materials

EFFICIENCY, STRENGTH, AND LONGEVITY, all highly desirable attributes of life, are equally applicable to the world of inanimate, manmade objects. And just as medical researchers strive to bring these characteristics to the living, so too do materials scientists endeavor to make them a reality for artifacts.



>> Astrophysics

>> Nanoscience

>> Climate Change

>> Laser Physics

>> Computational Medicine

>> Radiation Transport

>> Computational Biology

>> **Materials Science**

And just as advanced technology has given new tools to those medical researchers, so too has it furthered the quest of materials scientists, primarily through the power of computer simulation.

Most of the inanimate objects in question are made of either metallic or ceramic materials, both of which are actually conglomerations of minuscule crystals. What looks like a solid aluminum spar of an aircraft wing, for example, is really a mass of microscopic crystals. And the spaces between those crystals, which are occupied by a world of rapidly moving atoms, constitute the weak links in the material. Hence, if that spar fails, it will likely crack along the boundaries between those crystals. While engineers know approximately how long that aluminum spar will last, what they don't know is where and how it will crack. So, to prevent any untoward surprises, they over-design that spar, making it heavier than it would have to be if the reasons behind a potential failure were more fully understood.

And that's where Dieter Wolf and his colleagues at Argonne National Laboratory (ANL) come in. Wolf is a senior scientist and leader of the Interfacial Materials Group, which is responsible for developing computer simulations to learn what is going on in those spaces between the crystals.

"Material's microstructure is what controls the properties of the material," explains Wolf. "The nature of bonding of the atoms in individual interfaces and the entire spatial network of these grain interfaces is what controls the properties, and that's what we try to understand by simulation."

And because Wolf's group uses simulation methodology that is not material specific, their work can apply to virtually everything from aircraft wings and jet engine turbine blades down to the submicron-sized features of modern electronic circuitry.

Predicting and Preventing

Two primary goals drive this work. One is to develop an understanding of the characteristics of materials so that engineers have a better understanding of the tolerances of the materials used in their designs. The other is to provide information that can be used to improve the characteristics of various materials for given applications during the manufacturing process.

An engine's turbine blades, for instance, are exposed to hundreds of degrees of temperature as they spin at thousands of revolutions per minute. As a result, small changes are constantly taking place in the blades' polycrystalline microstructure, but these changes cannot be empirically observed as the turbine blades turn.

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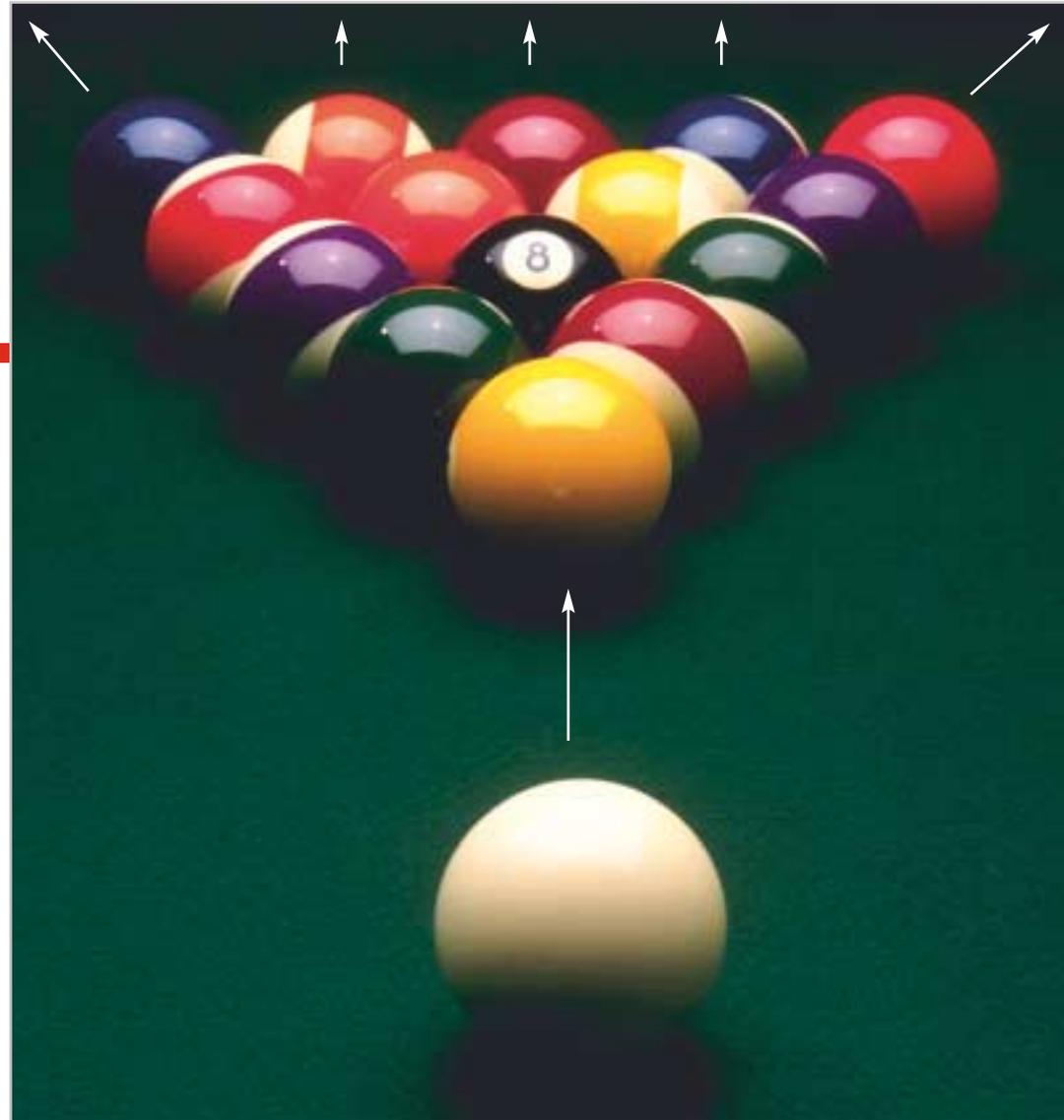
of this material under these high temperatures and stresses so you can predict how long it will last...The goal is to develop a predictive modeling tool such that the engineers one day down the road have a better way of predicting how the material will behave over time," says Wolf.

And, he adds, "if you want to reduce the weight of a jet engine, it would help enormously if you understood the underlying processes, so the goal of materials simulation is to put a lot more of the physics of the microstructure into [engineering] models," says Wolf. "If you could do that, you could tailor the microstructure of the materials. The big goal is to increase the power-to-weight ratio by a factor of 50 to 100 percent over the next 20 years."

A "Catch-22"

The fact that most solids have crystalline structures has been known for about 100 years, but only since the mid-1990s — as a result of the development of powerful computers — have researchers had the ability to use multi-scale materials simulation to probe the secrets of the microstructures within these polycrystalline materials.

Yet the microscopic boundaries between crystals do not readily reveal their secrets. One of the



quandaries they pose is the "Catch-22" of materials science: to view the internal boundaries of a material would logically require cutting into the material, but once that is done, the interior surfaces become the exterior surfaces and their very nature is changed. It was to overcome such empirical limitations that researchers turned to computer simulation.

And that brought them right up against yet another seemingly insurmountable blockade. Specifically, to create computer simulations requires at least some

empirical evidence of what is going on in the crystals' boundaries, or else the models would be pure guesswork. To skirt this problem the researchers devised an ingenious two-pronged approach.

First, they applied a basic understanding of physics, such as Newton's laws of motion. These same laws of motion apply to atoms as much to a large ball. And while understanding this is

DIETER WOLF

Dieter Wolf received his PhD from the Max-Planck-Institute for Metals Research in Stuttgart, Germany. He has been the Senior Physicist and Group Leader of the Interfacial Materials Group, Materials Science Division at Argonne for over 15 years. Dieter won the Basic Energy Sciences Award for Sustained Outstanding Research in Metallurgy and Ceramics for work on Computer Simulation of Interfacial Materials and Phenomena in 1997.

Further Reading

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Exact Method for the Simulation of Coulombic Systems by Spherically Truncated Pairwise 1/r Summation, D. Wolf, P. Keblinski, S.R. Phillpot and J. Eggerbracht, *J. Chem. Phys.* 110, 8254-82 (1999).

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important to the development of materials simulations, it is also important for the scientists to realize that at the microstructural level — one of the three length scales that multi-scale materials simulation examines — the physics is different. Specifically, as polycrystalline materials are subjected to stresses, the boundaries between their crystals move. As they do so, they follow a viscous law, in that the forces exerted upon them cause them to move at a constant speed — much like a glass bead sinks slowly and steadily in a glass of water. The result of this motion is heat rather than increasing velocity. This distinction between Newton's law and the viscous law of motion is important when it comes to modeling the activity of materials.

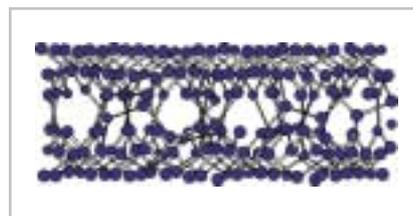
Wolf, himself a physicist, and his group apply this knowledge to building models that look at both the activity within individual grain boundaries and the interaction of all the boundaries within a material. They take this approach, rather than examining what happens to all of the boundaries at the atomic level, simply because the number of atoms involved make such a task onerous. There are simply too many of them. Hence, says Wolf, "You throw away thinking about the atoms, but you incorporate what the atoms do in the grain boundaries."

A Physicist's Best Friend

In addition to applying these basic physics concepts to the development of materials simulations, "in some very specialized cases there are experimental techniques available to statically probe the atomic structure of the interface," says Wolf. But even then, he adds, "it's extremely difficult to obtain that information and you can only get such information on certain types of internal interfaces."

Nanocrystalline diamonds provide a case in point, since their innards can be probed nondestructively by light in a technique known as Raman scattering. Nanocrystalline diamonds are synthetic diamonds being developed at Argonne, which have grain sizes in the nanometer range. This is considerably smaller than the micron-sized grains found in conventional polycrystalline materials — a nanometer being one-billionth of a meter, or about 10 times the size of a single atom. And, in fact, natural diamonds, such as those used in jewelry, are single crystals and therefore have no grain boundaries.

The non-invasive Raman light scattering applied to nanocrystalline diamonds is possible because, though different chemically and structurally, diamond and graphite are two different phases of the same material: carbon. Diamond is the hardest material known, while graphite is soft enough to be used as pencil lead. And, in fact, industrial diamonds are created by compressing graphite.



Above:
Atomic structure of a representative grain boundary in nanocrystalline diamond, revealing that approximately half of the atoms are graphite-like. The top and bottom perfect-crystal grains are terminated by diamond surfaces which are rotated relative to each other, thus forming the grain boundary.

By probing a nanocrystalline diamond with light and observing how the light is scattered, the extent to which graphite is present can be determined, and from that, other characteristics of the material can be extrapolated. "The Raman scattering gives a peek inside" the diamond, says Wolf, but "the simulations teach you a lot more than the experiments."

These experiments have shown that two to three percent of all the atoms in a nanocrystalline diamond are graphite-like. And since it is known that the crystals in a diamond are pure and contain no graphite, whatever graphite shows up in the light-scattering experiment should be in the boundaries between the crystals. It is also known from experimentation and simulation that about five percent of all the material in a nanocrystalline diamond is in the grain boundaries.

"In some very specialized cases there are experimental techniques available to statically probe the atomic structure of the interface."

diamond



“When we perform simulations on these grain boundaries to find out what their atomic structure might be, we find that about half of the atomic bonds in the boundaries are graphite-like. Therefore, 50 percent of five percent of all the atoms in nanocrystalline diamond, or 2.5 percent of all the atoms, exhibit graphite-like bonding,” says Wolf.

This both verifies the accuracy of the simulation, since it arrives at the conclusion observed from the light-scattering experiments, and gives more detailed information than does the Raman scattering, which leads to a better understanding of the material, which gets to the heart of multi-scale materials modeling.

Reversing Diamonds

Nanocrystalline diamonds also provide an example of how materials modeling is being used to help tailor specific materials to give them desirable characteristics. In this case the nanocrystalline diamond program at Argonne is reversing the characteristic of conventional diamonds, which are normally

very good insulators, by turning them into conductors of electricity. These ultra-small crystal diamonds are created using vapor deposition, a process similar to that used in the manufacture of semiconductor chips. “The idea is to choose deposition conditions such that as the vapor gets deposited on an amorphous substrate, little crystallites form,” says Wolf. The result is diamond crystals with grain sizes in the 5 to 10 nanometer range, which gives the nanocrystalline material unique properties.

“You have steep gradients in the structure, which gives an opportunity to develop entirely new materials with properties that one never expects for these materials, and to understand those we use computer simulation,” he says. It was just such simulation that showed that these diamonds are conductive because of the graphite found in their grain boundaries.

This new type of diamond material is also being tested for use as a virtually friction-free coating that holds promise for extending the life of machines in which severe operating conditions create significant wear.

Purpose of the Work

“The whole purpose of the work here is to develop a fundamental understanding of materials microstructure, which is relevant to many different technologies,” explains Wolf.

“We develop the fundamental knowledge that allows the application-oriented programs to develop more sophisticated approaches to the

processing of their materials to understand why they fail and how they fail. The ultimate goal is to develop an industrial type modeling tool which connects with the fundamental materials physics in a much more truthful way than has ever been possible.”

He adds, “To have physically faithful models that properly incorporate all of the atomic-level physics into the long time-scale and spatially large-scale problem of predicting the lifetime of engineering structures is a real challenge.”

A SCANDINAVIAN WARRIOR

>> ***Wolf and his crew have proven to be as resourceful in fashioning the computer hardware on which they run their highly complex simulations as they are in developing the materials modeling software itself.***

Their computer configuration is known as a *Beowulf* cluster, after a Scandinavian warrior whose name is the title of an Old English epic. In this case, the warrior’s super powers are those of a supercomputer composed of off-the-shelf personal computer components. The idea of tying a cluster of less powerful computers together to make one superpowerful computer originated during the mid-90’s and has since become popular with researchers and academics.

Wolf and his colleagues opted for the *Beowulf* approach for a very simple reason: money.

True supercomputers cost millions of dollars, and demand for time on them is great. On the other hand, “We have a cluster supercomputer that you can buy at Circuit City for \$50,000,” says Wolf. And, they have access to their homemade supercomputer 24/7. Actually, Wolf’s Interfacial Materials Group splurged and spent \$65,000 on their 100 node cluster, but that includes the graphics terminals and the switching equipment that allows the processors to be connected in parallel so they can communicate with each other while working on the same problem.