

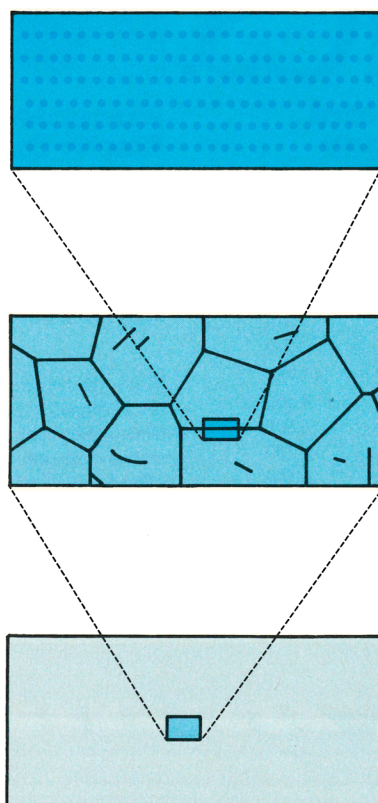
WHAT IS MATERIALS PHYSICS, ANYWAY?

Sokrates T. Pantelides

"Materials" have become a dominant theme in discussions of our national science and engineering agenda. Several reports have concluded that US competitiveness increasingly hinges on our ability to develop materials for improved energy efficiency, function and reliability at lower cost. The research community has been marching with the times: Witness the growth of the Materials Research Society and the materials physics division of the American Physical Society; witness the fact that last year 25 universities responded to a call from the National Science Foundation for proposals for new materials research laboratories, even though it was uncertain whether more than one new MRL could be funded.

This column will address some relevant questions: What is materials *physics*? Is the physics community playing an appropriate role in the "materials revolution"? And what should the community's agenda be for the next decade? I will give my own perspective, which was formed during years of physics research and management.

For several decades, the members of the physics community working in the field variously called solid-state physics, condensed matter physics or materials physics have focused their attention and energy on elucidating the atomic, electronic and magnetic properties of bulk prototype solids (metals, semiconductors, insulators, superconductors and disordered systems), crystal surfaces, interfaces, artificial structures (superlattices, quantum wells and quantum dots) and defects. They have developed a vast array of powerful experimental



Schematic illustration of the microscopic (top), mesoscopic (middle) and macroscopic (bottom) length scales in a polycrystal.

and theoretical techniques to study electronic and magnetic properties, the positions and dynamics of atoms, and various phase transformations. The success of this discipline and its impact on technology and industrial development have been phenomenal. For example, the invention of the transistor directly resulted from the recognition of the significance of hole conductivity in semiconductors. Solid-state lasers and the scanning tunneling microscope are other examples from a long list of such successes.

The mainstream physics community, however, has largely ignored a

wide range of key materials issues. Real materials are highly heterogeneous. Except for semiconductor devices, virtually all other industrial materials are polycrystalline, amorphous or composite. Most properties of these materials are determined by their collective microstructure, namely the size and orientation of grains, dislocation networks, inclusions, precipitates and microvoids (see the figure). Such microstructure is not in an equilibrium state and therefore evolves through deformations and diffusive processes, especially under external stresses or current. Clearly, in such materials the link between atomic structure and macroscopic properties is not direct. An intermediate length scale exists that provides the link. This intermediate length scale is pervasive even in the cases where single crystals are used: Impurity profiles determine the electrical properties of semiconductors, magnetic domains determine the magnetic properties of magnetic materials and so on. The term "mesoscopic" is appropriate for this intermediate scale.

The practices of the physics community illustrate my point. Take the standard solid-state physics textbooks of the last 30 years: Polycrystalline materials, microstructure, mechanical properties and diffusion-mediated phenomena are barely mentioned. They typically focus on electrons and phenomena related to elementary excitations in prototype crystals. Real materials have been mostly left as the domain of other academic disciplines.

The same pattern is evident in the contents of the premier US physics journals and in the programs of APS March meetings. At the 1992 meeting, there were 11 sessions labeled "materials theory." Virtually without exception, all papers reported atomic-scale or electronic-structure calculations. In fact this pattern was pervasive throughout the entire meeting. Only a few sessions and papers dealt with issues other than atomic-scale and electronic properties. This

Sokrates Pantelides is a research staff member at the IBM T. J. Watson Research Center in Yorktown Heights, New York. His research has been primarily in atomic-scale theory of materials. He has served in several science and technology management positions.

decade-old trend has persisted even with the advent in 1984 of the materials physics group, which recently became an APS division.

An examination of the *Bulletin of the American Physical Society* from previous meetings reveals another significant trend: Every few years a new theme captures the imagination of a large fraction of the community. Recall the days of electron-hole drops, charge-density waves, the TTF-TCNQ compounds, surface reconstruction, and quasicrystals; interest in high-temperature superconductivity continues to be strong, and buckyballs are causing the latest stir. There is always excitement about the *prospective uses* of novel phenomena, materials and devices. But the community has not been driven by any major themes that underlie the industrial use of materials.

In reality, a substantial gap exists between the usual focus in physics and the materials physics actually relevant to industry. The physics community has had its biggest impact on industry in electronic applications. Manufacturability and mechanical properties are, however, pervasive and important industrial concerns. Though the fundamental physics underlying these concerns boils down to atomic rearrangements, advances in atomic-scale physics usually do not affect industrial competitiveness. The problem is the link between the atomic scale and the length and time scales that are relevant to industry. In most cases, the link is the regime of mesoscopic atomic dynamics. Two examples help make the point.

First, we take a materials processing issue, namely the etching of Si by F ions in microelectronics. Atomic-scale physics has successfully probed experimentally and theoretically the underlying atomistic processes, such as the breaking of subsurface Si-Si bonds by F ions. Theory even accounted for the observed dependence of the etch rate on the Fermi level. But the crucial question for technology is the shape of the etched trench. The relevant physics would need to fold the atomistic understanding into a mesoscopic formulation in terms of atomic fluxes and surface strains, a task that poses both experimental and theoretical challenges.

As a second example, we return to polycrystals and microstructure. Atomic-scale probes of grain boundaries and dislocations are essential but are not the whole story. Most properties of polycrystals are determined by their collective microstructure. For example, microstructure controls the strength of steel and "earring" in

aluminum cans—a deformation of sheet aluminum shaped into cylindrical cans. In microelectronics, thermal stresses and current induce voids and extrusions in polycrystalline metal interconnects.

Traditionally, the collective behavior of the microstructure is captured into a set of constitutive relations. This is the continuum mechanics approach, a venerable and mathematically rigorous discipline that describes successfully many macroscopic phenomena. Describing the microstructure and its evolution is a tougher problem, however. Existing theories are based on continuum mechanics—for example, elasticity theory of dislocations or plasticity theory of crystals—or on hybrid approaches that combine continuum and atomistic concepts. But no comprehensive theoretical framework exists that is directly derivable from atomic-scale theories, that describes the formation and evolution of microstructure at the appropriate length and time scales, and that establishes a connection with corresponding macroscopic properties. New experimental techniques and new theories are needed to advance this frontier.

These observations naturally raise questions about basic versus applied physics. There is a common misconception that basic is synonymous with atomic-scale physics and that the study of properties at higher-order scales such as microstructure or plasticity belong to applied science. In reality the long-term intellectual challenges in these latter areas are just as compelling as those ordinarily defined as basic. They also transcend specific products, as my two examples illustrate, and they are "basic" in the sense that the primary objective is to unveil nature's mysteries, as manifested in industrial materials.

Basic physics does not and should not stop with atomistic understanding, but should follow through to higher-order scales. The physics community needs to strike a better balance between the atomic scale and higher-order length and time scales and to enter into new relationships with other materials-related disciplines such as metallurgy and mechanics. At the same time, the long-term industrial needs for materials physics need to be articulated. It will take a new type of partnership among universities, national labs and industry to chart out an agenda for materials physics that will directly enhance national competitiveness. Government funding agencies and APS can play a key role in formulating and promoting such an agenda. ■

Principles of Science



A Grand Unified Theory of All Science

Joseph M. Brown

The Neutrino

Donut flow of ether gas twists and translates with velocity of $v_r - v_m$

Completely condenses ether at core

Core "mass" varies greatly from one neutrino to next

Most basic organization element of the universe

Geometric size limited by mean free path of background ether

Inflow independent of core mass

Outflow momentum jump and thus propelling force is independent of core "mass"

Angular momentum unbalance is produced by velocity jump $v_r - v_m$ and with constant flow for all energy neutrinos the angular momentum unbalance is constant at $\pi/2$

Basic Research Press

120 E. Main Street
Starkville, MS 39759
(601)323-2844
FAX (601)324-5619

218 pg. 1991

\$39.95

ISBN 0-9626768-0-2

Visa/MC/AMEX/Discover/Checks

Circle number 28 on Reader Service Card