
THE SUPERDISCIPLINE

A Commentary On The Emergence and Evolution of 'Materials Science'

By David Turnbull

David Turnbull is a former recipient of the Arthur Von Hippel Award of the Materials Research Society. In this insightful essay, he demonstrates that materials science is significant for its interdisciplinary nature, and argues that this cooperative spirit is threatened by the mounting pressure toward specialization.

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Materials Science might be defined broadly as the characterization, understanding, and control of the structure of matter at the ultramolecular level and the relating of this structure to properties (mechanical, magnetic, electrical, etc.). In professional and educational practice, however, Materials Science is viewed rather more narrowly (1) as the science of the more complex features of ultramolecular behavior, especially those controlled by the various point and extended imperfections. Indeed, the unique role of those who would label themselves as Materials Scientists *primarily* is, perhaps, to provide instruction and guidance on the structure delineated by the extended imperfections (interphase and intercrystalline boundaries, dislocations, etc.)—its characterization, origin, and property effects. Of course, the research activities of these scientists are typically much broader, often ranging far into condensed-phase physics and chemistry.

Materials technology is, of course, thousands of years old and a science of materials, though labeled only recently, has existed for a long while. We might even trace the beginnings of Materials Science back to the Ionian atomists who seem to have been led to their atomic theory from realization that the identity and quantity of a material persists through a succession of transformations (e.g., freezing→melting→evaporation→condensation) (2, 3).

In the modern era the early preoccupations in the science from which Materials Science developed were with the characterization and understanding of perfect crystals and the conditions for the coexistence of phases. Early in this century this science had progressed to a stage where it became clear that some of the most important transport and mechanical properties of solids could not be explained by



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ideal crystal models. To resolve these problems the point and line imperfection models for crystal behavior were devised. It is quite remarkable that these models achieved success by requiring that only a minute fraction (typically less than one per million) of the atoms be displaced from their positions in the ideal structure. Such extreme structure sensitivity of properties seemed offensive to some but fascinating to others.

The point defect models for transport (electronic, ionic, or atomic) were accepted rather quickly, owing perhaps to the realization that point defects, despite their considerable energy cost, would be stabilized entropically to appreciable concentrations at higher temperatures. In contrast, extended imperfections increase entropy so minutely that, at

thermodynamic equilibrium, they should be virtually absent from finite crystals to quite high temperatures. Nevertheless, models for crystal plasticity and growth required that line imperfections, despite their metastability, be present and operative under nearly all experiential conditions. Without clear mechanisms for the introduction and retention of such imperfections in crystals, models based on their operation met with considerable resistance.

However, this resistance collapsed as a result of some quite remarkable investigations in several laboratories around mid-century. There were the studies of Bragg, Nye, and Lomer (4, 5) showing the introduction and movement of dislocations, when a shear stress was applied, in rafts to uniform soap bubbles in crystalline arrays. There followed the microscopic observations demonstrating that dislocations existed and acted in actual three-dimensional crystals in the ways that had been forecast (6-11). [Ed. Note: Cited here is the work of the MRS's 1983 Von Hippel winner, Sir Peter B. Hirsch.] Also occurring in this period were discoveries, more or less guided by the new knowledge, of methods (12, 13) for preparing virtually dislocation-free crystals that exhibited mechanical strength (14, 15) or growth resistance (16-18) nearing the levels predicted by the ideal crystal models (17).

These achievements were impressive, not only for vindicating the slightly defective crystal models, but also for the remarkable interdisciplinary interaction—especially between physicists, metallurgists, and chemists—with which they were made. It was, I think, the manifest effectiveness of this interdisciplinarity that gave rise to the consciousness of a sort of superdiscipline, which came to be labeled Materials Science.

How such interdisciplinary cooperation developed is not obvious. A key role probably was played by certain leading physicists—Mott, Seitz, Shockley, and Zener, [Ed. Note: Clarence Zener, the 1982 Von Hippel winner.] among others—who were attracted by the challenge that the more complex features of solid structure and behavior posed to the new understanding of interatomic cohesion. Also of great importance was the growing realization that, depending on the processing, very different metastable, or even unstable, configurations and densities of imperfections could, at constant composition, be frozen into solids with consequent wide property variations. Thus it appeared that, guided by the new understanding of defective crystal behavior, new materials formation and processing methods might be devised that would greatly improve important physical properties. It was thought that, ultimately, by such “ultramolecular engineering,” new materials might be made to fulfill a wide range of new applications demands. It was this prospect that

attracted applied scientists, from high technology industry as well as universities, and made them especially receptive to cooperation with those more motivated toward theoretical understanding. Interdisciplinary groups were formed in certain industrial laboratories to carry out wide-ranging solid state research programs, which frequently led to key contributions to basic understanding as well as to technology. Especially notable both for their achievements and interdisciplinary range were the Shockley Semiconductor group at Bell Laboratories and the Hollomon Metals and Ceramics group at General Electric. The authoritative structure of industrial research management, while having some serious drawbacks, is well suited to the promotion of interdisciplinary interaction. However, such interaction also marked solid state studies at certain universities, for example, in Nevill Mott's Bristol group and at Chicago's Institute for the Study of Metals under the leadership of Cyril Smith. The achievements, scientific and technological, in these and other laboratories provided much of the stimulus for the emergence in the 1950s of consciousness of a Materials Science “superdiscipline.” Especially impressive were the developments, based in large part on new methods of ultrapurification and impurity doping of materials, which led to the technology of solid state electronics.

In fields other than electronics the technological return from the new knowledge of materials seemed, initially, somewhat disappointing. For example, while the microscopic understanding of plastic deformations and internal structural evolution was greatly advanced in the 1940s and 1950s, the art of materials compounding and processing had been so well developed that Materials Scientists could do little more than assure technologists in these fields that their practices were, at long last, understood and, apparently, nearly optimum. However, the situation has, I think, been changed quite dramatically by advances in the past two decades leading to the synthesis of a wide variety of novel metastable structures. Stimulated by these discoveries, research on the synthesis and characterization of such structures has become one of the major activities in Materials Science, as is reflected by the considerable number of articles devoted to it in the present, as well as earlier, volumes of this series.

Actually, virtually all solids used technologically are configurationally frozen from states that often were metastable, or even unstable, before “freezing” (i.e., slowing of the atomic motions that alter local configurations to negligible rates). The most common type of metastability

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exhibited by these solids is the morphological, arising from the presence of considerable densities of extended imperfections—intergrain and interphase boundaries and dislocations. However, there is also in such solids quite widespread occurrence of nonequilibrium atomic level dispersions of impurities and of topologically metastable structures. The recent developments are most notable for the synthesis of metastable structures in all these categories, which are much further out of equilibrium as indicated by their excess energies relative to the stable states, than those known heretofore. Also they have exposed a state, the glassy metallic, not previously recognized. The discovery of this state by Pol Duwez and his students (19-21) provided much of the early stimulus, especially in metallurgy, for research directed at the synthesis and understanding of new metastable structures.

The general method in metastable structure synthesis is to energize a material and then deenergize or quench it (22). In the familiar high pressure technique, the new phase is “brought back alive” by configurational freezing before removal of the stabilizing pressure. In low pressure synthesis, materials are energized, for example by heating, dissolution, irradiation, or plastic deformation, and then rapidly deenergized, for example by quenching or some condensation technique.

The most recent advances in metastable synthesis have resulted in part from some application of newly developed techniques, such as laser pulsing, ion implantation, and ion beam mixing, and from exploitation of old techniques, such as cold working. The newer methods generally make possible much higher energy fluences, both into and out of thin sections or columns of materials, than could be attained with the older procedures. When thermalized, these fluences give rise to ultrahigh rates of up or down quenching (23). They can also produce local condensed regions with much higher energy content than can be reached in macroscopic thermalization.

Perhaps the most outstanding of the recent achievements have been the syntheses of several materials: (a) Glassy metallic alloys in a wide variety of compositions (20, 21, 24). (b) Amorphous solid phases of various elemental and compound semiconductors, including such a phase of Si formed by melt quenching (25-27). (c) Numerous crystalline and amorphous solid solutions with compositional homogeneities ranging far beyond those attained by conventional processing. In principle, it should be possible, by condensation, ion implantation, or ion beam mixing on substrates held at temperatures below those of configurational freezing, to form homophase solids of arbitrary composition (22). These possibilities seem to have been nearly realized in

some recent experience. An example is the formation by sputter codeposition (28) and also by ion beam mixing (29) of Ag-Ni solid solutions with solute concentrations about 50 times greater than at equilibrium in the liquid phases at the pure Ni melting point. (d) Structures with exceptionally high interfacial densities. These include compositionally modulated films (30) with modulation wavelengths as low as 1-2 atom diameters and one-dimensional superstructures (31, 32), e.g., of semiconducting compounds, with one-atom layer spacings. Also in this category are ultrafine interphase dispersions with relatively high interphase boundary energy formed by cold reduction (33). Some of these dispersions also are unique for the extremely high density ($\sim 10^{13}$ to 10^{14} cm/cm³) of dislocations trapped in one of the phases.

Probably it is much too early to predict the technological return from these advances. Since most of the methods make novel structures available only in thin section form, it seems likely that much of the return will be to the technology of thin films and surface modifications. It appears that the new structures (e.g., microcrystalline and amorphous alloys) formed in rapid melt quenching can be produced in large quantities at low cost. However, the difficulties and costs of quality and process control have not yet been adequately assessed.

There Is A Serious Danger The Trend Toward Specialization May Set Back The Development Of Materials Science

The novel structures produced in these low pressure syntheses are generally much more disordered compositionally and/or topologically than the structures on which the efforts of Materials Scientists were centered two decades ago. Indeed, the writer has suggested (1) that the historical emphasis in materials research might be viewed as having progressed from the highly ordered toward the more disordered states of matter—going from the ideal crystal through the “imperfections in nearly perfect crystals” stage to the current concentration on the formation, characterization, and understanding of highly disordered structures.

The opportunities for new discovery in this present phase of development are still so great that their pursuit will constitute a major part of the efforts of Materials Scientists for a considerable time to come. Much of the activity thus far has been concentrated on semiconducting and metallic materials but these still pose major challenges to understanding and new synthesis.

The low pressure techniques should hold great promise for the synthesis of ceramics in novel metastable forms but, as yet, there appears to have been little such exploitation. The application of the new understanding of materials to ceramics has lagged well behind that to metals and semiconductors, even though the technological return in ceramics (e.g., glass-ceramics, optical fibers, and Lucalox) has been quite impressive. While the use of concrete and bricks is obviously as widespread as that of steel and elemental silicon, the expenditure of research effort on ceramics has been far behind that of other materials. This disparity in the perception of opportunities by the scientific community may have been partly due to the greater difficulty of processing ceramics, e.g., melting and shaping them, especially in comparison with metals, which impedes the design of definitive experiments.

Studies on condensed organic materials—polymers, liquid crystals, and biological structures as well as molecular crystals—have become a prominent part of materials research in recent years. Those on the intermediately ordered liquid crystalline states have illuminated the nature of certain phase changes and extended imperfections (34). Also, some of the newly synthesized polymers have shown quite exceptional

electrical and mechanical behavior (35). These developments were achieved with quite effective interactions of physicists and chemists. They suggest that the field of condensed organic states research may become still more important, replete with challenging opportunities for Materials Scientists.

In summary, the emergence and past progress of Materials Science was marked by, and indeed crucially depended on, interdisciplinary interaction of physicists, chemists, metallurgists, and other applied scientists. While having diverse professional backgrounds, these scientists generally had in common a thorough grasp of classical thermodynamics and the atomic level structure of crystals, perfect and imperfect. Such interdisciplinary cooperation must continue and flourish if Materials Science is to remain a meaningful and viable superdiscipline. Certainly, the effectiveness of this cooperation is widely appreciated. However, the tremendous growth of science—in publications, personnel, and variety—especially in the applied areas, has greatly increased educational and professional trends toward specialization. There is a serious danger that these trends may hinder, or even set back, the interdisciplinary practice and development of Materials Science.

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