

### Workshop on First-Order Displacive Phase Transformations

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A workshop on First-Order Displacive Phase Transformations was held under the auspices of the Materials Sciences Division, Office of Basic Energies Sciences, U.S. Department of Energy, at the Claremont Resort Hotel—reputedly the largest wood frame structure in the world—in Oakland, California, on October 24-28, 1988. It was co-chaired by Lee E. Tanner of Lawrence Livermore National Laboratory and by M. Wuttig of the University of Maryland. The proceedings, with a long but not uncommon delay of over 21 months, appeared last August as a full issue of *Materials Science & Engineering*.

Displacive phase transformations in solids are fascinating phenomena which have, so far, refused to yield to a thorough basic understanding, even though they are of fundamental importance in many materials applications and have been the subject of intensive investigations—experimental and theoretical, basic and applied, fundamental and phenomenological—for well over a century. These transformations proceed by means of a cooperative displacement of the atoms from their original lattice sites: the displacements are a sizable fraction (approximately 10%) of the interatomic distance, very large in comparison with the ordinary lattice vibrations. During the transformation the crystal symmetry is profoundly altered, even though there is essentially no change in atomic order or chemical composition of the material.

Displacive phase transformations can be either first- or second-order; the former are usually subdivided into strong, moderate, and weak. Examples of second-order transformations are the ferroelectric insulators strontium titanate and barium niobate. Strong first-order transformations appear in steels—the primordial martensites—as well as in some ceramics (e.g. zirconia). Moderate first-order transformations are present in a large variety of alloys (the so-called shape memory alloys): In-Tl, Fe-Pd, Ni-Ti, Au-Cd, and (the prototypical example) the  $\beta_2$  phase of Ni-Al. Finally, weak (almost second-order) first-order displacive transformations appear, for instance, in the A15 intermetallic superconductors (e.g. Nb<sub>3</sub>Sn and V<sub>3</sub>Si) in In-Tl solid solutions.

The workshop, which aimed at cross-disciplinary stimulation and fertilization, could not completely eliminate the branching always present in most fields of materials science; whereas for these transformations the theorist tends to study the second-order or weakly first-order phenomena, emphasizing a search for universality and common trends, the applied scientist is mostly concerned with specific systems and well-defined phase diagrams with particular purposes in mind (these most frequently involve the alloys characterized by strong first-order effects); whereas the physicist mostly looks at precursors and order parameters which are susceptible to sensible—albeit not simple—mathematical formulations, the materials scientist examines the apparently overwhelming role of structure and defects; whereas the electron microscopist is concerned with thin enough samples which yield clear images but are dominated by surface and size effects, the materials engineer's main concerns are with the mechanical properties of bulk, macroscopic

structures. The length scales discussed in these contexts (and in the workshop) vary from the microscopic (less than  $10^9$  m, the realm of quantum physics), through the mesoscopic (between  $10^9$  to  $10^6$  m, the regime of electron microscopy) and up to the macroscopic one (greater than  $10^6$  m).

Some of the highlights of the workshop, all properly represented in the published proceedings, can be listed as follows:

- Electronic-structure theorists are now approaching the stage in which they can calculate, from first principles, the equilibrium structure and configuration of particular solids—elements, compounds and alloys, both ordered and disordered—as functions of temperature, concentration and other externally controlled parameters.

- The by-now venerable tradition of examining phase transformation using the Landau formalism and the nonlinear Ginzburg-Landau equations has produced physical and important results only for second-order and weakly first-order transformations. The approach may, however, experience a renaissance in the very near future and extend its range of validity if multiple—and sensibly chosen—order parameters (strains, composition, atomic order, phonon-mode amplitudes) are considered simultaneously.

- Singular solutions of nonlinear models and equations—the so-called “solitons”—remain primary theoretical tools to understand some aspects of the instabilities; they await however detailed applications to particular systems.

- Computer capabilities are approaching the point where molecular-dynamics simulations—combined in some cases with quantum-mechanical approaches—may produce results which are valid for real macroscopic systems. This approach

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of "numerical experimentation" eliminates the need for linearization and expansions, so pervasive in the more traditional, analytical theoretical methods.

■ Experimentally determined softening of particular vibrational modes of the lattice (phonons anomalies) give, in many cases, premonitory signatures of impending displacive transformations; study of these modes seems to yield, in some cases, considerable insight into the forces that drive the transitions. This mode softening, however, does not appear to occur in general, only in particular—albeit physically important and representative—systems.

■ Spectacular experimental data—based on neutron, x-ray and electron scattering, transmission electron microscopy and acoustic measurements—for the  $\beta_2$  phase of Ni-Al clearly demonstrate that this system "prepares itself" for the transition as the temperature is lowered towards the martensitic transformation. This "readiness" manifests itself by means of acoustic phonon softening, softening of modes at finite wavevector, elastic strain-diffuse streaking and satellite formation. All these effects are manifestations of fine-scale displacements consisting of homogeneous

shears and finite-wavevector "shuffles" in the lattice.

■ Temporal evolution of the transformations remains, at this point, an almost unexplored area, with promising possible experimental developments but little hard data or reliable information. From the theoretical point of view new formalisms to describe time-evolution of nonequilibrium systems are begging to be developed.

■ Trigger mechanisms in weakly-to-moderate first-order transformations are still poorly understood, with many factors remaining primary candidates as either fundamental or secondary players; harmonic and anharmonic effects, lattice defects, stochastic heterophase fluctuations.

■ Although the strongly first-order transformations have been the subject of intensive studies by metallurgists for a long time, their "nucleation and growth" approach remains plagued with inconsistencies, controversies and mysteries. The initiation of the phenomenon at a given site—the "nucleus"—in which an "embryonic fluctuation" produces the "embryo" for the transformation seems to be at this time the most favored model: the many ideas presented along these lines are still

awaiting experimental support.

■ Defects continue to be considered the primary cause of nucleation, and the essential factor in the first-order displacive transformations. Which defects and what is their specific role, however, are still subjects of controversy as well as of active research.

■ Diffusion studies in strongly anharmonic solids remain an as-yet poorly developed tool; they may, however, provide—if properly developed—some of the fundamental missing clues.

In summary, the workshop has highlighted a field of great theoretical, experimental and practical importance, a field which has had some spectacular advances in the last few years. It retains, however, a major wealth of unsolved problems and unanswered questions, and constitutes a fertile ground for continuing research which is expected to yield new discoveries and uninterrupted progress.

*Reviewer: L.M. Falicov is a professor in the Department of Physics at the University of California, Berkeley, and holds a joint appointment with the Materials Sciences Division of Lawrence Berkeley Laboratory.* □

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