

**05.X-01** STRUCTURAL STUDIES OF PHASE TRANSITIONS.

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The slow, correlated fluctuations that are now believed to dominate the mechanism of 'displacive' structural phase transitions, appear to predict precursor effects — above the transition temperature,  $T_C$  — in the probability distribution functions (PDF's) of those atoms that displace below  $T_C$ . Quite apart from this general sophistication of phase-transition theory, the acquisition of increasingly detailed information about the dynamics and phenomenology of a few 'classic' transitions (e.g. in  $\text{KH}_2\text{PO}_4$ ) has encouraged correspondingly detailed extensions of conventional theoretical models. Such extensions have often identified very small structural changes as being crucially important, and yet have been content to *guess* what those changes are — or, more commonly, have been forced to do so for want of the relevant structural information. Developments of these kinds have created a new need for accurate crystallographic studies of rather simple systems, carried out to high resolution and/or as a function of temperature (T) and pressure (P). Recent examples of such work are determinations of anisotropic anharmonicity in the X-ion PDF for cubic  $\text{ABX}_3$  perovskites like  $\text{SrTiO}_3$ , a comparison of the PDF's of H and D in  $\text{KH}_2\text{PO}_4$  and  $\text{KD}_2\text{PO}_4$  just above  $T_C$ , and a study of the small but significant changes in the  $\text{KH}_2\text{PO}_4$  structure with T and P. This and similar work will be presented, with an emphasis on the constructive role now being played — and to be played — by such crystallographic studies in developing the theory of structural phase transitions. Attention will also be given to the demands this enterprise now makes on crystallographic techniques both in experiment (e.g. the extension of data collection to higher resolution) and in analysis (e.g. in the description of anharmonic PDF's).

**05.X-02** FERROELASTIC PHASE TRANSITIONS. By V.K.

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Phase transitions resulting in the onset of "spontaneous strain" in a crystal are called ferroelastic phase transitions. Such transitions always entail a change of the crystal system (if we regard the rhombohedral and hexagonal crystal systems as one). The spontaneous strain can arise from a variety of mechanisms like mode softening (with or without electric or magnetic ordering), or the cooperative Jahn-Teller effect, or martensitic ordering. Although ferroelastic phase transitions can be regarded as the mechanical analogues of ferroelectric and ferromagnetic phase transitions, spontaneous strain differs from spontaneous polarization and spontaneous magnetization in some important ways. For example, spontaneous strain can be defined only with respect to a suitably chosen reference phase, called the prototype phase, whereas for spontaneous polarization and magnetization, the concept of a prototype phase, though very useful and convenient, is not essential.

Ferroelastic phase transitions can be categorized as being either "proper" or "improper," depending on whether or not the order parameter of the transition has the same symmetry properties as the appropriate spontaneous-strain components. Proper ferroelastic transitions may be either true-proper or pseudoproper. For the former type, a symmetry-adapted combination of the spontaneous-strain components is the actual order parameter, whereas for the latter type the order parameter is a Raman-active optical soft mode and the spontaneous strain arises only from a linear coupling with this mode. The onset of spontaneous strain at an improper (or faint) ferroelastic transition is also a secondary effect, resulting from its nonlinear coupling with the order parameter.

Recent applications of the renormalization-group theory to proper ferroelastic transitions show that the classi-

cal Landau theory, on which the above description is based, has a better range of validity for these transitions than for other types. This comes about as follows: since, in general, the velocity of acoustic waves is not isotropic in crystals, mode softening occurs only for certain selected directions in wavevector space. This limits the size of the correlated region, thus bringing down the marginal dimensionality to lower values as compared to the spin models.

From the point of view of the experimental verification of the current theories of critical phenomena, ferroelastic phase transitions offer a rich variety of opportunities. This is particularly true for tricritical or near-tricritical systems. In fact, in the nonferroelastic tricritical systems studied so far in detail, namely  $^3\text{He}$ - $^4\text{He}$  mixtures and the metamagnetic  $\text{FeCl}_2$ , since an external ordering field is largely inaccessible, the phase diagram cannot be explored in much detail in the tricritical "wings." Studies of proper ferroelectric and proper ferroelastic transitions are not expected to suffer from this handicap, because the ordering field for them is simply an electric field or a uniaxial stress, respectively. Moreover, hydrostatic pressure and composition control provide two readily available ways of approaching the tricritical point, because the orders of many such transitions are known to be sensitive to these influences.

Critical fluctuations are further restricted in the vicinity of a tricritical point; the marginal dimensionality for a three-dimensional tricritical system is only 3, instead of 4 for ordinary critical points. This means that approximate mean-field-type critical behavior (with possible logarithmic corrections) can perhaps be expected near a tricritical point even for improper ferroelastic phase transitions, driven by shorter-range interactions (zone-boundary modes). Results of recent birefringence studies on  $\text{Pb}_3(\text{P}_{1-x}\text{V}_x\text{O}_4)_2$ , which seem to indicate this tendency, will be presented.

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