

**13.X-01** THE STRUCTURE AND DYNAMICS OF INCOMMENSURATE PHASES. By R.A. Cowley, Department of Physics, University of Edinburgh, Mayfield Road, Edinburgh EH9 3JZ, Scotland.

Phases in which crystals are distorted by a modulation which is incommensurate with the underlying lattice have in the past few years been found to occur in many materials. The simplest structures occur when the modulations can be described by a simple sine wave distortion. Even in this case, however, there are unsolved difficulties in obtaining the structure from experimental observations. The excitation spectrum of these phases is also predicted to have a low frequency mode of oscillation associated with the phase fluctuations of the modulation. In a few materials this mode has been observed but in many other materials it has proved to be very elusive.

In many materials the wavevector of the modulated phase changes with temperature, and locks-in to a commensurate wavevector at low temperature. The lock-in transition can be described as an instability of the low temperature phase against domain walls in the phase modulations. Theoretically the diffraction pattern for these domain walls should consist of many Fourier components but experimentally these are not usually observed. Possible reasons for this and other discrepancies between theory and experiment at these transitions will be described.

**13.X-02** STRUCTURAL PHASE TRANSITIONS IN ANTI-FLUORITE CRYSTALS. By Robin L. Armstrong, Department of Physics, University of Toronto, Toronto, Canada M5S 1A7.

Many antiferroite crystals with room temperature static structure, belonging to space group  $Fm\bar{3}m$ , distort to form structures of lower symmetry as the temperature is reduced. The order parameter for each transition is describable by a particular normal mode of the crystal; the order parameter is a single irreducible representation of the high symmetry group. Group theoretical methods are used to develop a classification scheme for these phase transitions.

Specific examples of low symmetry static structures deduced from nuclear quadrupole resonance spectra and neutron diffraction patterns are introduced.

The dynamics associated with the structural changes may be studied using inelastic neutron scattering. The soft mode behaviour for a particular crystal undergoing a ferro-rotative phase transition is considered in detail. The data obtained are successfully modelled using a rigid-ion description of the crystal.

**13.X-03** PHASE TRANSITIONS AND INCOMMENSURATE STRUCTURES IN FERROELECTRIC CRYSTALS. By M. Iizumi, Division of Physics, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-11, Japan.

Structural phase transitions giving rise to incommensurately modulated structures have recently been found in numerous ferroelectric and related crystals. General survey is given of the recent results obtained by the author and others, especially in Japan, on those crystals, such as  $K_2SeO_4$ ,  $(NH_4)_2BeF_4$ ,  $Rb_2ZnBr_4$ ,  $[N(CH_3)_4]_2ZnCl_4$ ,  $[N(CH_3)_4]_2CuCl_4$ ,  $RbD_3(SeO_3)_2$  etc. The wave vector  $q_1$  characterizing an incommensurate structure is related to a commensurate structure characterized by  $q_c$  with  $\delta$  indicating the deviation:  $q_1 = q_c + \delta$ . According as the Lifshitz condition is satisfied or not at  $q_c$ , the incommensurate structures are classified into Lifshitz and non-Lifshitz types (Iizumi and Gesi, J. Phys. Soc. Jpn. (1980) 49, Suppl. B, 72). The distinction corresponds to whether an incommensurate structure is allowed by the symmetry of crystal or not. A substantial distinction has been observed in the magnitudes of  $\delta$ : they are small in the Lifshitz type ferroelectrics, no matter which values  $q_c$  takes among  $1/3$ ,  $2/5$  and  $1/2$  in the reduced unit, whereas  $\delta$  has substantial values for the non-Lifshitz type incommensurate structures. Various kinds of temperature change of  $\delta$  have been observed within the incommensurate phases with a unique result that the incommensurate-to-commensurate phase transitions are always of the first order. The successive phase transitions from the normal to incommensurate and then from the latter to the commensurate phases and the appearance of the secondary lattice distortion, e. g. spontaneous polarization in ferroelectric, commensurate phases, have been understood by the Landau-type theory by taking into account higher order terms with a proper order in the free energy expansion.

**13.X-04** HIGH RESOLUTION X-RAY STUDIES OF  $2H-TaSe_2$ : OBSERVATION OF THE STRIPED CDW PHASE. By D. E. Moncton and R. M. Fleming, Bell Laboratories, Murray Hill, NJ 07974.

Previous neutron scattering experiments (Moncton et al., Phys. Rev. Lett (1975) 34, 734) established the formation of an incommensurate charge-density wave (CDW) state in  $2H-TaSe_2$  at 122 K and the lock-in to a commensurate structure near 90 K. These CDW states were shown to consist of the superposition of displacement waves in the three equivalent [100] directions. Motivated by the observation of a third phase transformation at 112 K in dilatometry studies (Steinitz et al. Solid State Commun. (1979) 29, 519), high resolution X-ray studies were undertaken. These experiments (Fleming et al. Phys. Rev. Lett (1980) 45, 576) reveal the formation of a striped CDW phase in which one of the three CDWs is commensurate while the other two are incommensurate. We will discuss the detailed behavior of  $2H-TaSe_2$  as a function of temperature and pressure with emphasis on the nature of this new CDW state.