SYMMETRY AND THE CLASSIFICATION OF STRUCTURES

20.X-9 NMR STUDIES OF INCOMMENSURATE PHASES. By R. Blinc, J. Stefan Institute, E. Kardelj University of Ljubljana, 61000 Ljubljana, Yugoslavia

In incommensurate (I) systems where the translational lattice periodicity is lost there is an essentially infinite number of non-equivalent nuclear sites which contribute to the magnetic resonance spectrum. Instead of sharp lines as in commensurate (C) systems one thus finds in I systems a quasi-continuous distribution of NMR, NQR or EPR resonance frequencies.

Nuclear magnetic resonance (NMR) in structurally I systems enables one to obtain specific information on the following basic physical properties:
(a) the local nature of the modulation wave: devil's staircase, plane wave or multisoliton lattice type of variation of the I modulation wave phase in space, quantitative determination of the phase soliton density via a comparison between experimental and theoretical line shapes,
(b) pinning of the modulation wave, depinning and phase floating (via motional narrowing effects),
(c) temperature dependence of the amplitude of the modulation wave via the temperature dependence of line splitting,
(d) local spectral density of phason and amplitudon excitations in the plane wave and multisoliton lattice regimes via spin-lattice relaxation,
(e) commensurability or defect induced energy gaps in the phason spectrum (via spin-lattice relaxation).

Since NMR measures local properties it can give no direct information on the phason or amplitudon dispersion relation or the modulation wave vector.


In many cases the existence of an incommensurate displacive structure is due to the instability of a commensurate (basic) structure with respect to a given soft mode which becomes frozen after the corresponding phase transition. The relation between the transformation properties of this soft mode and the symmetry of the structure diffraction pattern (including extinction rules) is discussed in a general context. This relation can be expressed in a simple form by using an integral expression for the structure factor of the incommensurate phase. The connection between the structure super-space group, the symmetry properties (irreducible representation) of the soft mode and the diffraction symmetry are reviewed under this viewpoint.

The determination of incommensurate structures and soft mode characteristics by means of X-ray diffraction is then discussed. Practically all the structures determined up to the present exhibit a sinusoidal or near-sinusoidal modulation. This result can be sometimes an artifact of the determination method. The possibility of detecting structural modulations far apart from the sinusoidal regime like the so-called soliton regime is also analysed.

20.X-11 AN OVERVIEW OF NEUTRON SCATTERING STUDIES OF INCOMMENSURATE PHASES. By J.D. Axe, Physics Department, Brookhaven National Laboratory, Upton, New York, U.S.A.

This review will concentrate on what we have learned from inelastic neutron scattering studies of the nature of the quasiperiodic (incommensurate) instability in crystalline systems, and on the nature of the unique acoustic-like excitations (phasons) associated with the broken translational symmetry.

20.X-12 ORIGIN OF INCOMMENSURATE BEHAVIOR IN INSULATORS: THE PRINCIPLE OF LATENT SYMMETRY.* By J. K. Hardy, Department of Physics & Astronomy, University of Nebraska, Lincoln, Nebraska, U.S.A.

The existence of incommensurate phases in insulating materials will be explained in general terms based on specific a priori calculations for two very different systems: Sb$_2$ZnCl$_4$ and BaMnF$_4$. It will be demonstrated that the same basic principle is responsible for incommensurate behavior in both systems. Since this principle is basically structural in origin, it predicts very different behavior for different structures, and very similar behavior for isomorphs, in general accord with observation. To this underlying principle we give the name "latent symmetry" since, as will be demonstrated, it involves an imperfect and partially hidden symmetry, present in both normal and incommensurate phases, and distinct from the "broken symmetry" present in the incommensurate phase alone.

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