MOLECULAR DYNAMICS STUDY OF A MODEL WITH INCOMMENSURATE PHASES

K. Parlinski
Institute of Nuclear Physics
ul. Radzikowskiego 152, 31-342 Cracow, Poland

Abstract. The mechanism of the change of the characteristic wavevector of the modulation in the incommensurate crystal relies in the nucleation of striplles. The striplle is a finite object constructed from discommensuration planes. The nucleation and growth of the striplle is demonstrated by the molecular dynamics simulation of a two-dimensional model. The influence of point defects on striplle growth are discussed.

1. Introduction

Recently a number of crystals has been discovered which show in some temperature interval a long range modulation of some degree of freedoms with a period being incommensurate with the underlying lattice, i.e. the wavelength of the modulation is not an integral multiple of the unit cell edge. Such phases of a crystal are called incommensurate in contrary to the commensurate ones for which the wavevector is an integral multiplier of the lattice constant of high temperature unit cell. The modulation can propagate in one, two or three-dimensions but below we shall concentrate on the one dimensional modulations only.

The modulated degree of freedom of the incommensurate phase can be either of displacive or occupational type, in full analogy to the distorted degree of freedoms which form the low symmetry phase after structural phase transition. The averaged atomic arrangement in the one-dimensional incommensurate phase of displacive type relates in static displacements of some atoms from the positions in which they were residing in the high symmetry phase. The displacements form a periodic static wave propagating in one direction. No two atoms along the direction of the modulation are displaced by the same distance. The displacement in the plane perpendicular to this direction are the same in each unit cell. In real crystals the pattern of atomic distortions is usually complicated but the displacements can be combined to few static modes, which specify the incommensurate modulation.

The incommensurate modulation can be directly observed by the X-ray and neutron diffraction method. In the incommensurate phase the usual Bragg reflections are accompanied by satellite reflections
located in some distance from the main Bragg spots. The position of a satellite with regard to the main reflection defines the wavevector of the incommensurate modulation.

The incommensurate phase usually arises from a commensurate high symmetry phase below some critical transition temperature $T_c$. The phase transition to incommensurate phase can be well described by a generalization of the soft mode theory of structural phase transitions. According to this concept, in the high symmetry phase of the crystal exists a mode, which softens under temperature lowering. At the phase transition to the incommensurate phase the soft mode reaches the zero energy at the critical wavevector $q$. Below $T_c$, the diffraction satellite appears at position $q$ and the soft mode converts into the phason and amplitudon modes. The amplitudon mode is an optic-like mode and its energy increases under temperature lowering.

The cooling and heating runs define the global histeresis. The path ABCDA specifies a local histere-sis. Steps in (b) correspond to lock-in phases.

![Diagram](image)

The phason mode corresponds to oscillations of the phase $\epsilon$ of the displacement wave. In the continuum limit it is acoustic-like and gapless as it takes zero energy to slide whole condensed modulation throughout the crystal. The sliding mode comes from the fact that in the incommensurate phase the phase $\epsilon$ of the modulation is not fixed in space by any potential. If, however, the characteristic wavevector of the modulation is close to a commensurate value $q=n/m$, where $n$ and $m$ are small integers, then the crystal might gain energy if it forms a commensurate structure. Such a commensurate phases are called lock-in. In the lock-in phase the phase $\epsilon$ of the modulation is fixed and the phason is no longer an acoustic-like mode but exhibits