Phason mode in *n*-alkane/urea composites

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This work investigates the phason mode in *n*-alkane/urea compounds, where the alkane chains are situated in the hexagonal host structure of urea. For certain alkane molecules, for instance heptadecane (n=17), this compound is incommensurate in the channel direction. For weak interchain coupling, this aperiodicity leads to the appearance of a sliding or phason mode, an additional zero or low frequency mode. Until now, this mode has not experimentally been observed in *n*-alkane/urea. This work tries to find the conditions needed to measure this sliding mode.

The inclusion compound can be described by the double chain model, which consists of two harmonic chains with mutual incommensurate periodicities. The dynamical properties of this model were studied using a Lennard-Jones like interchain interaction. This potential introduces long range interactions between the host and guest sublattices at an atomic level, which in the one dimensional case led to an asymmetric behavior in the phase diagram in parameter space[1].

The use of values for the heptadecane/urea system found in literature for almost all system parameters in the one-dimensional model, shows that the window for a vanishing phason gap is very limited. In case of a vanishing phason gap, the sliding mode can be measured as an extra zero frequency phonon mode.

This study also discusses the feasibility of phason mode observation using higher dimensional models. Several ways of extending the model, for instance, by simply making the unit cell two or three dimensional or an iteration model in two dimensions, will be discussed. The dynamical matrix is used to calculate the dispersion relations and the eigenvectors to identify the phason mode. The possibility of phason mode detection in an experiment is revealed by the calculation of the intensities of phonon scattering.

1. L.A. Brussaard, A. Fasolino and T. Janssen, to appear in Phys Rev B (May 2001)