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TITLE TEMPERATURE DEPENDENCE OF THE SOFT MODE FOR STRUCTURAL PHASE
TRANSITIONS IN HIGHLY ANISOTROPIC SYSTEMS

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Temperature Dependence of the Soft Mode for Structural Phase Transitions in Highly Anisotropic Systems

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We describe here one result from an extensive molecular dynamics (MD) study of structural phase transitions [1]. The models which have been used for structural phase transition studies have a one-component displacement variable associated with each lattice site moving in a local double-well potential. This potential gives rise to two different excitations: phonons and domain walls. The frequency of the particular phonon with displacement pattern matching the distortion occurring at the transition decreases toward zero as the critical temperature T_c is approached (the "soft mode"). The domain walls separate correlated regions possessing short-range order. Nonlinear theory indicates that the phonon softening should not be complete and should reach its minimum at a temperature T_s greater than T_c . However for isotropic systems T_s and T_c are very close and phonon softening is almost complete. Therefore these major features expected from nonlinear theory can be probed more precisely by considering weakly coupled chains of double-well local potentials. In the limit of uncoupled chains, $T_c = 0$, whereas T_s is non-zero and depends on the energy to create a 1-d domain wall or soliton.

The potential energy function describing this situation is

$$\begin{aligned} \Phi = \sum_{i,n} \left\{ \frac{1}{2} A u_{i,n}^2 + \frac{1}{4} B u_{i,n}^4 + \frac{1}{2} C (u_{i+1,n} - u_{i,n})^2 \right. \\ \left. + \frac{1}{2} D (u_{i,n+1} - u_{i,n})^2 \right\}. \end{aligned} \quad (1)$$

Here $u_{i,n}$ is the displacement of the particle associated with the i -th position along the n -th chain; the parameters $A < 0$ and $B > 0$ describe the double-well potential at each lattice site, and C and D are the intra- and inter-chain coupling constants, respectively. For the simulations described here $C \gg D$.

The potential function (1) implies a certain nonlinear equation of motion. In the 1-d limit ($D = 0$) and the continuum limit, this equation becomes the 1-d ϕ^4 partial differential equation, which has the soliton solution

$$u(x,t) = u_0 \tanh[(x - vt)/\sqrt{2} \xi] \quad (2)$$

(u_0 and ξ are certain combinations of the parameters in (1)).

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This solution describes a moving boundary between regions where particles are in the left or right half of the double-well potential. Since our 2-d system ($D \neq 0$) is weakly-coupled, we can expect nearly one-dimensional domain walls to appear in our simulations.

We have carried out computer solutions of the equations of motion implied by (1) for a system of 10 chains, each consisting of 150 particles. The values used for the coupling constants were $C = 4.0$, $D = 0.01$. Thermodynamic properties (specific heat, susceptibility, etc.) have been calculated and indicate that the system has a continuous structural phase transition at the temperature $k_B T_c \approx 0.51(|A|^2/B)$. We have also carried out extensive calculations of dynamic properties, specifically frequency and wavevector dependent spectral functions for time-dependent correlation functions. Further details about the integration scheme and these results are contained in [1]. Here we concentrate on one particular aspect of the dynamics of this highly anisotropic system, namely the temperature dependence of the soft mode frequency. We will do this with a pictorial device that we call a "soliton detector" along with the power spectrum of the soft mode.

Since each particle is moving in a double-well potential, a coarse-grained way of viewing its motion is to record whether it is in the right- or left-hand well. To do this, we have made pictures which detect the sign of the displacement: as a function of time the two possibilities are distinguished by a black or white mark. Figure 1 shows one of the results from this "soliton detector". In this picture time is plotted along the horizontal axis [in units of $\sqrt{M/|A|}$]. The vertical axis shows three consecutive chains of the system; the chain number n is shown along the left side. Within each chain there are 150 positions corresponding to each of the sites along a given chain, labelled by i ; these are also plotted vertically. If the displacement $u_{i,n}(t)$ is positive, then a black dot is put at the (t,i) -th position on the n -th chain. If the displacement is negative, then a white mark is plotted at that position. With this scheme a soliton or domain wall is the boundary between large black and white regions (cf. (2)). This particular picture is at the temperature $k_B T = 0.90(|A|^2/B)$. At higher temperatures the soliton detector shows rapid incoherent change back and forth between black and white. At about this temperature the black and white regions begin to last for sufficient time intervals that it becomes reasonable to talk about the propagation of solitons. As T is lowered further, the extent of the black and white regions becomes larger both in the space and time directions, showing the growth of the correlated regions and their longer lifetimes. Below T_c the pictures become almost completely of one color, indicating the long-range order in the low temperature phase.

Fig. 1. Soliton detector at $k_B T = 0.90 (|A|^2/B)$

Further indications about the atomic motions can be obtained from the spectral function for the order parameter. The order parameter is proportional to the $\vec{q} = 0$ spatial Fourier component of the displacement field. That variable, the correlation function, and the corresponding spectral function are defined by

$$u(\vec{q}, t) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{-i\vec{q} \cdot \vec{R}} u_{i,n}(t); \quad D(\vec{q}, t) = \langle u(\vec{q}, t) u(-\vec{q}, 0) \rangle;$$

$$D(\vec{q}, \omega) = \int dt e^{i\omega t} D(\vec{q}, t). \quad (3)$$

[$\vec{R}$ denotes the lattice sites indexed by (i, n)]. Figure 2 shows the order parameter ($\vec{q} = 0$) spectral function at $k_B T = 0.99 (|A|^2/B)$. A central peak and a phonon peak are clearly evident in this spectrum. At higher temperatures the central peak has less weight, and at lower temperatures it grows to become the overwhelmingly dominant feature of the spectrum near T_c .

Fig. 2. Order parameter spectral function at $k_B T = 0.99$ ($|A|^2/B$)

Figure 3 shows the square of the soft mode frequency ω_s versus temperature both for the 2-d system and for the 1-d system obtained by setting the interchain coupling constant D to zero. The important point to note here is that the minimum in ω_s does not occur at the transition temperature T_c , but is at a so-called "soft mode" temperature T_s , which is near 0.90 ($|A|^2/B$). The softening occurs with the same temperature dependence for both the 2-d and 1-d systems, indicating that the mechanism is the same in the two cases.

For temperatures much above T_s the soliton detector pictures indicate that the particles oscillate completely across the double-well potential. For T near T_s , where solitons start to become evident in the soliton detector, the particles oscillate within one well and are flipped back and forth between the wells as the solitons pass by. Near T_s a separation of time scales takes place between the oscillation period within one well and the time between flips from one well to the other. Above T_s there is no such distinction. When the particles start to oscillate within one well rather than across both wells, then the soft-mode frequency starts to increase. The correlations producing this temperature dependence are essentially one-dimensional.

Two-dimensional correlations set in within a narrow temperature interval around T_c . These are shown by a strong narrowing and intensity increase of the central peak part of the spectral functions in the 2-d system relative to the central

Fig. 3. Square of the soft-mode frequency versus dimensionless temperature $k_B T / (|A|^2/B)$

peak in the 1-d system which is due to soliton propagation. The details of this argument are given in [1].

In conclusion we have shown that describing the dynamics of structural phase transitions in highly anisotropic systems requires the introduction of another characteristic temperature in addition to the transition temperature. This soft-mode temperature is identified with the minimum of the soft-mode frequency and results from the appearance of 1-d soliton propagation along the chains.

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