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Melting of Dislocation Vector Systems in Two Dimensions

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A Monte Carlo study of a system of interacting dislocation vectors reveals the possibility of two types of phase transitions. For a system with a large dislocation core energy, unbinding of dislocation pairs causes a continuous phase transition. With a small core energy a first-order transition is produced by formation of grain boundaries. This possibly resolves the discrepancy between the Kosterlitz-Thouless theory and previous computer experiments of atomistic systems.

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Among the various phase transitions taking place in two dimensions, melting is one of the still unresolved problems. On the one hand the renormalization method of Kosterlitz and Thouless[1] (KT) predicts a continuous phase transition due to dislocation unbinding, and its extension by Halperin and Nelson[2] and by Young[3] (HNY) predicts two continuous phase transitions due to dislocation and disclination unbinding. On the other hand previous computer experiments[4-9] on various atomistic systems indicate the melting transition to be first order.

The renormalization-group methods are calculating the free energy by the linear elasticity theory with additional dislocations,[10] whereas atomistic systems contain furthermore effects such as anharmonicities, vacancies, and so on. If these neglected effects are important, the dislocation model is not sufficient to describe the melting transition. Recently, however, Chui[11] has pointed out that the first-order transition is possible even in a dislocation model if one considers the grain boundary excitation.[12]

In this paper I perform Monte Carlo simulations of dislocation vector systems with long-range interactions and a core energy, and investigate the order of phase transition taking place there. The merit of simulating the dislocation vector system is that one can control the core energy directly.

The main finding is that both types of phase transition are possible depending on the core energy: a continuous phase transition for a large core energy and a first-order transition for a small core energy. The continuous transition is due to dislocation unbinding and the formation of free dislocations, as predicted by KT. The first-order transition is due to the nucleation of loops of grain boundaries, in agreement with computer experiments and Chui's prediction. Thus the disagreement between theories and experiments seems to be a consequence of differences in core energies.

I shall now explain details of the investigation. In the ground state, atoms order in a close-packed structure, i.e., triangular lattice in two dimensions. At high temperatures defects such as dislocations are possible as well as phonon excitations. Burgers vectors $\vec{b}$ can be in six directions; $(\pm a_0, 0)$ and $(\pm a_0/2, \pm \sqrt{3} a_0/2)$, where a_0 is the lattice parameter. Instead of assuming dislocations with core radius a, I assume here that dislocations can be situated only on a triangular mesh site with lattice parameter $2a$. I also as-

sume a "neutrality" condition $\sum \vec{b}_i = 0$. The interaction may be written as

$$\mathcal{H} = -\frac{J}{2}\sum_i \sum_{j\neq i} b_i{}^{\alpha} b_j{}^{\beta} V_N{}^{\alpha\beta}(\vec{r}_i - \vec{r}_j). \quad (1)$$

Here the coupling constant J is given in terms of the Lamé coefficients λ and μ by $J = \mu(\mu+\lambda)/\pi(2\mu+\lambda)$ and the Einstein convention of summation for components $\alpha, \beta = x, y$ is used. The interaction consists of two parts:

$$V_N{}^{\alpha\beta}(\vec{r}) = \delta^{\alpha\beta} G_N(\vec{r}) + U_N{}^{\alpha\beta}(\vec{r}), \quad (2)$$

with the orientation-independent term

$$G_N(\vec{r}) = \frac{2\pi}{\sqrt{3}LMa^2}\frac{1}{2}\sum_{\vec{q}}{}'' G_0(\vec{q})(1 - e^{i\vec{q}\cdot\vec{r}}) + e_1 \quad (3)$$

with a constant e_1 related to the core energy, and the orientation-dependent term

$$U_N{}^{\alpha\beta}(\vec{r}) = -\frac{\pi}{\sqrt{3}LMa^2}\frac{1}{2}\sum_{\vec{q}}{}''\left(\frac{\partial}{\partial q_\alpha} G_0{}^{-1}(\vec{q})\frac{\partial}{\partial q_\beta} G_0(\vec{q})\right)(1 - e^{i\vec{q}\cdot\vec{r}}). \quad (4)$$

$G_0(\vec{q})$ is the triangular-lattice Green's function,

$$G_0(\vec{q}) = 3/[3 - \cos 2q_x a - \cos(q_x + \sqrt{3}q_y)a - \cos(q_x - \sqrt{3}q_y)a]. \quad (5)$$

The Fourier summation runs over the coordinates $q_x = 2\pi l/La$ ($l = 0, \ldots, L-1$) and $q_y = 2\pi m/\sqrt{3}Ma$ ($m = 0, \ldots, M-1$), and two singular points $(q_x, q_y) = (0,0)$ and $(\pi/a, \pi/\sqrt{3}a)$ are excluded from the summation. By numerical calculation of the interation $V_N(\vec{r})$, the asymptotic behavior of G_N and U_N for a large system is found to be $G_N(\vec{r}) \sim \ln r/a + 1.13 + e_1$, and $U_N{}^{\alpha\beta}(\vec{r}) \sim \frac{1}{2}\delta^{\alpha\beta} - r^\alpha r^\beta/r^2$. In the thermodynamic limit the Hamiltonian (1) therefore reduces to[10]

$$\mathcal{H}_\infty = -\tfrac{1}{2}J\sum_i \sum_{j\neq i}\{\vec{b}_i\cdot\vec{b}_j \ln\vec{r}_{ij}/a - (\vec{b}_i\cdot\vec{r}_{ij})(\vec{b}_j\cdot\vec{r}_{ij})/r_{ij}{}^2\} + E_c\sum_i \vec{b}_i{}^2, \quad (6)$$

with a core energy $E_c = \frac{1}{2}J(1.63 + e_1)$. Two typical cases of core energies are considered; $E_c = 0.82J$ ($e_1 = 0$) and $E_c = 0.57J$ ($e_1 = -0.5$).

The Monte Carlo procedures are similar to the previous simulation of scalar Coulomb system[13]; the creation or annihilation of a nearest-neighbor (nn) dislocation pair, as well as the diffusion of dislocations is permitted. Two system sizes, $L \times M = 38 \times 22$ or 76×44, are considered, and normally 2000 to 4000 Monte Carlo steps (MCS) per nn bond are performed at each temperature.

I first describe results for the system with a larger core energy, $E_c = 0.82J$. The reduced energy per mesh site $E = \langle\mathcal{H}\rangle/NJa_0{}^2$ and the specific heat $C = (\langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2)/NT^2$ are shown in Fig. 1. Here N is total number of mesh sites $N = LM/2$, and the Boltzmann constant k_B is set equal to unity. No discontinuity nor hysteresis is found. The specific heat has a sharp maximum at a reduced temperature $t = T/Ja_0{}^2$ near 0.25. At low temperatures only a few dislocations are created and almost all of them are forming bound pairs. The dislocation density is found to follow the Arrhenius law $n = n_0 \exp(-\Delta E/t)$ for temperatures $t \lesssim 0.22$, with an activation energy ΔE corresponding to the minimum formation energy of a nn bound pair. At high temperatures one finds many dislocations as shown in Fig. 2. The Arrhenius law does not hold any more, since there are also many isolated dislocations. These isolated dislocations, however, do not destroy the global orientational order of the underlying crystal, and thus the system may be in a hexatic phase described by HNY. More precisely one expects an orientational stiffness K_A, defined by[2]

$$T/K_A = \lim_{q\to 0}\langle[\vec{q}\cdot\vec{b}(\vec{q})][\vec{q}\cdot\vec{b}(-\vec{q})]\rangle/q^2MLa^2,$$

to be finite in a hexatic phase, whereas K_A is infinite in a solid and zero in a liquid. In the simulation, the value of the correlation at the shortest wave vector ($q \sim 2\pi/76a$) is taken to be T/K_A. It is found to be less than 10^{-4} at $t \leq 0.23$, increasing from ~ 0.004 at $t = 0.24$ to ~ 0.03 at $t = 0.27$. This warrants the transition to be from the solid to the hexatic phase. By calculating a renormalized coupling K_R from the formulas (2.17) and (2.38) of Nelson and Halperin,[2] one finds a sharp decrease of K_R around the value $K_R = 16\pi$ at $t \sim 0.22$ as is shown in Fig. 1. This value $K_R = 16\pi$ at the transition point agrees with the universal value predicted by KT. Consequently the observed continuous phase transition is well described by the KT or HNY theory.

On the other hand, since the KT theory relies on the fugacity $[\sim \exp(-E_c/T)]$ expansion, systems with small core energies could shown different behavior. Now I will discuss the results of studies on a system with a small core energy, $E_c = 0.57J$. The energy and the specific-heat

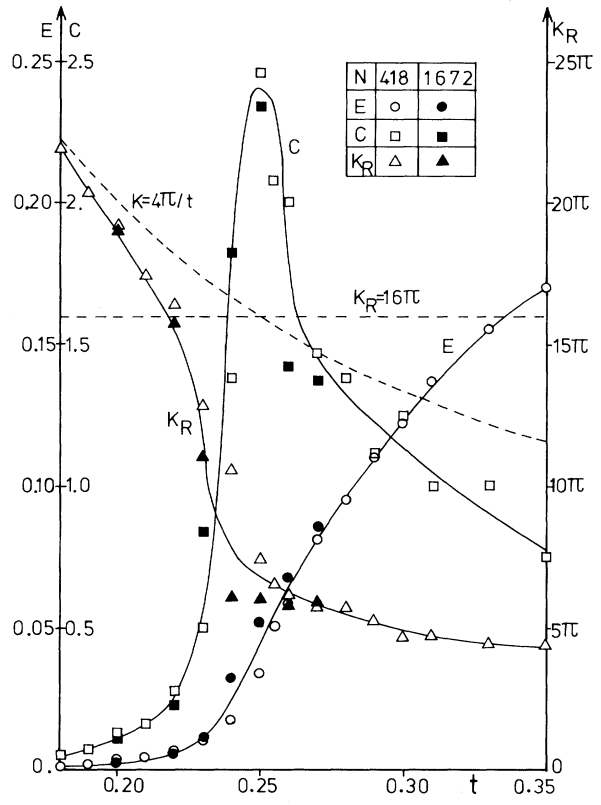

FIG. 1. Energy E, specific heat C, and renormalized coupling K_R as a function of reduced temperature t for systems with a large core energy $E_c = 0.82J$. Thin lines are just for the guide to the eyes. The unrenormalized coupling $K = 4\pi/t$ and the universal value $K_R = 16\pi$ are shown by broken lines.

curves in Fig. 3 show a large discontinuity at $t = 0.14$. Hysteresis is also found and the supercooled liquid stays metastable at low temperatures $t = 0.12$–0.135. Configurations of the low-temperature solid phase are similar to the corresponding configuration for $E_c = 0.82J$. One finds bound pairs and the dislocation density is found to be well described by the Arrhenius law. One difference is that in the course of simulation here loops of dislocations are created and destroyed. In fact, at high temperatures, configurations such as those in Fig. 4 have long lines of dislocations or grain boundaries, surrounding many crystal regions. Because of this entangled structure of grain boundaries, the orientational order of the underlying crystal may be globally destroyed. In fact the inverse of the stiffness T/K_A is found to jump from a value less than 10^{-4} at $t \leq 0.135$ to $\sim 0.3 \pm 0.1$ at $t = 0.14$ or 0.15. Despite the large fluctuation in T/K_A, the instability condition,[2]

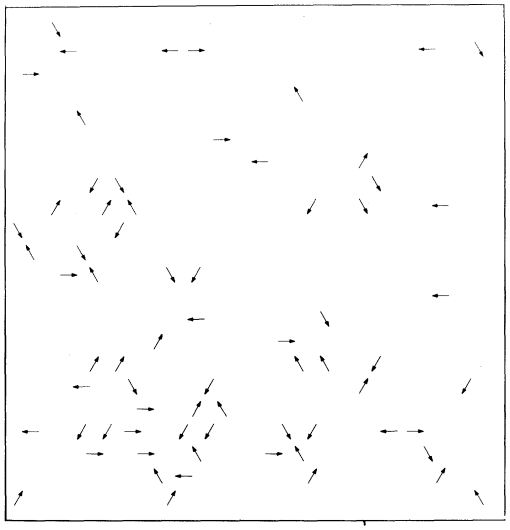

FIG. 2. Snap-shot configurations of dislocation vectors with $E_c = 0.82J$ at high temperature $t = 0.30$ for a system size $N = 418$.

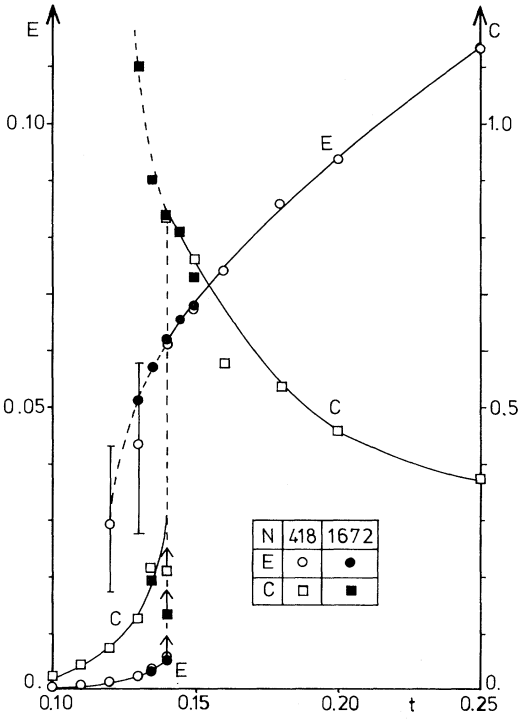

FIG. 3. Energy E and specific heat C for systems with a small core energy $E_c = 0.57J$. Thin lines are for the guide to the eyes. At $t = 0.14$ the lower branch becomes unstable and relaxes to the arrowed direction. The upper branch becomes metastable below $t < 0.14$ and fluctuations become very large as is shown by bars at $t = 0.12$ and 0.13.

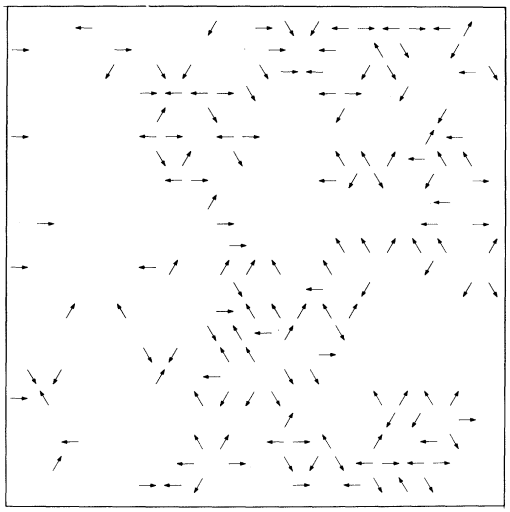

FIG. 4. Snap-shot configurations of dislocation vectors with $E_c = 0.57J$ at a high temperature $t = 0.15$.

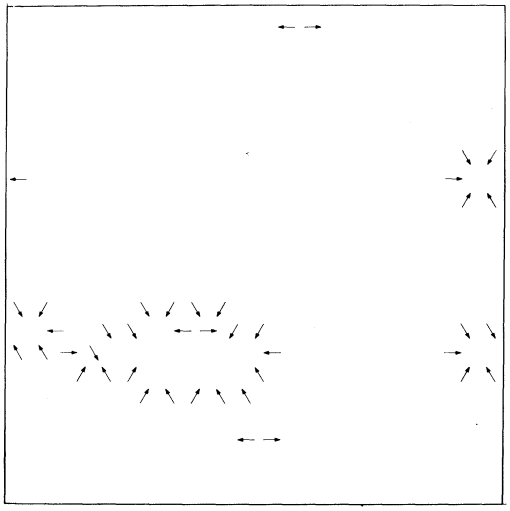

FIG. 5. Nucleation and growth of loops of dislocation vectors on melting at $t = 0.14$.

$T/K_A > \pi/72$, to form a true liquid without orientational order is satisfied at $t \geq 0.14$. The system now performs a solid-to-liquid transition. Similar loops of grain boundaries were also found in previous computer experiments of atomistic systems, and these loops may be the common and responsible feature of the first-order melting. Figure 5 shows grain boundary loops formed in the intermediate stage of melting at $t = 0.14$. These loops grow in size and also produce other loops, and they finally eat into the crystal region shown in the upper part of Fig. 5.

The above investigation indicates the importance of the core energy in determining the order of the phase transition. The change in the order of the melting transition is expected at a core energy somewhere between $0.57J$ and $0.82J$, which contradicts the Chui prediction of the multicritical point at $E_c = 0.92J$. More detailed investigation, for example, by the real-space renormalization method seems necessary. In atomic systems, as far as I know, there is only one calculation of the core energy, namely in the one-component plasma.[12] The value obtained, $E_c \approx 1.22J$, seems to support a continuous phase transition, although there is still no final agreement on the order of phase transitions among various computer simulations.[9-11] It seems therefore urgent to calculate core energies for other atomic systems to classify the order of phase transitions.

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