SIZE-MISMATCH MELTING IN TWO DIMENSIONS

Normand Mousseau and M. F. Thorpe

Department of Physics and Astronomy
and Center for Fundamental Materials Research
Michigan State University
East Lansing, MI 48824.

INTRODUCTION

Two dimensional systems present structural properties that differ markedly from those of three dimensional systems. It has been known for a long time that at any non-zero temperature the long range positional order is destroyed (Mermin, 1968). However, even if the crystalline structure disappears, the system remains a solid and presents so-called quasi-long-range order; the positional correlations vanish algebraically and the orientational order is maintained.

Following the work of Kosterlitz and Thouless (1971) on 2D phase transitions, Halperin and Nelson (1979) and, independently, Young (1979) proposed a melting theory (KTHNY theory). This theory, based on the dissociation of defects, introduced a new phase between the solid and liquid; the hexatic phase. In spite of numerous simulations and experiments, no clear picture has yet emerged and the situation remains highly controversial (Strandburg, 1988).

Thorpe and Cai (1991) proposed to examine 2D melting using size-mismatch disorder instead of temperature to drive the transition. In their paper they looked at size-mismatch caused by bonds of different lengths using a spring model. We present here results of size-mismatch induced melting using a pseudo-harmonic potential.

THEORY

For the analytical solution, we start with a triangular network interacting via a harmonic potential
Figure 1. Positional correlation as a function of distance for two different size-matches. The crosses are simulation results obtained on a 200x200 lattice and the squares from simulations on a 100x100 lattice. The solid curves are from Eq. (3).

\[
V = \frac{1}{2} K \sum_{<ij>} (L_{ij} - L_{ij}^0)^2.
\]  

(1)

We have a random distribution of two types of atoms A and B of different sizes but with the same elastic constant K and three natural (unstrained) lengths \(L_{AA}^0, L_{BB}^0\) and \(L_{AB}^0 = 1/2(L_{AA}^0 + L_{BB}^0)\).

Using this model and the formalism developed by Thorpe and Garboczi (1990), it is possible to define an effective temperature associated with the mismatch \((L_{BB}^0 - L_{AA}^0)/L_{AB}^0\) and concentration \(x\) of atoms B (Thorpe and Cai, 1991)

\[
k_B T_D = \frac{1}{2} K x (1 - x) (L_{BB}^0 - L_{AA}^0)^2.
\]

(2)

At low mismatch, as mentioned in the introduction, a two dimensional system is still a solid but no longer a crystal. The positional order \(C_Q(R)\) decays algebraically

\[
C_Q(R) = \frac{B(Q)}{R^n}
\]

(3)

where \(\eta\) is found to be (Chen and Thorpe, 1992)

\[
\eta = \frac{2}{3\pi \sqrt{3}} x(1 - x) \left[ Q \left( L_{BB}^0 - L_{AA}^0 \right) \right]^2.
\]

(4)

Even as the positional correlations vanish at large distances, the orientational (angular) correlations remain long-range and well-defined. Since each site on a triangular lattice has six neighbours, the orientational correlations are defined as

\[
C_\theta(R) = \left| \langle e^{i\theta_{ij}(R)} \rangle \right|
\]

(5)

where \(\theta\) is the angle between two bonds situated at a distance \(R\) from each other. For large \(R\), we find that the correlation approaches a constant and so the orientational order parameter becomes

\[
C_\theta(\infty) = \exp \left[ 35.2 \, x(1 - x) \left( \frac{L_{BB}^0 - L_{AA}^0}{<L>} \right)^2 \right].
\]

(6)
Figure 2. The solid line is the analytical curve for the orientational correlations as \( R \to \infty \); the diamond symbols are the simulation values of the same quantity. The square symbols are the simulation values for the fraction of coordination defects as a function of mismatch. The dashed and dotted lines are guides to the eye.

SIMULATIONS

We have checked these analytical results against computer simulations. In order to have a potential which would be harmonic around the minimum and also allow for the formation of coordination defects and hence melting, we constructed a continuous pseudo-harmonic potential, described by three parts

\[
V(r) = \begin{cases} 
(\frac{2}{3})^{12} + \epsilon_1 & \text{for } r < r_1 \\
k_2 (r - r_0)^2 + \epsilon_2 & \text{for } r_1 < r < r_2 \\
k_3 (r - r_3)^2 & \text{for } r_2 < r < r_3.
\end{cases}
\]

The simulations were performed on a triangular lattice supercell of 10000 sites with the two species A and B distributed randomly on the lattice with equal concentrations. By using mismatch instead of temperature to drive the disorder, we can find the minimum energy configuration by static relaxation. The disorder is quenched in the system, which would prefer to be locally ordered but the barrier is so large that phase separation is extremely unlikely on any reasonable time scale. This procedure allows the study of disorder at zero temperature and hence avoids some of the difficulties present in molecular dynamics and Monte-Carlo techniques.

RESULTS

At low mismatch, i.e. up to 20%, the simulation confirms the analytical predictions from the spring network described by (1). Fig. 1 shows the algebraic decay of positional correlations and Fig. 2, the value of the orientational order parameter. This agreement breaks down at \( \sim 20\% \) mismatch, when the first coordination defects (pairs of dislocations) appear (Fig. 2). The orientational order parameter falls below the theoretical prediction from (1) in which coordination defects are not permitted.

In contrast with the KTHNY theory predicting a phase transition when the defects unbind, we see an inflection point in the strained energy at \( \sim 20\% \) mismatch. Increasing the mismatch fills up the lattice with pairs of dislocations without showing any sign of the unbinding of defects (Fig. 3 (a)).
Figure 3. (a) Lattice with 32% mismatch relaxed using the pseudo-harmonic potential; (b) Lattice with 26% mismatch relaxed using a Lennard-Jones potential. The squares and the circles symbols are five- and seven-fold coordinated atoms respectively.

It is well known that the melting in two dimensions is very potential dependent. The pseudo-harmonic potential used here is very soft: the competition between lattice distortions and local rearrangements is not strong enough to allow for pair unbinding. Other short-range potentials can therefore present very different results. We have looked at the truncated Lennard-Jones potential, cut between the third and fourth neighbours. Preliminary results indicate that unbinding of dislocation pairs does occur (Fig. 3 (b)).

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REFERENCES