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PHASE TRANSITIONS IN TWO DIMENSIONS*

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Although a two-dimensional solid with long-range translational order cannot exist in the thermodynamic limit ($N \to \infty, V \to \infty, N/V$ finite) macroscopic samples of two-dimensional solids can exist. Such finite samples will exhibit a quasi long-range translational order which is virtually indistinguishable from the conventional long-range order of three-dimensional solids.

Halperin and Nelson,[1] applying the theory of Kosterlitz and Thouless[2] and Feynman[3] for dislocation-mediated melting, have speculated that the melting of two-dimensional films involves two second-order transitions At a lower temperature, they believe that there is a second-order transition from the solid phase to an intermediate phase (the "hexatic" phase) with translational disorder but with six-fold orientational order. At a higher temperature they believe that there is a second second-order phase transition from the hypothetical hexatic phase to the liquid phase which lacks both translational and orientational order.

Apparent support for these startling predictions comes from the computer simulations of Frenkel and McTague[4] who claim to observe a hexatic phase in a two-dimensional Lennard-Jones system. On the other hand, the simulations of Tsien and Valleau,[5] Toxvaerd,[6] Abraham,[7] and van Swol et al.[8] all show that the melting of two-dimensional Lennard-Jones systems is first-order and give no support for the existence of a "hexatic" phase.

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In order to investigate more fully the two-dimensional Lennard-Jones system, Barker, Henderson and Abraham[9] have determined the phase diagram of this system. Barker et al. calculated the energy and pressure of this system for a wide range of states by means of a computer simulation and then integrated these results to obtain the free energy. Constants of integration were determined either from virial coefficients[10] or from the properties[11] of the low temperature solid. The stability of the phase was determined by the usual method of equating the pressure and chemical potential of the phases. The resulting phase diagram is shown in Fig. 1. Melting is first-order and there is no evidence of the existence of any "hexatic" phase.

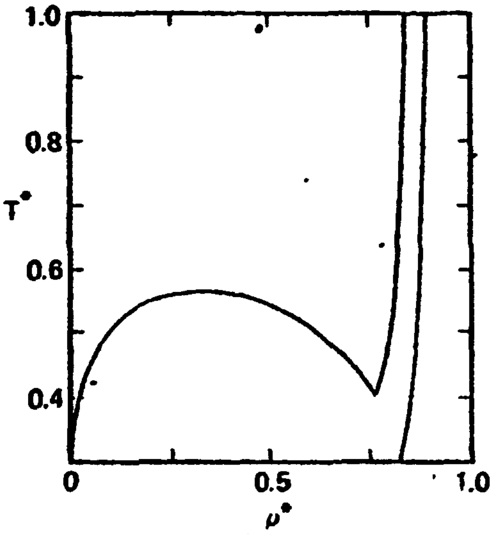

Figure 1. Phase diagram of Lennard-Jones system

Comparison of the results of Frenkel and McTague with Fig 1 shows that their simulations were largely in two phase regions Their purported hexatic phase is merely solid and fluid phases coexisting (as suggested by Toxvaerd[6] and Abraham[7]).

Recently Tobochnik and Chester[12] have simulated the melting of the Lennard-Jones system and, while unable to reach any definitive conclusions, they call in question the conclusion that melting is first-order. Comparison of their results with the phase diagram in Fig. 1 shows that Tobochnik and Chester's simulations are in the two phase region. Their results are completely consistent with a first-order phase transition.

Melting in two dimensions is qualitatively similar to three-dimensional melting. In particular, the transition is first-order and there is no exotic phase.

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