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LETTER TO THE EDITOR

Monte Carlo study of defect melting in three dimensions

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Abstract. Using Monte Carlo methods, we analyse a simple model of defect melting in three-dimensional crystals. The model undergoes first-order transitions for all values of the elastic constants. This substantiates and extends a previous mean-field analysis performed for the isotropic model. For materials where the model is expected to work, we find good quantitative agreement with experiment: Lindemann parameters for FCC metals whose volume expansion coefficients are not too large are correctly predicted to within a few percent.

Over thirty years ago, Shockley suggested that the primary reason for the breakdown of crystalline order during melting was the sudden proliferation of line-like translational defects (dislocations) (Shockley 1952, Kosterlitz and Thouless 1973, 1978, Halperin and Nelson 1978, Edwards and Warner 1979, Cotterill 1980, Nelson and Toner 1981 (and references therein)). Once this mechanism sets in, the ensuing liberation of translational degrees of freedom along the basis vectors of the crystal allows the formation of orientational defects (disclinations) which are no longer energetically suppressed, as they are in the crystalline state. The proliferation of disclinations eventually leads to complete isotropy and the resulting state corresponds to that of a proper liquid (Halperin and Nelson 1978, Nelson and Toner 1981).

In a series of recent developments, a consistent picture of the melting transition based on the proliferation and interactions of both types of defects has emerged (Kleinert 1982a, b, c, 1983a, b, c). The old puzzle as to why crystal melting is always a first-order transition as opposed to the apparently similar vortex-line transitions in superfluid ^{4}He can be resolved within this framework: In crystals, dislocation lines can combine to form disclination lines, a possibility which does not exist in the superfluid. Conversely, a dislocation line can be viewed as a bound state of two oppositely oriented disclination lines with a confining potential proportional to their separation. As dislocation lines proliferate, a disorder analogue of the Meissner effect (Kleinert 1982b) screens the potential from linear to Coulomb and the bound states break up. A mean-field analysis of the disorder field theory for the grand canonical ensemble of defect lines indicates that the combined effect of proliferation plus deconfinement leads to a first-order transition (Kleinert 1983a).

The effects of fluctuations are, of course, difficult to assess in a mean-field approximation. For this reason, we have performed a Monte Carlo study of the crystal defects.

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Because of the long-range nature of the interactions between defect lines, a direct numerical analysis becomes extremely cumbersome. This difficulty can be circumvented by making use of a convenient dual formulation of the model (Kleinert 1982b). The dual model is a local statistical theory describing non gauge-invariant interactions of U(1) spins on a lattice. There is a striking formal resemblance of this model to ordinary lattice gauge theory (Kleinert 1983b), for which Monte Carlo methods are well developed (Creutz *et al* 1983). These techniques can be easily adapted to the study of the gauge theory of dislocation melting.

The model we shall study in this letter is described by the partition function

$$Z=\prod_{n,i}\int_{-\pi}^{\pi}\frac{\mathrm{d}A_{ni}}{2\pi}\exp-\beta\left(\sum_{n,i<j}\Omega_{ij}(\boldsymbol{n})+2x\sum_{n,i}\Omega_{ii}(\boldsymbol{n})+\frac{\lambda}{\mu}\sum_{n}\Omega_0(\boldsymbol{n})\right), \tag{1}$$

with

$$\Omega_{ij}(\boldsymbol{n})=1-\cos(\nabla_i A_{nj}+\nabla_j A_{ni}),$$

$$\Omega_0(\boldsymbol{n})=1-\cos\left(\sum_i \nabla_i A_{ni}\right).$$

In (1), $\boldsymbol{n}$ represents a general lattice site and $i, j=1, 2, 3$ denote spatial directions and ∇_i is the lattice gradient operator. A_{ni} is a U(1) angle variable, located at $\boldsymbol{n}$ in the direction i, which is related to the atomic displacement vectors, $u_i(\boldsymbol{n})$, in the lattice (Kleinert 1982a). The parameters appearing in (1) are written in terms of the elastic constants of the crystal as $\mu=c_{1212}$, $\lambda=c_{1122}$, and $x=(c_{1111}-c_{1122})/2\mu$, appearing in the definition of the elastic energy, $\frac{1}{2}c_{ijkl}\partial_i u_j \partial_k u_l$, and $\beta=\mu a^3/(2\pi)^2 T$ with a^3 the volume per site. The model given above is the symmetric analogue of the usual Wilson U(1) lattice gauge model (Wilson 1974), which involves the discrete curl of A_{ni}. The difference between the two systems is physically crucial. The mean-field approximation to both models predicts first-order transitions. However, when fluctuations are properly taken into account, the mean-field transition of the U(1) lattice gauge theory disappears (Polyakov 1975, 1977, Gopfert and Mack 1982). On the other hand, as our results strongly indicate, the symmetric model undergoes a first-order transition when the full spectrum of fluctuations is included in the analysis.

Using standard Monte Carlo methods (Creutz *et al* 1983), we have simulated the above model with lattices varying in size from 12^3 to 20^3 sites with periodic boundary conditions and approximated the U(1) group by its discrete subgroup $Z(32)$, an approximation known to be excellent for values of β which are not too large.

To study the critical behaviour of the model we used a strategy which has been very successful in the study of ordinary lattice gauge theory. An initial state in which all A_{ni} were set to zero was run at a value of β, β_0, which clearly corresponded to the ordered phase. After a few iterations (between 5 and 20), the inverse temperature was reduced by a small amount $\delta\beta$. This operation was repeated until $\beta=0$, and then reversed back to β_0; thus simulating a thermal cycle. The presence of hysteresis loops (in the internal energy, for example) signals the existence of a phase transition. For each value of x, once the region of hysteresis was determined a different type of simulation was performed to obtain the critical value of β (Creutz *et al* 1979); An initial state was prepared in which half of the lattice was initialised at zero temperature (all $A_{ni}=0$) and the other half of the spins were set to random angles in the group (which is an equilibrium state at $\beta=0$). This state was then run in the range of values of β where hysteresis was observed. At any temperature other than the critical one,

if the system undergoes a first-order transition, one of the two halves of the lattice will be highly unstable (rather than metastable) and a clear, linear evolution to the corresponding stable state will be observed. At the critical temperature, however, each half of the system evolves into a different stable equilibrium state and the evolution of values of the internal energy as function of the Monte Carlo iteration time will show no drift. The gap between the energies corresponding to the two temperatures neighbouring the critical point is determined by the latent heat if the transition is first order. For all values of x explored, this gap was sufficiently large (i.e. much larger than typical thermal fluctuations) to exclude the possibility of a continuous transition. The results of this kind of simulation at a continuous transition are drastically different. That the transitions were indeed first order was further ascertained by the usual method of making long runs at the estimated critical temperatures of initial states which are either totally ordered or totally random. A stable evolution to two distinct values of the internal energy is, again, an exclusive property of first-order transitions. The accuracy in the determination of β_{melt} using the mixed-state technique is basically only limited by numerical resolution and surface effects. Generally (depending on the value of x), we were able to determine the critical temperatures with an uncertainty of less than 0.04 in β for $x<1$, and less than 0.01 for $x\geqslant 1$. At present we do not have a precise determination of the λ-dependence of β_{melt}, but preliminary evidence indicates this dependence is weak. Unless otherwise stated, all the results presented below correspond to the case $\lambda=0$. In this case, the resulting functional dependence of β_{melt} on x turns out to be a surprisingly simple power law. Using a least-squares linear fit to the logarithms, we found

$$\beta_{\text{melt}}(x)=\tfrac{1}{2}(2/x)^{\alpha}, \tag{2}$$

with $\alpha=0.597\pm0.002$. This fit is shown in figure 1. (Note that a simple Lindemann criterion would give $\beta_{\text{melt}}\propto x^{-0.5}$ for small x, in welcome agreement with our results). By measuring the discontinuity in the internal energy at β_{melt} we determined a transition entropy, ΔS, as a function of x, which was found to be almost independent of λ. For

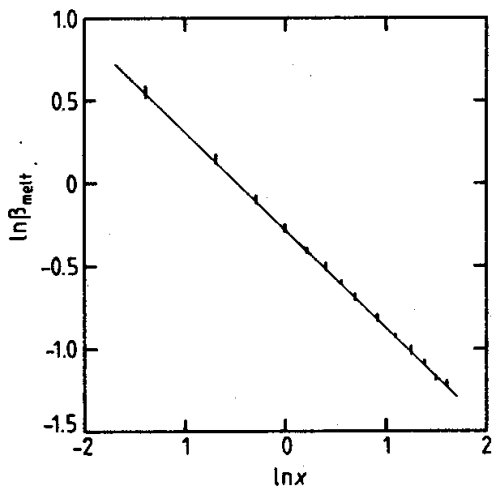

Figure 1. The critical temperature as a function of x. Error bars correspond to resolution uncertainty. The straight line is a least-squares fit to equation (2) for $\alpha=0.597$.

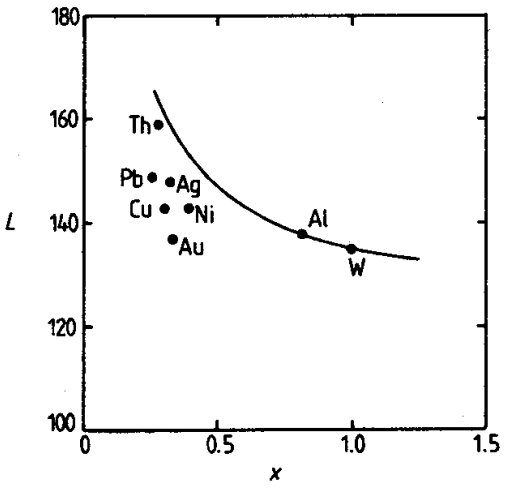

Figure 2. Comparison of the predicted and experimental values of the Lindemann parameter for FCC metals. The continuous line is given by equation (4) with the β_{melt} given by equation (2). Experimental values are taken from Lasocka (1975).

isotropic crystals ($x=1$), the transition occurs at $\beta_{\text{melt}}=0.76$ with an entropy change of about 1.4 per site, in rough agreement with experiments observation (Lasocka 1975). Although we have no explanation as to the origin of the simple power law given in (2), its qualitative behaviour is easy to understand. For $x\to 0$, the crystal melts at zero temperature due to elastic instability. As $x\to\infty$, the system decouples into three independent one-dimensional systems, which have no melting transition at all.

The Lindemann parameter can be expressed as a function of β_{melt}. It is defined as

$$L=\theta_D V^{1/3}(A/T_{\text{melt}})^{1/2}, \tag{3}$$

where θ_D, T_{melt} are the Debye and melting temperatures measured in Kelvin, V is the molar volume in cm^3/mole, and A is the atomic number. In a polycrystalline sample, the three elastic constants average out to two isotropic Lamé constants,

$$\bar{\mu}=\tfrac{1}{5}\mu(3+2x), \qquad \bar{\lambda}=\lambda-\tfrac{2}{5}\mu(1-x),$$

and longitudinal and transverse sound propagate with velocities $c_{\text{L}}^2=(2\bar{\mu}+\bar{\lambda})/\rho$, $c_{\text{T}}^2=\mu/\rho$, where ρ is the density of the sample. Writing the Debye temperature in terms of these parameters, the Lindemann number becomes

$$L=2\pi L_0\bar{\gamma}[\tfrac{1}{5}(3+2x)\beta_{\text{melt}}]^{1/2}, \qquad \bar{\gamma}=(1-\tfrac{1}{3}c_{\text{T}}^3/c_{\text{L}}^3)^{-1/3} \tag{4}$$

where $L_0=22.76$. In figure 2 we have plotted (4) as a function of x as well as the corresponding experimental values for several FCC metals (Ubbelhode 1978). We have omitted materials which have a strong volume expansion at the transition point, since our model works at constant volume and is thus not expected to describe such cases.

The specific heats predicted by the model were obtained by either differentiation of the internal energy (when this variation was reasonably smooth) or by a direct measurement of the average fluctuations in the internal energy. Consistency of the two results was checked in those regions in β where the statistical uncertainties of both were comparable. These results can be compared with experiment by including the contribution of the kinetic energies, $\Sigma_n m\dot{u}_i^2(\boldsymbol{n})/2$. These give, at the classical level, a factor of $(2\pi/\beta)^{3/2}$ in the partition function. Far below the transition they lead to the correct Dulong–Petit value of 3 ($\frac{3}{2}$ for the kinetic terms and $\frac{3}{2}$ for the potential energy) and approach $\frac{3}{2}$ as $T\to\infty$ (when there are only kinetic degrees of freedom in the liquid). Around the transition, there is some excess heat capacity in the present model when compared with such materials as lead (Borelius 1963), as shown in figure 3. This indicates that defects in nature form less easily than in this model and points to the necessity of including an additional core energy in the model to correct this discrepancy.

Apart from the above observation, the present model calls for several improvements. First of all, the simple cubic lattice must be abandoned in favour of a proper lattice structure. Second, and very important, cubic terms have to be included in the elastic energy in order to account for volume expansion, without which a quantitative comparison of transition entropies is very difficult. Nonetheless, we feel that the simplicity of the model, together with the fact that it gives reasonably accurate results, as the present work indicates, justify pursuing a detailed analysis and improvement of its general structure.

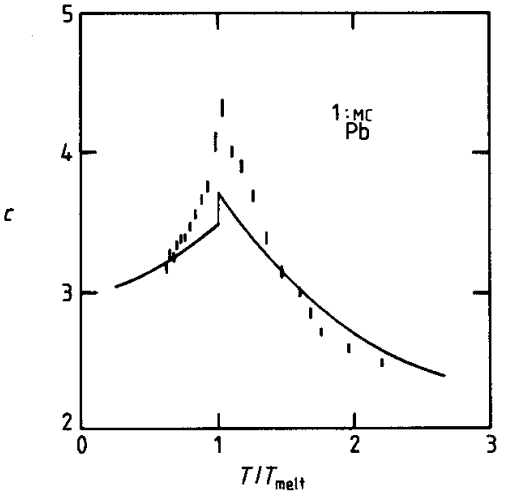

Figure 3. Comparison of the predicted specific heat for $x = 0.25$ and the experimental values for lead. Experiment (full line) is taken from Borelius (1963).

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