Disorder-Induced Phase Transitions in Two-Dimensional Crystals

Min-Chul Cha and H. A. Fertig
Department of Physics and Astronomy and Center for Computational Sciences, University of Kentucky, Lexington, Kentucky 40506-0055
(Received 26 January 1995)

We analyze a model of a two-dimensional crystal subject to a slowly varying random potential, and find evidence for the existence of a zero-temperature phase transition via the appearance of isolated dislocations above a critical disorder strength. The result is in contrast to earlier analyses of the model, which found that the crystal is always unstable with respect to dislocation formation. The argument is generalized to finite temperature and a phase boundary is derived. Molecular dynamics simulations of a model electron crystal show strong evidence of this phase transition at low temperatures.

PACS numbers: 64.60.Cn, 05.50.+q, 05.70.Fh

It has long been appreciated that topological defects can drive interesting phase transitions in two-dimensional systems as a function of temperature. These defects, which carry a topological "charge," are bound together into neutral pairs at low temperatures, and unbind above the Kosterlitz-Thouless transition temperature [1]. For the case of XY ferromagnets, these excitations are vortices; for crystals, they may be dislocations or disclinations [2,3]. The appearance of isolated defects in the system generally changes the behavior of certain correlation functions from power-law (quasi-long-range) to exponential (short-range) behavior.

An interesting question is whether this phenomenology has an analog for zero-temperature systems subject to various strengths of disorder. This question arises in a variety of situations: ferromagnets subject to random fields and/or random exchange interactions [4,5], Josephson junction arrays with positional disorder [6], and crystal systems on disordered substrates [7,8] or with random substitutional impurities [9,10]. In this Letter, we will focus on crystal systems, with particular emphasis on their stability with respect to defect formation in the presence of a slowly varying random potential. In particular, we will give evidence, both analytical and numerical, that one may have a zero-temperature transition in which isolated dislocations appear above a critical disorder strength. Specifically, we will show within our model that, in a finite size system, the number of locations at which it is energetically favorable to include an isolated dislocation in the ground state configuration vanishes below a well-defined threshold disorder strength, and diverges above it, in the infinite size limit. A generalization of the argument to finite temperature may also be made, resulting in the phase diagram presented in Fig 1. Analogous arguments for the appearance of isolated disclinations for stronger disorder [8(b)], as well as isolated vortices in XY ferromagnets with appropriate random exchange interactions, [5] may also be constructed. These generalizations will be discussed elsewhere [11]. We note that recent numerical simulations have shown strong evidence of a disorder induced disclination unbinding transition in the electron crystal [8].

To further strengthen the case that such a transition is possible, we have performed large scale simulated annealing molecular dynamics simulations of electron crystals in a slowly varying random potential. Our results show behavior indicative of such a transition: the positional correlation length rises sharply to above the system size at a critical disorder strength (see Fig. 2), and simultaneously one finds that the number of isolated dislocations in the low-temperature configuration drops sharply as the transition is approached from above. Results for the ground state configurational energy also show structure at the transition (see Fig. 3).

We begin with a continuum elasticity theory model of the two-dimensional crystal, in which the energy to create a strain field $u_{ij}(\vec{r}) \equiv \frac{1}{2}(\partial_i u_j + \partial_j u_i)$, where $\vec{u}$ is the displacement field of the lattice and $i, j = x, y$ is given by

$$E = \frac{1}{2}\int d^2r\{2\mu u_{ij}^2 + \lambda[u_{kk} - \delta\rho(\vec{r})]^2\}. \quad (1)$$

We have taken our unit of length in the above to be the lattice constant (i.e., $a_0 \equiv 1$), and μ and λ are Lamé

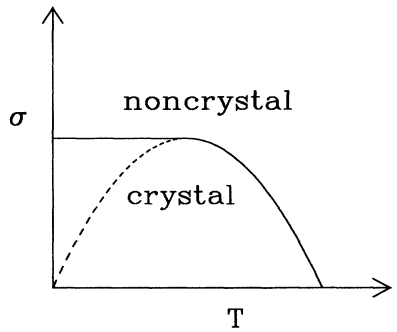

FIG. 1. Schematic phase diagram of the disordered two-dimensional crystal as temperature and disorder strength change. The solid line represents the phase diagram suggested in this work. The dotted line is found in Ref. [9].

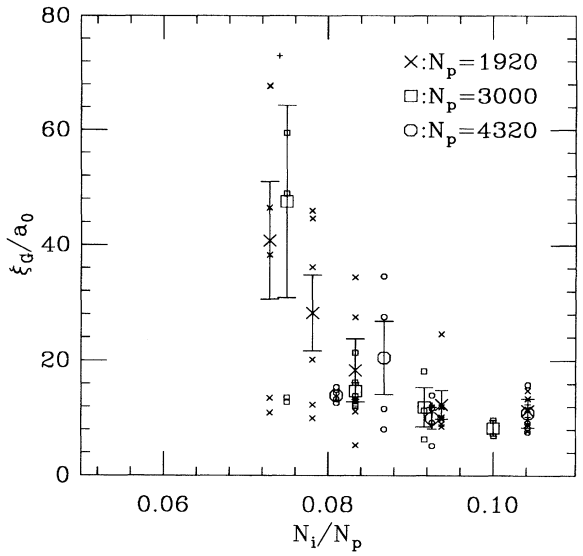

FIG. 2. The positional correlation lengths of two-dimensional electron solid in finite size systems at zero temperature where N_p is the number of electrons and N_i is the number of quenched impurities. Small symbols represent actual data, while bigger symbols represent corresponding average values. The correlation lengths rise sharply as the disorder strength approaches a finite critical value from above. Samples with $N_i/N_p \leq n_c$ are not shown, because long-range behavior is present in correlation functions and correlation lengths cannot be defined.

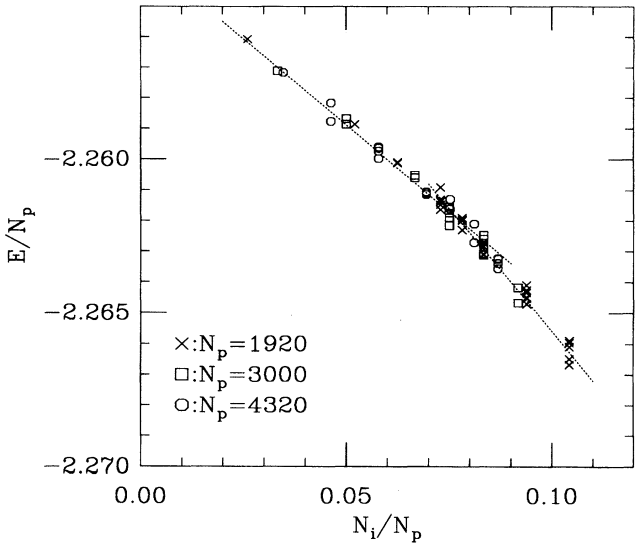

FIG. 3. The configurational energy per particle of the model system given in Eq. (6) in units of e^2/a_0. There is a cusplike behavior coincident with the sharp rise of the positional correlation lengths. The dotted lines are guides to the eye.

coefficients. The quantity $\delta\rho$ represents a random field, which for simplicity we assign an uncorrelated Gaussian distribution, $P[\delta\rho(\vec{r})] = (1/\sqrt{2\pi\sigma})e^{-\delta\rho(\vec{r})^2/2\sigma}$. One can see in this model that the coupling of the strain field to the disorder has the effect of forcing in fluctuations in the lattice density, which is proportional to u_{kk}. This model has been studied previously to describe a crystal with random substitutional disorder [9]; it has also been argued that the $\lambda \to \infty$ limit of this model may be used to describe the electron crystal in a random neutralizing background [8,12,13].

The strain field in Eq. (1) may be separated into a smoothly varying part ϕ_{ij} and a part due to dislocations with cores at sites $\vec{r}_j$ and Burgers vectors $\vec{b}_j$. The energy of the resulting configuration turns out to be separable in these two contributions [9]. The contribution to the energy due to the presence of dislocations has the form

$$E_0^{\rm dis} + \frac{K'}{4\pi}\int d^2r\,\delta\rho(\vec{r})\sum_j \frac{z\cdot[\vec{b}_j\times(\vec{r}-\vec{r}_j)]}{|\vec{r}-\vec{r}_j|^2}, \qquad (2)$$

where $K' = 4\mu\lambda/(2\mu+\lambda)$, and $E_0^{\rm dis}$ is the energy of the dislocations in the absence of the disorder field [3,9].

Suppose one attempts to find the ground state for a given disorder realization in a finite size system of area A. We can first minimize the energy with respect to the smooth displacements ϕ_{ij} without introducing any dislocations. We now ask: can one find a site in the sample for which the introduction of a dislocation lowers the energy? The energy to create a dislocation with Burgers vector $\vec{b}$ in the absence of disorder has the form $E_0 = (Kb^2/16\pi)\ln A$ for large A, where $K = 4\mu(\mu+\lambda)/(2\mu+\lambda)$; to be energetically favorable, the interaction energy between the dislocation and the disorder E_1 [i.e., the second term in Eq. (2)] must more than balance this energy cost. For a given site, the ensemble of disorder configurations will generate a distribution of interaction energies $P(E_1)$ that in the limit of large sample sizes should be independent of the site location. The probability distribution $P(E_1)$ may be computed *exactly* by a functional integral, with the result $P(E_1) = (1/\sqrt{2\pi\eta})e^{-E_1^2/2\eta}$, with

$$\eta = \left(\frac{K'}{4\pi}\right)^2 \frac{\sigma\pi b^2}{2}\ln A. \qquad (3)$$

The probability that a site is energetically favorable for creation of a dislocation is then given by $p = \int_{-\infty}^{-E_0} P(E_1)\,dE_1$, which for large A is easily shown to have the form $p \sim e^{-E_0^2/2\eta} = A^{-(bK/4K')^2/\pi\sigma}$. Since the number of sites in the sample scales as A, the number of sites for which it is energetically favorable to create the dislocation scales as $A^{1-(bK/4K')^2/\pi\sigma}$, so that it will only be possible to find sites for the dislocation in the thermodynamic limit if

$$\sigma > \sigma_c = \frac{1}{\pi}\left(\frac{K}{4K'}\right)^2,$$

where we have set the Burgers vector to its lowest nontrivial value, $b = a_0 \equiv 1$.

Several comments are in order. First, this is clearly the generalization of the original Kosterlitz-Thouless argument [1] for entropy-driven phase transitions in two-dimensional systems; one is balancing the probability due to its energetics of a given lattice site being occupied by a dislocation with the number of available sites. As in that work, we must expect that screening by dislocation pairs will affect the precise value of σ_c. One also cannot rule out the possibility that this phase transition will be circumvented by a first order phase transition, for example, to a state with grain boundaries [2].

A finite temperature version of this argument may be constructed by assigning a thermal probability $1/(1 + e^{(E_0+E_1)/k_BT})$ that a site will be occupied by a dislocation, even if the energy to do so is positive. The probability that a given site will have a dislocation then takes the form $p = \int_{-\infty}^{\infty} dE_1 P(E_1)/(1 + e^{(E_0+E_1)/k_BT})$. The behavior of this integral for very large areas may be computed by breaking the integral up into two parts: $p = \int_{-\infty}^{0} dE' P(E' - E_0)/(1 + e^{E'/k_BT}) + \int_{0}^{\infty} dE' P(E' - E_0)/(1 + e^{E'/k_BT})$. We then expand the thermal factor in powers of e^{E'/k_BT} in the first term, and in powers of e^{-E'/k_BT} in the second. The resulting integrals may be expressed as sums over complementary error functions, from which one finds for the asymptotic behavior $p \sim e^{-E_0^2/2\eta}$ for $\beta\eta > E_0$, $p \sim e^{-\beta E_0 + \beta^2\eta/2}$ for $\beta\eta < E_0$, with $\beta \equiv 1/k_BT$. The resulting asymptotic behavior for large areas has the form $p \sim A^{-\alpha}$, with

$$\alpha = \begin{cases} \frac{1}{\sigma\pi}\left(\frac{Kb}{4K'}\right)^2, & \beta\sigma > \frac{2K}{K'^2}, \quad (4) \\ \frac{\beta b^2}{16\pi}[K - \beta K'^2\sigma/2], & \beta\sigma < \frac{2K}{K'^2}. \quad (5) \end{cases}$$

Recalling that the number of sites for the dislocation scales as A, the probability of a site being occupied with a dislocation for $A \to \infty$ diverges if $\alpha < 1$. With Eqs. (4) and (5), this defines a phase boundary illustrated in Fig. 1.

It is interesting to compare these results with earlier work on this model. In particular, it was found in Ref. [9] that the phase boundary is the dotted line illustrated in Fig. 1. The results coincide precisely for the high-temperature half of the phase boundary, but are markedly different on the low-temperature side. Indeed, it was found in Ref. [9] that the crystal state is always unstable to dislocation formation at zero temperature, for arbitrarily small disorder strengths. This result is based on a more sophisticated renormalization group (RG) analysis than the approach presented here; however, one can identify precisely why the present work obtains different results at low temperatures. The RG analysis relies on an expansion in the fugacity e^{-E_c/k_BT}, where E_c is the core energy of a dislocation. This expansion turns out to be necessary to derive scaling relations for the system parameters, and arises quite naturally in the RG approach. It has been employed with great success in the theory of two-dimensional melting in the absence of disorder [3]. Such an expansion is completely equivalent in our approach to expanding in e^{-E_0/k_BT}; in particular, one is then led to approximate the thermal factor $1/(1 + e^{(E_0+E_1)/k_BT}) \approx e^{-(E_0+E_1)/k_BT}$. Substituting this into our expression for p, one obtains *precisely* the same result as in Ref. [9]. The failure of the fugacity expansion occurs because of rare but non-negligible disorder configurations in which E_1 is large and negative, leading to unboundedly large values of $e^{-(E_0+E_1)/k_BT}$. However, this thermal probability should never exceed 1 when properly normalized; thus, the fugacity expansion breaks down when the fluctuations in the dislocation energy due to disorder are larger than those due to thermal effects. A very similar breakdown in perturbation theory is known to occur for random field Ising models [14].

In order to find the evidence of this zero-temperature transition, we performed a simulated annealing molecular simulation. We use a model electron system subject to a random potential, whose configurational energy is given by

$$E[\{\vec{r}_i\}] = \sum_{i \neq j}^{N_p} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_{i}^{N_p}\sum_{j}^{N_i} A_i \exp(-|\vec{r}_i - \vec{R}_j|^2/\xi_i^2) + \text{uniform neutralizing background}, \quad (6)$$

where e is the electronic charge, $\vec{r}_i$ are the positions of particles, $\vec{R}_j$ are the positions of randomly quenched impurities, N_p and N_i are the number of particles and impurities, respectively, and ξ_i is the range of the random potential. A neutralizing uniform background is assumed to cancel out the diverging energy due to the long-range electron-electron interactions. ξ_i is fixed to be $\xi_i = 0.3\sqrt{A/\pi N_i}$ so that most particles are under the influence of the random potentials. The disorder strength is characterized by A_i and N_i. In order to maximize the competition between interaction and disorder, we take $A_i = 0.805e^2/a_0$ which is roughly the energy cost in a perfect triangular lattice when a particle is moved by a half lattice spacing along one of its symmetry axes. In our simulation, we tune N_i to change the strength of the disorder. We employ a periodic boundary condition and use the Ewald sum technique to take into account the interaction with image boxes. To obtain the zero-temperature configurations, we use the simulated annealing molecular dynamics technique [8]. The discretized time step size is $\delta t \approx 1.11 \times 10^{-13}$ s and $(1-2) \times 10^5$ steps are devoted to cooling-down processes in 15–30 temperature decrements. Grain boundary formation occurred in some samples at temperatures a little below the melting temperature, but these essentially disappeared when such samples were annealed more slowly.

The positional correlation is characterized as the correlation function of the field $\rho_{\vec{G}}(\vec{r}_i) = e^{\vec{G}\cdot\vec{r}_i}$ where $\vec{G}$ are reciprocal vectors. In practice the correlation function is averaged over six $\vec{G}$'s with $|\vec{G}| = 4\pi/\sqrt{3}a_0$,

which give peaks of structure factors. It is important to determine such $\vec{G}$'s carefully because the positional correlation length is sensitive to $\vec{G}$. The positional correlation length ξ_G is determined by fitting the correlation function to an exponential form. Figure 2 shows a rapid increase of the positional correlation lengths as N_i/N_p approaches to $n_c = 0.075 \pm 0.005$ from above. When $N_i/N_p \leq n_c$, either the correlation lengths are much longer than the system size or the long-range correlation cannot be fitted in an exponential form [15,16].

It is also interesting to observe the configurational energy per particle. Figure 3 shows there is cusplike behavior whose location is consistent with the position of the positional correlation length divergence. This behavior suggests a possible second order phase transition. The argument provided in this paper is, however, analogous to the Kosterlitz-Thouless dislocation-unbinding picture, which usually predicts an infinite order transition. Further investigation of this issue will be necessary.

In conclusion, we argue that there is a dislocation-unbinding transition due to a quenched random potential at a finite strength of disorder down to zero temperature. The difference of our approach from the previous theoretical works resides on the failure of the fugacity expansion on which previous RG studies are based. Numerical simulations of a model electron system in a slowly varying random potential shows evidence of this transition.

The authors would like to thank J. P. Straley and E. Kolomeisky for helpful discussions. This work was supported by the NSF through Grant No. DMR-92-02255, as well as by the Sloan Foundation and the Research Corporation.

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[15] The transition observed in this simulation was not observed in the simulations of Ref. [8]. The difference lies in the disorder potential used in the latter work, which was essentially a correlated disorder potential, in which the correlation length was varied by changing the distance between the impurity plane and the electron plane. However, the *magnitude* of the random potential fluctuations is not affected by controlling the disorder in this way. The theory presented here may be easily extended to describe such a correlated impurity potential [11]; one finds that the probability of a given site being energetically favorable for a dislocation depends only on the long-wavelength limit of the disorder field fluctuations. Since this is unaffected by the setback between the impurities and the electrons, the system should always contain sites favorable for the formation of dislocations. This is precisely what was observed in Ref. [8].

[16] It was also found by inspection that isolated dislocations appeared in the low-temperature configurations only for $n > n_c$. This phenomenology is consistent with the solid line phase boundary of Fig. 1 and not with the dashed line. However, as with any finite size simulation, one cannot rigorously rule out the possibility that new physics will appear at length scales much larger than can practically be simulated, leading to qualitatively different results. Nevertheless, it seems highly unlikely that there is a very large length scale associated with the dotted line in Fig. 1 that is not present in the physics leading to the solid line.