Vortex lattice melting in layered superconductors with periodic columnar pins

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The melting transition of the vortex lattice in highly anisotropic, layered superconductors with commensurate, periodic columnar pins is studied in a geometry where magnetic field and columnar pins are normal to the layers. Thermodynamic properties and equilibrium density distributions are obtained from numerical minimizations of an appropriate free-energy functional. We find a line of first-order transitions that ends at a critical point as the pin concentration is increased. A simple Landau theory providing a semi-quantitative explanation of the numerical results is proposed.

Thermodynamic and transport properties of type-II superconductors in the mixed phase can be altered in a controlled manner by the introduction of artificial pinning centers. Columnar pinning in high-temperature superconductors (HTSCs), produced by damage tracks from heavy-ion bombardment, has been extensively studied experimentally [1,2] and theoretically [3,4] because such pinning enhances the critical current. A random array of such pins leads to a glassy phase, known as Bose glass [3]. The interplay between the lattice constant of the pin array and the intervortex separation should produce [5] commensurability effects. Such effects have been observed in imaging experiments [6] and magnetization measurements [7] on thin-film superconductors with periodic arrays of artificially produced pinning centers.

In this Letter, we investigate the effects of a commensurate, periodic array of columnar pins on the vortex-lattice melting transition [8] in highly anisotropic, layered, HTSCs in a magnetic field. Both the field and the columnar pins are assumed to be normal to the layers. We consider values of the field for which the pin areal density is smaller than that of the vortex lines. Although vortex lattice melting in HTSCs in the absence of pinning has been studied extensively [8], not much is known about the effects of columnar pins on this transition. Since columnar defects produce strong pinning, at temperatures near the melting temperature of the vortex lattice in the pure system each defect should pin a vortex. However, interstitial vortices, present when there are more vortices than pins, should [4] undergo a melting transition at a temperature slightly higher than the melting point of the pure vortex lattice [9]. Evidence for such melting of interstitial vortices has been found in experiments [6,7] on thin-film superconductors with periodic pinning, but the thermodynamics of this transition has not been studied.

Since the defect-pinned vortices produce a periodic potential for the interstitial ones, the melting transition of the latter provides a physical realization of three-dimensional melting in the presence of an external periodic potential. For small concentrations of pinning centers, we find a first-order melting transition from a crystalline solid to an inhomogeneous liquid. As the pin concentration is increased, the transition temperature increases and the latent heat and the jump in the crystalline order parameter at the transition decrease. This line of first-order transitions terminates at a critical point beyond which the thermodynamic transition is replaced by a sharp crossover. This critical point is a rare, experimentally realizable example of continuous melting in three dimensions. We show that a simple Landau theory provides a semi-quantitative understanding of most of our results. Such melting transitions are of interest in other systems such as atoms adsorbed on crystalline substrates [10], colloidal particles in interfering laser fields [11] and arrays of optical traps [12]. Our work is of relevance to these systems also.

Our study is based on a model free energy functional [13,14] for a system of "pancake" vortices [8] in a highly anisotropic layered superconductor. The commensurate array of columnar pins is accounted for by an appropriate "external potential" term [5] in the free energy functional. By numerically minimizing a discretized form of this functional, we have studied the effects of periodic pinning on the structure and thermodynamics of the liquid and crystalline states of this system. We consider a layered superconductor with vanishingly small Josephson coupling between layers (vortices on different layers are coupled via their electromagnetic interaction only). In this limit of effectively infinite anisotropy, which is appropriate [14] for extremely anisotropic Bi- and Tl-based compounds, the energy of a system of pancake vortices residing on the superconducting layers may be written as a sum of anisotropic two-body interactions $v(n, r)$ where n is the layer separation and r is the separation in the plane of the layers. The Fourier transform of v is [14]

$$\beta v(\mathbf{k}) = \frac{2\pi\Gamma\lambda^2[k_\perp^2 + (4/d^2)\sin^2(k_z d/2)]}{k_\perp^2[1 + \lambda^2 k_\perp^2 + 4(\lambda^2/d^2)\sin^2(k_z d/2)]}, \quad (1)$$

with $\Gamma \equiv \beta d \Phi_0^2 / 8\pi^2 \lambda^2$ and $\beta = 1/k_B T$. Here, $k_z(k_\perp)$ is the component of $\mathbf{k}$ perpendicular (parallel) to the layer plane, d is the layer spacing, $\lambda(T)$ the penetration depth in the layer plane, and Φ_0 the flux quantum. The intralayer potential $v(n = 0, r)$ is repulsive and $\propto \ln(r)$, whereas the interlayer potential $v(n \neq 0, r)$, also $\propto \ln(r)$, is attractive, weaker than the intralayer potential by the factor d/λ, and decreases exponentially with n as $e^{-nd/\lambda}$. We use parameters appropriate to BSCCO i.e. $\lambda(T = 0) = 1500 \text{Å}$ and $d = 15 \text{Å}$, and assume a two-fluid T dependence of λ with $T_c(0) = 85$K.

In density functional theory [13–15], the free energy of a state in a density configuration specified by $\rho(i, \mathbf{r})$, the time averaged areal density of vortices at point $\mathbf{r}$ on the ith layer, is given in terms of equilibrium correlation functions of the layered liquid of pancake vortices. We use the Ramakrishnan-Yussouff free energy functional [13] which is known [14] to provide a quantitatively correct description of the melting transition in our system in the absence of pinning. Since the potential produced by a set of straight columnar pins perpendicular to the layers is the same on every layer, the *time-averaged* density of vortices at any point $\mathbf{r}$ must be the same on all layers: $\rho(i, \mathbf{r}) = \rho(\mathbf{r})$ for all i. Then, the free energy per layer may be written in a two-dimensional form:

$$\beta(F[\rho] - F_0) = \int d^2r \left[\rho(\mathbf{r}) \ln \frac{\rho(\mathbf{r})}{\rho_0} - \delta\rho(\mathbf{r}) \right]$$
$$- \frac{1}{2} \int d^2r \int d^2r' \tilde{C}(|\mathbf{r} - \mathbf{r}'|) \delta\rho(\mathbf{r}) \delta\rho(\mathbf{r}')$$
$$+ \beta \int d^2r V_p(\mathbf{r}) \delta\rho(\mathbf{r}). \qquad (2)$$

Here, $\delta\rho(\mathbf{r}) \equiv \rho(\mathbf{r}) - \rho_0$, F_0 is the free energy of the uniform liquid of areal density ρ_0 ($= B/\Phi_0$ where B is the magnetic induction), $V_p(\mathbf{r})$ is the pinning potential, and $\tilde{C}(r) \equiv \sum_n C(n, r)$, where $C(n, r)$ is the *direct pair correlation function* [15] of a layered liquid of pancake vortices. We use the results for $C(n, r)$ obtained [14] from a hypernetted chain calculation [15].

The pinning potential at point $\mathbf{r}$ is given by $\beta V_p(\mathbf{r}) = \sum_{\mathbf{j}} V_0(|\mathbf{r} - \mathbf{R_j}|)$, where the sum is over all pinning centers located at the points $\{\mathbf{R}_j\}$ on a plane, and $V_0(r)$, the potential at $\mathbf{r}$ due to a pinning center at the origin is assumed to have the truncated parabolic form

$$V_0(r) = -\alpha\Gamma(1 - r^2/r_0^2) \qquad (3)$$

for $r \leq r_0$ and $V_0(r) = 0$ if $r > r_0$. Here, r_0 is the range and α is a "strength" parameter chosen to ensure that on the average a pinning center traps $\lesssim 1$ vortex in the temperature range of interest.

We find the minima of the free energy of Eq.(2) using a methodology quite similar to that in our earlier studies [16,17] of hard-sphere systems. We discretize space by defining density variables $\{\rho_k\}$ at the sites of a periodic grid, and use a gradient descent method [16] to locate the minima of the free energy of Eq.(2) written as a function of $\{\rho_k\}$. The use of fast Fourier transforms in the calculation of lattice sums [18] speeds the computations and allows studies of larger systems. To accommodate a triangular lattice, we use a triangular grid with periodic boundary conditions.

We have performed our studies for $B = 2$kG and 3kG. We first checked the results for crystallization without pinning. For this purpose, the computational system was one triangular lattice unit cell with lattice constant a (all lengths are in units of a_0, with $\pi a_0^2 \equiv 1/\rho_0 = \Phi_0/B$), and the spacing h of the computational grid was chosen to have the values a/n with $n = 16, 32, 64$ and 128. The free energies of the crystal obtained [19] for all these values of n are essentially the same, indicating that the effects of discretization are minimal for $h \leq a/16$. The equilibrium value a_m of the lattice parameter a was determined by finding the value of a that minimizes the free energy at a given B and T. The value of a_m is found to be slightly *higher* than the spacing of a perfect triangular lattice of density ρ_0. This reflects the well-known result [8] that the density of a vortex lattice *increases* slightly at melting.

The free energy of the crystal crosses zero at the transition temperature $T_c = 18.45$K at $B = 2$kG. As expected, T_c is slightly higher than that obtained from approximate treatments [14] of the same free energy. The entropy change Δs per vortex is $0.29k_B$, and the jump in the order parameter m, (m is the magnitude of the Fourier component of $\rho(\mathbf{r})$ at the shortest reciprocal lattice vector of the triangular lattice) is $\Delta m = 0.52$. The Lindemann parameter calculated from the density distribution [19] at the crystalline minimum is $\mathcal{L} = 0.26$ at melting. Very similar results were obtained for $B = 3$kG ($T_c = 15.10$K, $\Delta s = 0.28k_B$, $\Delta m = 0.52$, $\mathcal{L} = 0.25$). The close agreement of these results with those of other studies [8,14] establishes the validity of our numerical approach.

Next, we considered the effects of a single pin and a pair of pins on the liquid-state properties. The single-pin calculation was done to fix the value of the parameter α of Eq.(3). Using $r_0 = 0.1a_0$ ($\simeq 60 \text{Å}$ for $B = 2$ kG), we find that in the temperature range of interest ($T \approx 15$-25K), the integrated density inside the range of the pinning potential is close to one if $\alpha \approx 0.05 - 0.06$ ($V_0(r = 0) \approx 7$-9). The density distribution near the center of the defect is gaussian, $\rho(r) \propto \exp(-\alpha\Gamma r^2/r_0^2)$, expected from Eq.(3). Since pinning of multiple vortices at radiation-induced defects is not found in experiments, higher values of α were not considered. Our two-pin calculations show [19] the expected oscillatory behavior [5] of the free energy as a function of the distance between the pins.

To study melting in the presence of a commensurate, periodic array of pins, we considered a triangular lattice of pins with spacing equal to la_m where l is an integer. Thus the pin concentration is $c \equiv 1/l^2$. The computa-

tional cell used was one unit cell of the pin lattice (which contains l^2 unit cells of the vortex lattice) with one pin located at the center of the first unit cell of the vortex lattice. The value of h was fixed at $a_m/64$. The crystalline (or liquid) minimum of the free energy was located by starting the minimization from a crystalline (or liquid-like) initial state, usually that obtained at a nearby T. For both values of B and smaller c, ($l = 10$, 8, 7 and 6) we found a first-order transition (two distinct local minima whose free energies cross at the transition temperature). Results for $B = 2$kG are shown in Fig.1. As expected, the presence of columnar pins increases T_c. The discontinuities in s and m decrease as c increases (inset in Fig.1) because pinning-induced order in the liquid increases with c. The results for $B = 3$kG are very similar, with T_c reduced by approximately 3.4K for all these values of c.
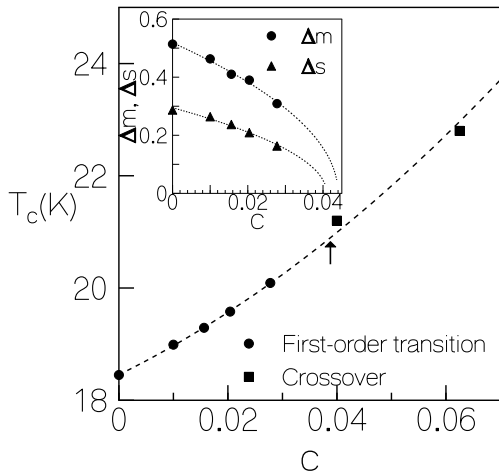

FIG. 1. The phase diagram (T_c vs. pin concentration c) for $B = 2$kG. The dashed line is a polynomial fit. Inset: Entropy change Δs (in units of k_B) and order parameter jump Δm vs c. Dotted lines are fits to the form $const. \times (c_c - c)^{1/2}$. The approximate position of the critical point is indicated by the arrow.

In Fig.2, we have shown the variation of the local density ρ along a line joining two neighboring pinning centers for the coexisting crystalline and liquid minima at the transition temperature for $c = 1/64$ and $B = 2$kG. This plot brings out the differences between the structures of the coexisting crystal and liquid phases and illustrates the ability of our numerical method to provide detailed information about the density distribution in inhomogeneous states. In the liquid state, we find [19] the expected six-fold angular modulation [5] of the density.

At larger values of c, ($l < 6$) the behavior found (for both values of B) is significantly different. Here, the apparent minima obtained in "heating" runs (increasing T in steps from a crystalline state at low T and using the minimum obtained for the last T as the input for the current minimization) and in "cooling" runs (decreasing

T in steps from a liquid state at high T) have almost the same free energy, but significantly different density distributions [19] and values of m. At $c = 1/25$, ($l = 5$) the difference in the values of m peaks at $T = T_x \simeq 21.2$K for $B = 2$kG, as shown in Fig.3. These results suggest
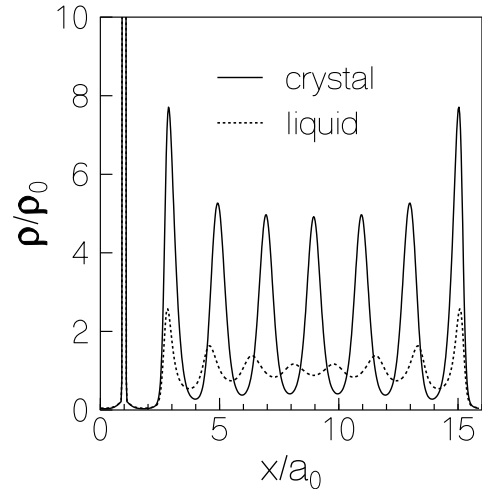

FIG. 2. The normalized local density ρ/ρ_0 along a line joining two adjacent pinning centers. Data for the coexisting crystal (solid line) and liquid (dotted line) for $c = 1/64$, $B = 2$kG are shown. The peak near $x/a_0 = 1$ is at the location of a pinning center.

that F has only one minimum that becomes very "flat" near $T = T_x$: our minimization routine, which assumes that a minimum has been reached when the gradient of the free energy becomes smaller than a small convergence parameter, stops at slightly different points when approaching a very flat minimum from different directions. To check this, we have calculated the free energy of configurations $\{\rho_i(x)\}$ defined by $\rho_i(x) = x\rho_i^{(1)} + (1-x)\rho_i^{(2)}$, where $\{\rho_i^{(1)}\}$ and $\{\rho_i^{(2)}\}$ are the configurations obtained in heating (crystal) and cooling (liquid) runs, respectively, and $0 \leq x \leq 1$ is a mixing parameter. A plot of the free energy as a function of x (or of $m(x) = xm^{(1)} + (1-x)m^{(2)}$, where $m^{(1)}$ and $m^{(2)}$ are the order parameters in the two configurations) exhibits a minimum at $x = x_0 \sim 0.5$ at all temperatures. A typical plot, for $B = 2$kG, $T = 21.2$K, is shown in the inset of Fig.3. In contrast, similar plots for smaller values of c exhibit a clear *maximum* at an intermediate value of x. These results confirm that for $c = 1/25$ or more, the free energy has a unique minimum that lies between the configurations obtained in heating and cooling runs. Thus, no first-order transition occurs at $c = 1/25$, and the line of first-order transitions found for smaller values of c must end at a *critical point* lying between $c = 1/36$ and $c = 1/25$. At $c = 1/25$, the change from liquid-like to solid-like behavior occurs as a sharp crossover. We identify the temperature T_x, which coincides with the temperature at which the temperature-derivative of the "equilibrium" value,

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$m(x_0)$, of the order parameter peaks, as the crossover temperature. The sharpness of the observed crossover (see Fig.3) suggests that $c = 1/25$, $T = T_x \simeq 21.2$K is close to the critical point for $B = 2$kG, as shown in Fig.1. For $c = 1/16$ the crossover is smoother. Our results for $B = 3$kG are very similar, with $T_x \simeq 17.7$K for $c = 1/25$.

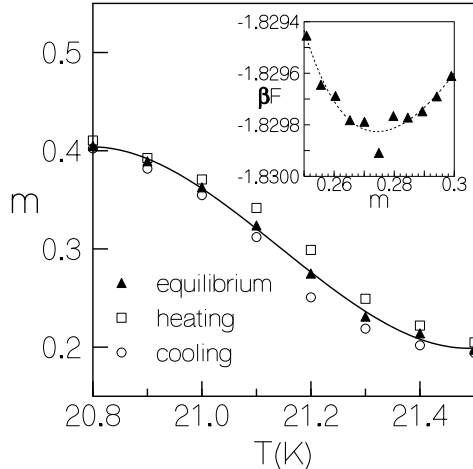FIG. 3. The "heating", "cooling" and "equilibrium" values of the order parameter m (see text) as functions of T for $c = 1/25$, $B = 2$kG. The solid line is a polynomial fit to the equilibrium data. Inset: Plot of the free energy vs. $m(x)$ at $T = 21.2$K. The dotted line is the best fit to Eq.(4).

We can describe the basic Physics underlying this phase diagram as follows. In the presence of commensurate periodic pinning the liquid and the crystal have the same symmetry. Since the degree of order in the liquid increases with c, the liquid and the crystal become indistinguishable beyond a critical value of c. Thus, it is possible to go from one phase to the other without crossing a phase boundary. A simple Landau theory illustrates this. Symmetry considerations [20] suggest the following Landau expansion for F:

$$\beta F = \frac{1}{2}a_2 m^2 - \frac{1}{3}a_3 m^3 + \frac{1}{4}a_4 m^4 - hm, \qquad (4)$$

where a_3 and a_4 are positive constants, a_2 is a decreasing function of temperature, and the "ordering field" h is proportional to the pin concentration c. This free energy leads to a first-order transition for $h < h_c = a_3^3/27a_4^2$ and a critical point at $h = h_c$, $a_2 = a_{2c} = a_3^2/3a_4$. The transition temperature increases with h, and the latent heat and Δm vanish as $(h_c - h)^{1/2}$ as h approaches h_c from below. As shown in Fig.1 (inset), our data for Δs and Δm are well-described by the form $\propto (c_c - c)^{1/2}$ with c_c close to $1/25$. For a more quantitative comparison, we have fitted the βF vs. m data for $B = 2$kG, $T = 21.2$K to the form of Eq.(4) (inset of Fig.3). The values of a_{2c} and h_c, calculated from the best-fit values of a_3 and a_4,

are [19] less than 1.5% lower than the best-fit values of a_2 and h, indicating that the critical point for $B = 2$kG is very close to $c = 1/25$, $T = 21.2$K. This explains the sharpness of the crossover at $c = 1/25$. Our results for $B = 3$kG are very similar. The simple Landau theory, thus, provides a semi-quantitative account of our density functional results and suggests that a critical point lies very close to $c = 1/25$ for both values of B. This critical point is analogous to the liquid-gas critical point in mean-field theory. Fluctuations are expected to change this correspondence because the symmetry of our order parameter is different from that for the liquid-gas transition.

Theoretical and experimental investigations of the nature of this critical point in highly anisotropic HTSCs would be welcome. The critical point should be experimentally accessible: the pin lattice spacing for $B = 2$kG, $c = 1/25$ should be ~ 0.55 μm, close to the spacing of the radiation-induced pin array of Ref. [6]. Applications of our numerical method to other condensed matter systems [11,12] of a similar nature would also be very interesting.

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