Flux-lattice melting in artificially layered superconductors

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(Received 18 March 1996; revised manuscript received 28 May 1996)

We apply a previously described lowest-Landau-level formalism to treat flux-lattice melting in artificially layered superconductors, using Monte Carlo methods. For a pin-free layered system, the model predicts a single phase transition with simultaneous ordering both within one layer and between layers. The melting curve calculated using this model agrees reasonably well with experiments of Koorevaar *et al.* on NbGe/Ge multilayers. [S0163-1829(96)00942-3]

One of the most striking features of the high-T_c superconductors is the large region in the H-T phase diagram where the superconducting order parameter ψ is nonzero, yet the material has a finite resistivity.[1] This phenomenon is believed to be due to the melting of the Abrikosov vortex lattice well below the mean-field upper-critical field line $H_{c2}(T)$.

Flux-lattice melting can also be seen in artificial multilayers of alternating low-T_c materials and nonsuperconductors,[2–4] or of two different kinds of low-T_c materials.[5–7] In a thick layer of a pure low-T_c material, the melting line occurs very close to the mean-field transition temperature $T_{c0}(B)$. The multilayers introduce anisotropy and large thermal fluctuations artificially, thereby lowering the flux-lattice melting temperature significantly below $H_{c2}(T)$, as in the high-T_c materials. Instead of weak Josephson coupling between adjacent CuO_2 planes, the interlayer coupling in the artificial multilayers is produced by coupling through spacer layers of nonsuperconductor. Thermal fluctuations are sizable in the multilayers in part because the Ginzburg-Landau parameter κ can be very large, even though in the multilayers the critical temperature and the mass ratio of the individual layers are quite small. The flux-lattice melting temperature of the multilayers can be tuned by varying the thicknesses of the normal and superconducting layers. The former controls the anisotropy while the latter determined the thermal fluctuations in a single layer.

This paper presents some calculations which approximately describe the experimental results of Ref. 2 on NbGe/Ge multilayers, for a magnetic field applied perpendicular to the layers. We consider a material consisting of alternate layers of two types of materials, denoted 1 and 2, of thickness d_1 and d_2, respectively. Material 1 is assumed to be superconducting, while material 2 is taken as a nonsuperconducting component. The free energy is described by a Ginzburg-Landau free-energy functional of the form[8]

$$F[\psi(\mathbf{r})]=\int d^3r\left[a(T,z)|\psi|^2+\frac{b}{2}|\psi|^4+(2m)^{-1}|(-i\hbar\nabla - q\mathbf{A}(\mathbf{r})/c)\psi|^2\right], \tag{1}$$

where $q=-2e$ is the charge of a Cooper pair. For simplicity, we assume that the coefficient b and the mass m are the same in materials 1 and 2, while a is z dependent (z is the coordinate perpendicular to the layers), taking on different values in the superconducting and nonsuperconducting material (a z-dependent mass could readily be included, although such a change is unlikely to affect the numerical results significantly). It is also assumed that the material as a whole lies in the extreme type-II limit, so that **B** can be approximated by the applied field **H**, and the field energy can be omitted from Eq. (1). Finally, we assume $a(T,z)=\alpha[T-T_{c0}(z)]$, where α is independent of z. Note that $a(z)$ is periodic in the z direction, with period $d=d_1+d_2$.

Following the work of Ref. 9, we include only states in the lowest-Landau level (LLL) of the operator

$$H_\perp=(2m)^{-1}(-i\hbar\nabla-q\mathbf{A}(\mathbf{r})/c)^2 \tag{2}$$

and the lowest band of Bloch states. [Such LLL calculations have already been used with considerable success to describe flux-lattice melting in two dimensions,[10–12] the three-dimensional (3D) high-T_c superconductors $YBa_2Cu_3O_{7-\delta}$ (Ref. 13) and $Bi_2Sr_2CaCu_2O_{8+\delta}$,[9] and a more general model of Josephson-coupled superconducting layers.[14]] In particular, the free-particle Hamiltonian in the z direction is

$$H_\parallel=-\hbar^2/(2m)\cdot\nabla_\parallel^2+\alpha[T-T_{c0}(z)], \tag{3}$$

We now assume that $T_{c0}(z)$ is a square well potential with values T_{c1} and T_{c2} in layers with width d_1, and d_2 in 1 and 2, respectively. With this choice, the Hamiltonian Eq. (3) is equivalent to the Kronig-Penney model, whose solution and band structure are well known. If the band is sufficiently narrow, it is reasonable to approximate it by the nearest-neighbor tight-binding form, $E_\parallel(k)=E_\parallel^{(0)}-2t\cos(kd)$. The tight-binding matrix element t can be estimated by fitting it to the effective mass at $k=0$. The required overlap integral $u_{0000}=\int_0^d|u(z)|^4dz/[\int_0^d|u(z)|^2dz]^2$ can be obtained from the tight-binding Wannier functions $u(z)$. We use the notation $E_\parallel^{(0)}=\alpha T+E_0$, where E_0 is the value of the band minimum $E_\parallel^{(0)}$ at $T=0$.

With these approximations, all the terms in the free-energy function F are identical in form to those of the single crystal case, and the thermodynamic properties can be evaluated by Monte Carlo simulations exactly as in the case of the high-T_c materials.[9,10,13,14] The most significant formal differ-

TABLE I. Parameters for the NbGe/Ge multilayer system (various samples, as described in Ref. 2).

Symbol		$M22$	$M26$	$M30$	$M60$
d_2	(nm)	2.2	2.6	3.0	6.0
t	(10^{-17} erg)	7.4400	7.1385	6.8515	5.0795
$-E_0$	(10^{-16} erg)	4.8449	4.8035	4.7617	4.5272
u_{0000}	(10^6 cm^{-1})	3.8085	3.3855	3.0575	1.9113

ence is that the boundary conditions in the z direction are most appropriately free rather than periodic. We have carried out simulations as described previously,[9,13] generally on cells of dimensions $N_x l_0 \times N_y \sqrt{3}/2 l_0 \times N_z d$, where $l_0=[2\Phi_0/\sqrt{3}H]^{1/2}$ is the intervortex spacing, and typically $N_x=12$, $N_y=12$ and $N_z=6$ or 18. We take periodic boundary condition in the ab directions, and free or periodic boundary condition in the c direction. We use about 10^4 passes through the sample for equilibration, and Monte Carlo averages are evaluated using an additional 10^4 passes through the sample.

It is straightforward to connect the parameters in this model to NbGe/Ge multilayers. First, the coefficient $\alpha=(2mc/\hbar|q|)dH_{c2}/dT|_{T=T_{c1}}$, where $H_{c2}(T)$ is the mean-field transition temperature of the superconducting layer. This condition determines α in terms of the slope of the mean-field upper critical field line. Similarly, $b=2\pi\kappa^2(\hbar|q|/mc)^2$, where $\kappa=\lambda/\xi$, and λ and ξ are penetration depth and correlation length of the superconducting layer. Effectively in this model, we are really assuming superconductor–normal-metal–superconductor coupling through the Ge layers, by treating these layers as Ginzburg-Landau superconductors with transition temperature $T_{c2}=0$.

The remaining tight-binding parameters can be obtained from other experimental quantities in the NbGe/Ge superlattices,[2] or can be evaluated numerically, as enumerated in Table I. For the other parameters, we use $T_{c1}=3.16$ K ($S90$), $T_{c2}=0$ K, $|dH_{c2}/dT|_{T=T_{c1}}=2.5\times10^4$ Oe/K, $d=20.2$ nm, and $\kappa=78.5$. d_1 and d_2 are the thicknesses of the NbGe and Ge layers, respectively.

We describe our numerical results in terms of various correlation functions, as introduced in previous papers[9,13] These include the two-point correlation function $\Gamma^{(2)}(\mathbf{r},\mathbf{r}')\equiv\langle\psi(\mathbf{r}')\psi^*(\mathbf{r}')\rangle$, the density-density correlation function $\Gamma^{(4)}(\mathbf{r},\mathbf{r}')\equiv\langle|\psi(\mathbf{r})|^2|\psi(\mathbf{r}')|^2\rangle$ (where the brackets $\langle\cdots\rangle$ denote a canonical average), and their Fourier transforms $\Gamma^{(p)}(\mathbf{q}_\perp,q_z)$ ($p=2,4$). Another quantity of interest is the helicity modulus tensor,[15] for which a general expression can be found in Ref. 13. As discussed previously, only the c component, γ_{zz}, is nonzero in the *pin-free* crystal, since the Abrikosov lattice can then slide freely in the ab plane.

Figure 1 shows the ''structure factor'' $\Gamma^{(4)}(q_x,0,0)/G_{at}^{(4)}(q_x)$ as function of q_x for sample $M22$ and sample size $12\times12\times6$ at several temperatures, where $G_{at}^{(4)}(q_x)=[(L_yL_z/d)\exp(-q_x^2/4\beta^2)]^2$, $\beta^2=|q|H/(\hbar c)$. The intensity of the sharp Bragg-like peaks diminishes with increasing temperatures, which is indicative of Debye-Waller-like fluctuations of the flux lines. Similar structure is observed for other Bragg peaks in other symmetry directions.

Analogous structure is seen in real-space correlation func-

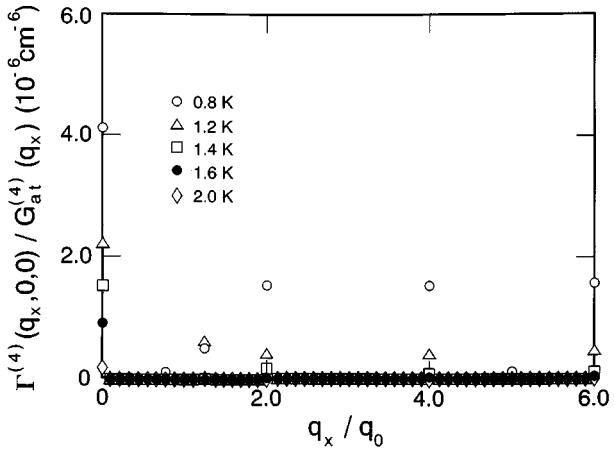

FIG. 1. Calculated structure factors $\Gamma^{(4)}(q_x,0,0)/G_{at}^{(4)}(q_x)$ for model NbGe/Ge (in cm^{-6}), at a field $H=1.2\times10^4$ Oe. The wave-number scale is defined by $q_0=2\pi/l_0$, where $l_0=[2\Phi_0/\sqrt{3}H]^{(1/2)}$ is the intervortex spacing, and $\Phi_0=hc/|q|$ is the flux quantum. The sample size is $12\times12\times6$. In this and the following figures, unless otherwise stated, the calculations are carried out with free-boundary conditions in the z direction.

tions. Figure 2(a) shows the two-point correlation function $\gamma^{(2)}(x,0,0)=\Gamma^{(2)}(x,0,0)/\Gamma^{(2)}(0,0,0)$. At low temperatures, this quantity shows peaks at positions reflecting the periodicity of the crystal. In order to see similar structure in $\gamma^{(2)}(0,0,z)=\Gamma^{(2)}(0,0,z)/\Gamma^{(2)}(0,0,0)$, it is necessary to carry out calculations with a larger number of layers. Figure 2(b) shows the results of such calculations for a $12\times12\times18$ sample. They show, as expected, that $\Gamma^{(2)}(0,0,z)$ decreases with increasing temperature and separation, as observed previously in $BiSr_2Ca_2CuO_{8+\delta}$.[9]

Figure 3 shows $\gamma_{zz}(T)$ for two cases: free (FBC) and periodic (PBC) boundary conditions in the z direction. In both cases, the sample size is $12\times12\times6$. As one might anticipate, γ_{zz} is smaller at any given temperature for FBC than for PBC. Since γ_{zz} measures the stiffness against long-wavelength twists of the phase of ψ, the toroidal structure implied by PBC presumably increases the difficulty of twisting the phase, relative to FBC, thereby increasing the helicity modulus. We have found that the difference between PBC and FBC increases with decreasing numbers of layers. In the monolayer limit, γ_{zz} is, of course, not defined, since a monolayer is a 2D system.

In Fig. 4, we show the calculated phase diagram for the $M22$ material, as obtained using free-boundary conditions in the z direction for a $12\times12\times6$ sample, i.e., six *pairs* of layers in the z direction. The phase boundary is taken as the point where γ_{zz}, as calculated using free-boundary conditions, vanishes. The agreement between theory and experiment is satisfactory, given uncertainties in the various parameters of the model.

We have not done a detailed comparison between theory and experiment for the other samples studied in Ref. 2. Nevertheless, one other feature of the experiments can be deduced from the LLL model, even without a full numerical study. It is found in the experiment that, for sufficient small thickness of the Ge spacer layers, the flux-lattice melts as if the entire multilayer system were *one single layer*. In our

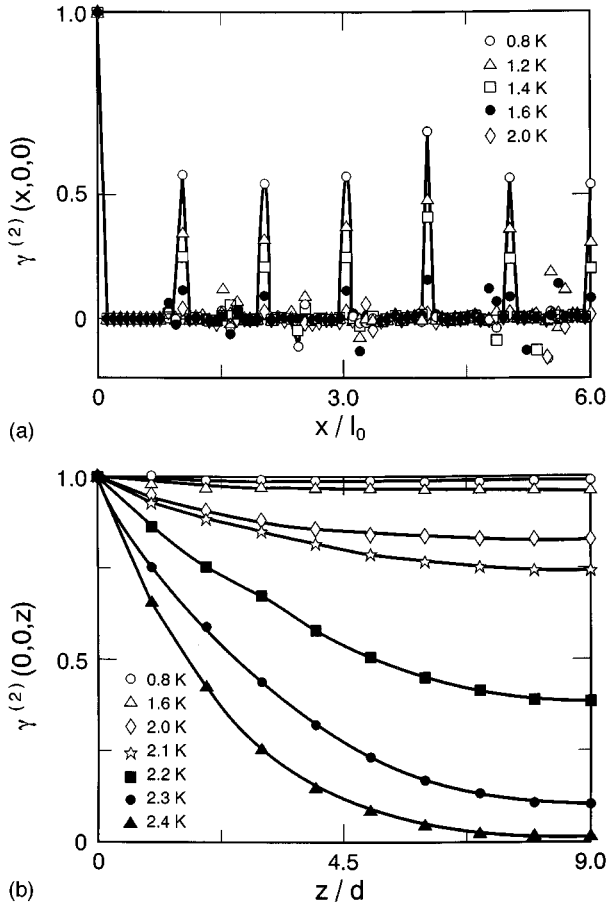

FIG. 2. (a) Normalized two-point correlation function $\gamma^{(2)}(x,0,0) \equiv \Gamma^{(2)}(x,0,0)/\Gamma^{(2)}(0,0,0)$, plotted as a function of x/l_0 at several temperatures for model NbGe/Ge. The sample size is $12\times12\times6$. (b) $\gamma^{(2)}(0,0,z) \equiv \Gamma^{(2)}(0,0,z)/\Gamma^{(2)}(0,0,0)$ vs temperature, where d is the period in the c direction. The sample size is $12\times12\times18$ with FBC. Solid lines are to guide the eye. Other conditions as in Fig. 1.

model, a small spacer layer would correspond to a large coupling constant t. For sufficiently large t, the allowed fluctuations are restricted: all c_{kn}'s for the same k but different n should be equal, since other fluctuations would be energetically too expensive (these coefficients are defined in Ref. 9). In that case, the free-energy functional simply reduces to that of a single layer, with renormalized coefficients. Thus, it follows from the structure of the Hamiltonian [Eqs. (4) and (5) in Ref. 9] without any detailed calculations, that the melting transition in this strong coupling case should behave like that of a single layer.

Finally, we comment on another possible experimental consequence of the fact that only $\gamma_{zz} \neq 0$ in the flux-lattice state, in this model. If a sufficiently defect-free multilayer could be constructed, this effect would be seen experimentally as a vanishing of the c-axis resistivity, while the ab resistivity would remain finite even below freezing. Such behavior has been reported experimentally by Safar *et al.*,[16] where it was interpreted as the onset of a line liquid. While a line liquid remains a possibility, the present model shows that the same behavior could also occur in a highly pin-free layered system where the flux lattice could slide under an

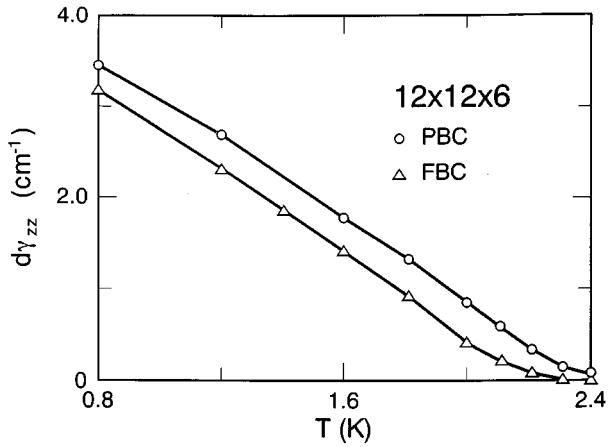

FIG. 3. γ_{zz} in Gaussian units) for a NbGe/Ge multilayer, with periodic (PBC) and free- (FBC) boundary conditions in the z direction. The sample size is $12\times12\times6$.

applied current even below the melting temperature. With pinning present, all three components of γ would become nonzero, leading to a simultaneous resistive transition in all three directions. In a finite sample, also, the sliding of the flux lattice is probably prevented by the sample surfaces. For these reasons, it seems rather unlikely that such behavior could be observed in an artificially layered material. Hence, the cause of the ''line transitions'' observed by Safar *et al.* remains unknown.

In summary, we have presented calculations describing flux-lattice melting in artificial multilayers within the LLL model. This model predicts that the melting transition (in an ideally clean, pin-free sample) is a single phase transition. Below it, long-range order develops simultaneously both parallel and perpendicular to the layers. The transition temperature predicted from this model is in reasonable agreement with the measurements of Koorevaar *et al.*[2] We conclude that the LLL model is an adequate starting point for describing the superconducting transition in multilayer filmsof low-T_c as well as high-T_c superconductors.

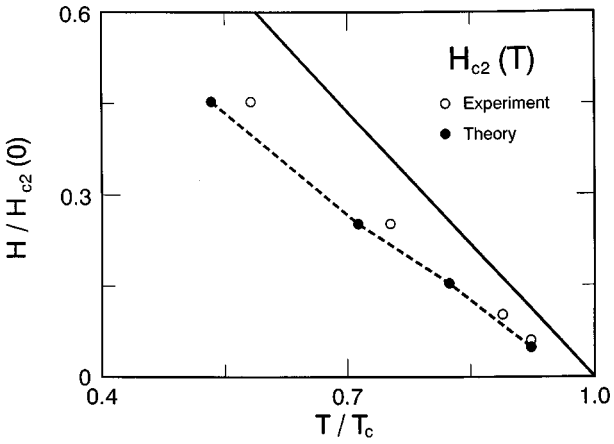

FIG. 4. Flux-lattice melting curves for NbGe/Ge for sample $M22$. Open circles: simulation results, obtained with free-boundary conditions in the z direction. Full circles connected by a dashed line: experiment (Ref. 2). Full line: mean field theory for NbGe layer.

This work was supported by DOE Grant No. DE-FG02-90 ER45427 through the Midwest Superconductivity Consortium, and by NSF Grant No. DMR94-02131. We are grateful for useful conversations with D. E. Farrell. D. S. thanks Professor S. Doniach and the Department of Applied Physics at Stanford University for their warm hospitality while this work was being completed.

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