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Simulations of the onset of diffusion in a flux-line lattice in a random potential

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We simulate the finite-temperature dynamics of flux lines in a thin film. It is shown that a weak random potential significantly reduces the temperature, T_D, at which flux lines start to diffuse and dissipation sets in. The diffusion starts to take place along grain boundaries in the flux-line lattice. These findings are discussed in relation to the magnetic properties of the high-temperature superconductors.

It has now become apparent that the electrical properties of high-temperature superconductors in magnetic fields are strongly influenced by the finite-temperature behavior of the Abrikosov flux-line system in these materials. Many interesting features have been observed. The resistive transition becomes very broad when a magnetic field is applied.[1,2] An irreversibility line is found in the field-temperature phase diagram.[3,4] Flux creep rates are unusually high,[4] and thermally assisted flux flow has been proposed as an explanation for these high rates.[5] Aging and memory effects also seem to have been observed.[6] Although the experimental evidence for melting of the flux-line lattice[7] is not conclusive,[8] theoretical considerations suggest that melting might take place at low temperatures compared to the superconducing transition temperature.[9]

All the above-mentioned phenomena are related to the mobility of the flux lines. This problem is complicated by the fact that due to inhomogeneities in the superconducting material, the flux lines always experience a random potential background. The mobility is thus determined by the combined effect of the random potential and thermal fluctuations.

We have simulated the onset of diffusion in the flux-line lattice in a thin-film superconductor. We prefer to discuss our results in terms of mobility rather than in terms of melting. The reason is that even a weak random potential at zero temperature destroys the order of the lattice,[10] resulting an amorphous glass-liquid-like (static) structure.

In this paper, the temperature T_D at which vortices start to become mobile is studied as function of applied magnetic field and strength of the random pinning potential. We find that *weak* randomness *reduces* T_D significantly, and that the diffusion takes place in channels along grain boundaries in the flux-line lattice. The random potential facilitates the creation of these grain boundaries and thereby assists the thermal fluctuations in making the vortices diffuse.

Details of the simulation method have been published previously.[11] We consider a set of vortices with velocity $\mathbf{v}$ determined by an over-damped diffusive equation of motion

$$\mathbf{v}=\frac{1}{\eta}\mathbf{F}+\chi \ , \tag{1}$$

where η is the friction (or viscosity) coefficient, and $\mathbf{F}$ is the total force on a vortex due to the other vortices and the random potential. The function χ is a Gaussian white-noise velocity that models the coupling to a heat bath at a given temperature T. To make the simulation computationally manageable we consider straight, parallel flux lines, in which case the vortex-vortex force is determined by the potential[12]

$$U_{vv}(\mathbf{r}_i)=\varepsilon_0(0)(1-b)(1-t^4)\sum_{j\neq i}\{K_0[r_{ij}\sqrt{(1-b)}/\lambda]-K_0[r_{ij}\sqrt{(2-2b)}/\xi]\} \ , \tag{2}$$

where the energy scale $\varepsilon_0(0)=\phi_0^2/[8\pi^2\lambda(0)^2]$ [ϕ_0 is the flux quantum and $\lambda(0)$ is the zero-temperature penetration depth]. $b=B/B_{c2}(T)$ is the reduced magnetic field at the temperature T, $t=T/T_c$ is the reduced temperature (T_c is the superconducting transition temperature), K_0 is a modified Bessel function, and ξ the Ginzburg-Landau coherence length. The random potential is modeled by a set of randomly positioned pinning centers of density n_p at position $\mathbf{R}_p$. For concreteness we use a Gaussian form of the individual pinning wells

$$U_{vp}(\mathbf{r}_i) = -A_p \sum_p \exp\left[-\left\{\frac{|\mathbf{r}_i - \mathbf{R}_p|}{\xi}\right\}^2\right] . \qquad (3)$$

We have chosen the radius ($=\xi$) of the flux-line core as the range of the pinning centers (point pinning) and for the amplitude we take a fraction σ of the condensation energy stored per length in a cylinder of the size of the flux-line core[13]

$$A_p = \sigma \frac{B_{c_2}^2}{16\pi\kappa^2}(1-b)\pi\xi^2 , \qquad (4)$$

where $\kappa = \lambda/\xi$. It should be emphasized that the temperature enters both through the stochastic term in Eq. (1) and through the phenomenological temperature dependence of all the superconducting parameters.[11,14]

The important energy scales in the problem are the vortex-vortex interaction energy and the superconducting transition temperature $k_B T_c$ (k_B is Boltzmann's constant). We consider a system with[15]

$$k_B T_c / d\varepsilon_0(0) = 2.5 \times 10^{-3} ,$$

d being the thickness of the sample, and $\kappa(0)=2$. This choice of parameters is dictated by numerical requirements: Small number of interacting neighbors,[16] and reasonable speed of the stochastic dynamics.[11] A typical high-temperature superconducting sample with $d=\lambda$ should be described by

$$k_B T_c / d\varepsilon_0(0) \simeq 2 \times 10^{-4}$$

and $\kappa(0) \simeq 100$. A conventional superconductor like Niobium-Germanium has

$$k_B T_c / d\varepsilon_0(0) \simeq 7 \times 10^{-6}$$

and $\kappa(0) \simeq 60$. Although, the parameter set we consider does not directly describe a specific material, we find it useful as a model for the study of the effect of the random potential on the mobility of the vortices.

We show in Fig. 1 the onset of diffusion for a flux-line lattice, consisting of 340 flux tubes in the presence of 170 randomly placed pins, as a function of temperature and strength of the random potential. The external magnetic field is kept constant[17] at $b(0) = B/B_{c_2}(0) = 0.1$. The criteria of the onset of diffusion are that the mean-square displacement approaches the normal diffusive behavior (Fig. 2); and that the correlated stringlike motion occurs (Fig. 4).

One sees clearly that even a weak random potential has a dramatic effect on the mobility of the vortices. The flux-line lattice is softened by the disorder. The same effect has been observed at zero temperature,[19] where numerical measurements of the shear modulus of a model system showed a linear decrease of the shear modulus as the amplitude of the random potential was increased. This decrease in the shear modulus reduces the barrier for diffusion. The diffusion onset temperature $T_D(\sigma)$ saturates as the pinning strength σ exceeds about 0.4.

One might have expected that the strong random potential, since it consists of attractive centers, would have increased the diffusion temperature due to its pinning effect. The saturation behavior of T_D may be due to the fact that the density of pins used in this particular simulation is less that the density of the vortices. Since each pinning center can trap only one vortex, the number of mobile vortices approaches a constant value for strong pinning potentials. These mobile vortices diffuse by overcoming an energy barrier that is determined by the density of the pinned vortices. Therefore for low pinning density and strong pinning strength, one expects that the diffusion onset temperature T_D is a function of the pinning density only, and that $T_D(n_p)$ increases with increasing n_p.

In Fig. 2 we show the mean-square displacement

$$R^2(\tau) = \langle [\mathbf{r}_i(\tau+\tau_0) - \mathbf{r}_i(\tau_0)]^2 \rangle$$

as function of τ. The average is over the vortices and over τ_0. The presence of a random potential cause $R^2(\tau)$ to behave as τ^α with $\alpha \sim 0.2$ to 0.4 at times shorter than a

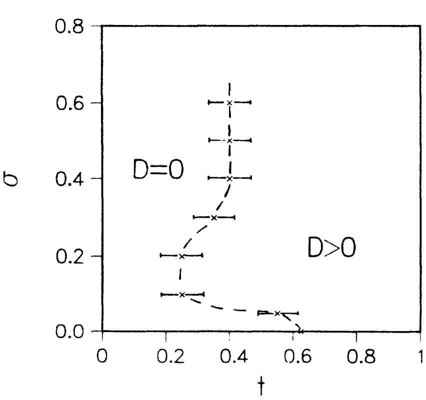

FIG. 1. Diagram of the diffusive and nondiffusive regions for a fixed external magnetic field $b(0)=0.1$. The bars indicate the temperature T_D at which the vortices start to diffuse for a given value of the amplitude of the random potential. The dotted line is a guide to the eye. The system consists of 340 vortices and 170 pinning centers. Periodic boundary conditions are used.

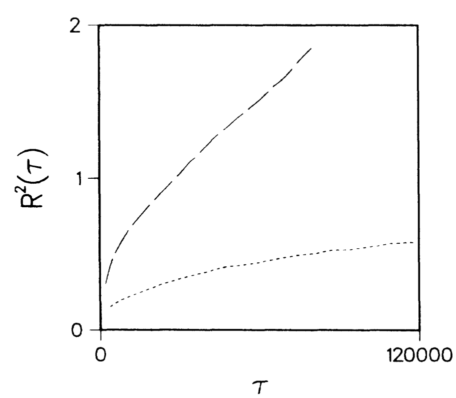

FIG. 2. The mean-square displacement as function of time for three different values of temperatures ($t=0.1$, 0.3, and 0.7 from bottom to top) at a given amplitude of the random potential $\sigma=0.3$. The magnetic field is $b(0)=0.1$.

crossover time τ_{cr}. For times longer than τ_{cr} normal diffusive behavior is observed; i.e., $R^2(\tau) \propto \tau$. The crossover time τ_{cr} increases with increasing σ and decreases with increasing temperature. The anomalous slow diffusion at short times is probably due to the restricting effect of the local minima in the random potential.[18] At longer times the vortices have experienced many thermal fluctuations among which many are large compared to the fluctuations in the random potential. Hence the effect of the random potential is lost at long times.

The diffusion is exponentially activated as is seen from Fig. 3. Here we plot the logarithm of the diffusion constant D as a function of the inverse temperature. The slope of the dashed line indicates that the temperature dependence of D follows a form $D = D_0 \exp(-\Delta E / k_B T)$ with an activation energy $\Delta E \simeq 2 \cdot 10^{-3} d\varepsilon_0(0)$. The activation energy measured this way decreases for small σ ($0 \leq \sigma \leq 0.1$). As σ becomes larger than 0.1, ΔE starts to increase slowly. The crossover from decreasing to slowly increasing $\Delta E(\sigma)$ presumably takes place when the fluctuations

$$\Delta E_p = [\langle U_{vp}^2 \rangle - \langle U_{vp} \rangle^2]^{1/2}$$

in the pinning potential become equal to the vortex-vortex energy barrier, ΔE_{bar}, for a string of vortices to move past the surrounding vortices. This barrier is connected with the shear properties of the lattice and hence is expected to decrease for small increasing σ due to the softening of the lattice.[19] An upper bound of ΔE_{bar} can be estimated from the potential barrier (per vortex) for a string of vortices to move in, say, the $\langle 10 \rangle$ direction in the ideal lattice configuration. Using Eq. (2) we have (for $b = 0.1$)

$$\Delta E_{\text{bar}} \simeq 5 \times 10^{-3} d\varepsilon_0(0) .$$

The fluctuations in the pinning potential are easily estimated if one neglects the distortion of the lattice. The result is

$$\Delta E_p = \left[\frac{\pi n_p}{2} \right]^{1/2} \xi \frac{(1-b)\sigma}{8} d\varepsilon_0(0) . \tag{5}$$

For $b = 0.1$ we have $\Delta E_p = \Delta E_{\text{bar}}$ at $\sigma \sim 0.4$, this value compares reasonably with the value in Fig. 1 at which the crossover occurs.

That the onset of diffusion takes place in the form of correlated string motion, as anticipated by the energy argument given before, can be seen from Fig. 4. Here we show the trajectories of the vortices for $\sigma = 0.1$ at temperature $t = 0.3$, i.e., just as diffusion has started. One notes that the fluctuations in the commensurability between the random potential and the flux-line lattice produce two different types of regions. The pinning centers act more efficiently in places where the random potential matches the vortex lattice. The mobility of the vortices is therefore low in these regions. The less mobile areas are separated by channels in which the vortices diffuse more easily.

We do not observe any qualitative magnetic-field dependence in the range accessible to us, $b(0) = 0.05$–0.2. For $b(0) = 0.1$ and 0.2, the diffusion temperatures for the pure system ($\sigma = 0$) are

$$t_D \equiv T_D / T_c = 0.625 \pm 0.025$$

and 0.675 ± 0.025, respectively. For $\sigma = 0.1$, we have $t_D = 0.25 \pm 0.025$ and 0.525 ± 0.025, respectively. This behavior is to be expected since the flux-line lattice becomes more rigid as the induction is increased for small inductions (see, e.g., Ref. 12).

Some comments about finite-size effects are appropriate. Since the change from no observable diffusion to observable diffusion is difficult to pinpoint numerically, it is difficult to test for finite-size effects. For strong random potentials the correlation length of the vortex lattice is of a few lattice spacings at any temperature. In this range we do not expect our results to change with system size.

The situation is different for weak randomness. It was argued earlier that the activation energy for diffusion in the weak random potential, $\Delta E(\sigma \ll 1)$, is connected with the barrier for plastic shear flow in a random potential background. The latter we expect to be related to the energy needed to produce topological defects in the vortex lattice. In a previous zero-temperature study[10] we

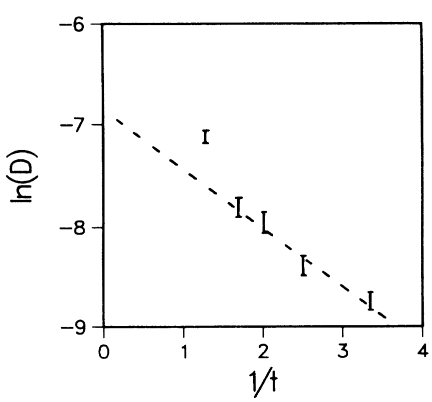

FIG. 3. The diffusion constant as function of temperature. The system is the same as in Fig. 1. The strength of the random potential is $\sigma = 0.1$.

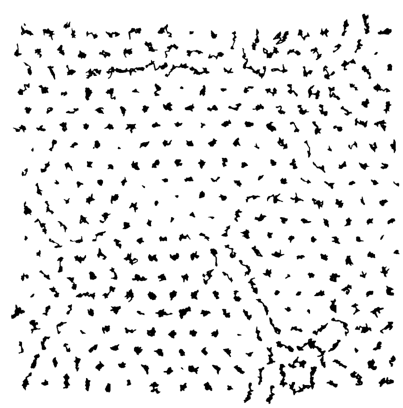

FIG. 4. Plot of the trajectories of the vortices for the same system as in Fig. 1. The temperature is $t = 0.3$, diffusion has just started. The field and random potential is $b(0) = 0.1$, $\sigma = 0.1$.

found that the amplitude of the random potential A_{plas} at which the disorder is able to produce plastic deformations decreases logarithmically with the size of the system. Hence, we also expect $\Delta E(\sigma \ll 1)$ to be logarithmically decreasing with the system size. We estimate that the zero-temperature value of A_{plas} for the system described in Fig. 1 corresponds to $\sigma \simeq 0.1$.

Markiewicz (see Ref. 9) has considered an analytical model of two-dimensional flux lattice melting and the influence of pinning potentials on the melting temperature. For the Kosterlitz-Thouless[20] mechanism, the melting temperature is given by

$$k_B T_M = \frac{a_0^2}{4\pi} C_{66} d \ , \qquad (6)$$

where

$$a_0 = (\tfrac{4}{3})^{1/4} \sqrt{\Phi_0 / B}$$

is the lattice spacing, and C_{66} is the shear modulus of the flux-line lattice. Using Brandt's[21] expression for C_{66} the melting temperature predicted by Eq. (6) for the system described in Fig. 1 at $\sigma = 0$ is found to be $t_M = 0.92$, while the diffusion temperature determined in the simulation is much lower, $t_D = 0.65$. The reason for this discrepancy could be that the onset of diffusion is connected with correlated string motion as shown in Fig. 4, rather than with unbinding of dislocations. As mentioned in Ref. 11, it is not possible from the simulation to distinguish unambiguously between Kosterlitz-Thouless-like behavior or an alternative mechanism. Markiewicz also points out that—as observed in the present simulation—the effect of a pinning potential can be to lower the diffusion temperature.

We want now to associate the preceding discussion with the magnetic properties and resistive transition in the high-temperature superconductors. It is well known[22] that the pinning energies in Bi-Sr-Ca-Cu-O are much smaller than those found in Y-Ba-Cu-O. Hence, the bismuth compound is located in the low-σ regime of the diagram in Fig. 1. The yttrium compound is, on the other hand, in the upper part of the $\sigma - t$ diagram. Kleiman, Gammel, Schneemeyer, Waszczak, and Bishop[23] have published Bitter patterns for both yttrium and bismuth samples. The decoration of two samples was performed simultaneously, and it was found that the flux lines in the bismuth sample had diffused much more than the flux lines in the yttrium sample. This observation is compatible, for example, with $\sigma = 0.1$ for the bismuth sample, and $0.2 < \sigma < 0.4$ for the Y-Ba-Cu-O sample.

A much broader resistive transition[24] is observed in the bismuth compounds than found in the yttrium compounds. This difference is also likely to be connected with the different position of the two materials in an $\sigma - t$ diagram. The weak pinning potential in Bi-Sr-Ca-Cu-O can lower the diffusion temperature and hence makes resistivity occur at a much lower temperature, whereas the strong pinning potential in Y-Ba-Cu-O helps to prevent flux motion.

Finally, we mention that the onset of diffusion in the form of chainlike shear motion might explain why Tinkham's shear-limited phase slip model of the resistive transition[2] is so successful in spite of the fact that the model ignores the pinning potential.

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[15]This is the same system as the one used in Ref. 11. The value for $\lambda^2 T_c/d$ given in Ref. 11 contains a misprint. The correct value is $\lambda^2 T_c/d = 10^{-2}$ cm.

[16]The lattice constant of the triangular Abrikosov lattice is given by $a_0 = (\frac{4}{3})^{1/4} \sqrt{2\pi/b}\, \lambda/\kappa$.

[17]It should be noted that since B_{c_2} is temperature dependent the actual *reduced* field varies with temperature like $b(t) = b(0)(1+t^2)/(1-t^2)$. In the temperature range con-

sidered in Fig. 1 $b(t)$ varies from 0.11 at $t=0.2$ to 0.45 at $t=0.8$.

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