Monte Carlo Simulations of a Disordered Lattice London Model

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The effects of uncorrelated disorder in three-dimensional type-II superconductors are studied by means of Monte Carlo simulations of the current-voltage characteristics of a disordered lattice London model. Vortex motion observed at any temperature and current in the simulations suggests that there is no finite-T glass transition in this model because there are finite barriers against vortex motion at any temperature. [S0031-9007(96)01705-X]

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The mixed state of type-II superconductors is still not fully understood [1]. A largely unresolved question of great theoretical interest is how point disorder affects the phase diagram. While there now seems to be strong theoretical [2] and experimental [3] evidence for a first-order melting transition of the flux line lattice (FLL) in pure bulk materials, uncorrelated pointlike defects modify this transition in a way that remains unclear. Theoretical predictions [1,4,5] have not been satisfactorily confirmed by experiments, which yield somewhat conflicting results [6–9], certainly because disorder cannot be entirely controlled, either in density, nature, or strength. In particular, a transition to a "truly superconducting" glassy phase, characterized by a phase pattern that is random in space but frozen in time, a vanishing linear resistivity, and a highly nonlinear exponential current-voltage relation, has been predicted to occur at a temperature T_g (possibly equal to 0) for sufficiently strong pinning centers [5,10]. Early experimental evidence (the glass transition *should* manifest itself in the inversion of concavity of log-log I-V curves) for such a glassy transition [6] is inconclusive [11] because the observed transition could be due to correlated pinning. Finally, recent resistivity measurements indicate a suppression of the melting transition [9] in the presence of weak disorder.

It seems therefore that Monte Carlo (MC) simulations could bring new insight into this problem. But most (3D) simulations so far have either addressed questions related to the melting transition of the pure system [12,13], or focused on a particular model of strong disorder, the gauge-glass model, where there is no applied magnetic field [10] (see also [14,15]). The relevance of the latter to the modeling of real disordered materials in the mixed state has yet to be firmly established; Bokil and Young [16] recently reported results on this model where screening, which was neglected in previous simulations, was found to destroy the finite T_g glass transition. In order to study the effects of pointlike disorder on the melting transition, we performed MC simulations of a lattice London model, used by several authors to investigate the behavior of the pure system [12], supplemented with an uncorrelated random potential accounting for the presence of defects. This is, to the best of our knowledge, the first attempt to explore the effects of disorder by means of simulations with a realistic model containing the essential physics of bulk superconductors in the London limit. Only the isotropic case is considered here; results should therefore apply to moderately anisotropic materials such as YBCO. Because most characterizations of the glassy transition rely on transport properties, we have measured current-voltage (I-V) characteristics with a method used previously in a related context [17,18].

Model.—Simulations are performed on a cubic grid. The unit cell is of size d, that we take equal to the bare correlation length ξ. Vortex lines are constructed from finite elements e_μ, $|e_\mu| = d$, $\mu = 1, 2, 3$, located at the center of each cell. The vorticity $q_{j\mu} = 0, \pm 1, \pm 2, \ldots$ indicates the number of flux quanta carried by cell j in the μ direction. Solving the lattice London equation without disorder and with periodic conditions in all directions [12] yields the energy $E = \sum_{i,j} \sum_{\mu=1}^{3} G(r_i - r_j) q_\mu(r_i) q_\mu(r_j)$. The couplings $G(r_i - r_j)$ are defined through their Fourier transforms $G(p) = 4\pi^2 J/(\kappa^2 + \lambda^{-2} d^2)$, where $\kappa^2 = 4 \sum_{\mu=1,2,3} \sin^2(p_\mu d/2)$, λ is the London penetration depth, $J = \phi_0^2 d/16\pi^3\lambda^2$ sets the energy scale. In the following, $k_B T$ will be defined in units of J and distances in units of d. We use a finite penetration depth λ such that $\lambda = 20d$. We include the effect of the pinning potential by supplementing the energy with a potential term: $E = \sum_{i,j} \sum_{\mu=1}^{3} G_\mu(r_i - r_j) q_\mu(r_i) q_\mu(r_j) + \sum_i U_{\mathrm{pin}}(r_i) \rho(r_i)$, where $U_{\mathrm{pin}}(r_i)$ is the pinning energy lost or gained by a vortex segment passing through cell i and $\rho(r_i)$ is the vortex density at that cell (Fig. 1). Note that since d is the atomic displacement in our model, the approximate range of the pinning potential is about d and a vortex segment feels the potential only when it reaches the corresponding cell. The distribution of pinning energy U per site is given by $P(U) \propto \exp(-U^2/U_0^2)$, where U_0 is a characteristic pinning energy. U_0 can be evaluated as follows: The total average pinning energy of a cell is $\langle U_{\mathrm{pin}}^2(\xi) \rangle^{1/2} \approx 2\pi J \xi^{-1} (n_i \xi^{-2} \sigma_i^2)^{1/2}$, where n_i is the average number of

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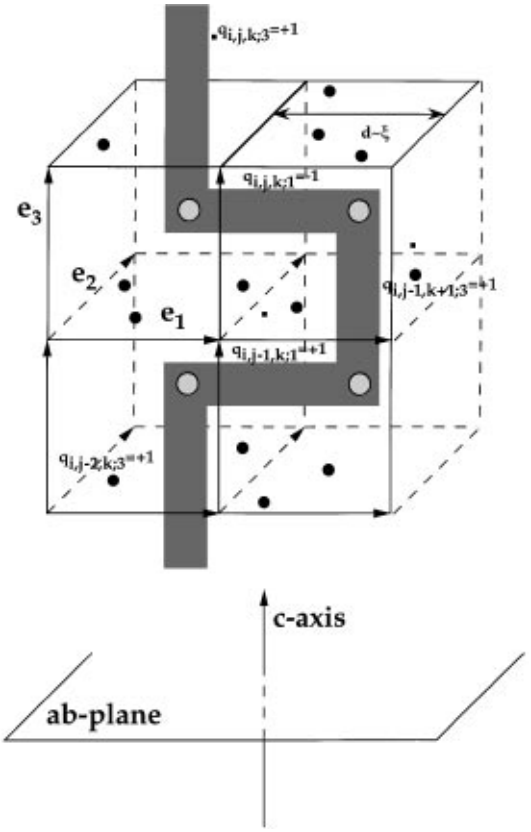

FIG. 1. Plaquette in the presence of disorder. Black circles represent impurities and grey circles plaquette centers. Four plaquettes are shown and a five-segment vortex is represented with a kink (dark grey tube). Corresponding vorticities are indicated.

defects per cell and $\sigma_i \approx 2\pi(\xi/5)^2$ is the scattering cross section, so that $\langle U_{\rm pin}^2(\xi)\rangle^{1/2} \approx 3J$ and $U_0 \approx 1J$-$10J$ (a usual irradiation dose creates approximately 0 to 8 oxygen defects per ξ^3 volume [1]). We have explored strengths ranging from $0.5J$ to $10J$, and report results for $U_0 = 2J$, $3J$, and $10J$.

Simulations start with a fixed number n_i of straight vortex lines along the c axis, arranged in an approximate (Abrikosov) triangular lattice. New configurations, generated by adding at a randomly chosen site of nonzero vorticity a randomly selected elementary loop of unit vorticity, are accepted or rejected according to a standard Metropolis procedure. One MC step corresponds to $\Omega = L_1L_2L_3$ such elementary trials, where L_μ is the linear size of the grid in the μ direction. The update procedure conserves both the local vorticity and the total magnetic induction $B_\mu = (\phi_0 d\Omega^{-1})\sum_j q_\mu(r_j)$. Spontaneous nucleations and subsequent fluctuations of closed loops are neglected; this should not alter too much the results in this isotropic case. This, and the fact that only occupied sites can be updated, allows us to trace individual vortices and their motion. The first 5000 MC steps are used to reach thermal equilibrium with no applied current. Then a current j is applied perpendicularly to the vortices, and measurements start, following a procedure identical to the one used in Refs. [17,18]: Each time an elementary move is made, a term $\delta U \equiv \alpha J = \Phi_0 j\xi^2/c$ is substracted from the corresponding energy change ΔE if the move is in the direction of the Lorentz force, or added to ΔE if the move is in the direction opposite to the Lorentz force; ΔE is not modified for moves perpendicular to the Lorentz force. This procedure generates a net flux of vortices in the direction of the Lorentz force. The voltage V is proportional to $\Omega^{-1}\langle\langle\frac{\Delta M}{\Delta t}\rangle\rangle$, where ΔM is the number of moves in the direction of the Lorentz force minus the number of moves opposite the Lorentz force. $\langle\langle\cdots\rangle\rangle$ denotes thermal averaging and averaging over disorder. Simulations were run for 10 000 MC steps after equilibration with $n_i = 30$ vortices in a $30 \times 30 \times 30$ grid. Twenty simulations were performed for averaging over different realizations of the quenched disorder. The fact that we obtain reasonably small error bars shows that averaging over 20 realizations of disorder is sufficient, especially for our purpose, which is to study the overall shapes of the I-V curves below and above, and not precisely at, the (possible) glass transition. As will be shown below, this procedure allows one to detect a Bose-glass transition when point defects are replaced by columnar defects (Fig. 5).

Results.—In the case of a defect-free material, we find a melting transition at $T_m \approx 0.9$, characterized by the disappearance of the Bragg peaks exhibited by the normalized in-plane structure factor in the low T phase. The introduction of weak pointlike disorder ($U_0 = 2J$) does not drastically modify the static behavior observed in the pure system. Bragg peaks are still observed in the low T phase, so that the melting transition of the weakly disordered system can still be characterized by a quick decay of the structure factor evaluated at the vortex system reciprocal lattice vectors. At this point, we need to evaluate the various length scales involved in the problem, especially to make sure that the collective bundle pinning scales are not far beyond the system's size, a situation that would weaken the significance of the results. To do so, let us define the mean-square relative displacement of two vortices separated by a distance x in the FLL $B(x) \equiv \langle\langle u(x) - u(0)\rangle^2\rangle$, where u is the lateral displacement of a vortex with respect to its equilibrium position. The largest relevant length scale R_a is defined by $B(R_a) \approx \max(\langle u^2\rangle, \xi^2)$. The theory of collective pinning [1,19] allows one to compute R_a: $R_a = (C_{66}/C_{44})^{1/2}2a^4C_{44}/[\pi^3U^2\xi^{-3}(C_{66}^{-1} + C_{11}^{-1})]$, where U is a characteristic pinning energy, $a \approx (\phi_0/B)^{1/2}$ is the FLL constant, and $C_{11} \approx C_{44} \approx B^2/4\pi$ and $C_{66} \approx \phi_0 B/(8\pi\lambda)^2$ are the elastic moduli. Injecting the values of the parameters used in the simulations, we see that R_a is of the order of a few d even for $U_0 = 2J$, because we chose a value of λ which is not much larger than the intervortex distance a. Screening is therefore important for the relevance of our results, since R_a varies as

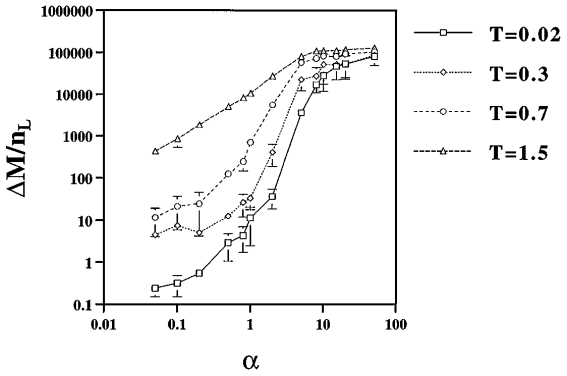

FIG. 2. Log-log plot of I-V curves for a disorder strength characterized by $U_0 = 2J$. ΔM is the number of moves in the direction of the Lorentz force minus the number of moves opposite the Lorentz force. α is a measure of current intensity: $\alpha = \Phi_0 j \xi^2 / cJ$, $n_1 = 30$, $30 \times 30 \times 30$ cubic grid, error bars correspond to averaging over 20 realizations of the quenched disorder.

λ/a (here $\lambda/a \approx 5$, and this makes the large scale behavior of the system, i.e., beyond R_a, accessible).

When a current is applied to the disordered system according to the procedure described above, no transition is observable from the I-V characteristics. In particular, the concavity of these curves in logarithmic representation does not change, even if simulations are performed at very low values of T. In the weak pinning case ($U_0 = 2J$), the I-V response smoothly becomes Ohmic as T increases (see Fig. 2, where error bars correspond to statistical averaging over disorder), and the linear resistivity does not vanish at low T. The Ohmic regime is observed over more than two decades at high enough T. In the stronger pinning case ($U_0 = 10J$), the same conclusion holds, except that the Ohmic regime is not observed within the explored temperature range (Fig. 3). The vortex liquid viscosity becomes stronger for strong pins. Note that these simulations suffer from several drawbacks: (1) One cannot be sure that the MC dynamics captures the way vortices actually move; (2) the MC procedure, which assumes an overdamped dynamics, saturates at large current because vortices cannot move more than a distance d per MC step; this limitation makes the large current region unreliable; (3) the low current–low T region suffers from another limitation, namely, the discreteness of the underlying grid (an artifact of the model), which may prevent vortices from moving because the energy necessary to perform an elementary move is finite; this may result in a reduced observed motion of vortices in that region, all the more as the rigid, collective motion of the whole lattice is not permitted by the MC procedure. We see, however, that disorder promotes the displacement of vortex segments, since V is never equal to 0. At extremely low values of the applied current (e.g., $\alpha = 10^{-7}$), vortex motion is still observed, although it is no longer Ohmic (the slope of the I-V curve is close to 0; see Fig. 4). These remarks might give the impression that an inversion of the concavity of the I-V curves could never be observed owing to limitations intrinsic to MC simulations. However, I-V MC simulations in the presence of correlated defects along the c axis (columnar defects) with $U_0 = 10J$ show an inversion of concavity when the induction is close to the matching field (Fig. 5): This property indicates the existence of the predicted Bose glass at low T [1] and validates the present MC approach.

In conclusion, we observe no inversion in the logarithmic concavity of the I-V curves measured on a lattice London model, including screening, and supplemented with weak or strong point defects. This suggests that there are finite barriers against flux motion *in this model* at finite T, in agreement with the results of Bokil and Young on the 3D gauge glass model with screening [16]. We find a progressive freezing of vortices at low current as T is lowered, with vortex motion observed at any current and temperature. Lee and Stroud [15] found results consistent with a finite T glass transition from I-V measurements on the 3D gauge glass model, yet in the absence of screening and magnetic field; apparently, the 3D disordered lattice London model does not share the dynamic properties of their model, but more extensive simulations, particularly on larger systems, are required. On the experimental side, Fendrich *et al.* [9] have reported the suppression of the (first-order) transition observed in their pure, untwinned $YBa_2Cu_3O_{7-\delta}$ single crystal, after 1 MeV electron irradiation, which is known to induce weak point disorder:

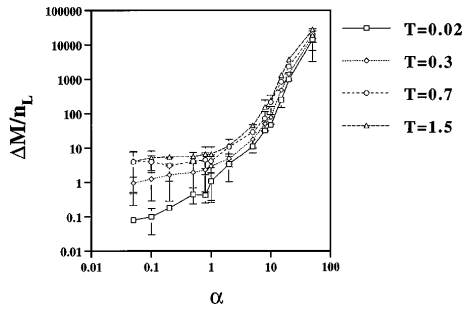

FIG. 3. Same as Fig. 2 but with $U_0 = 10J$.

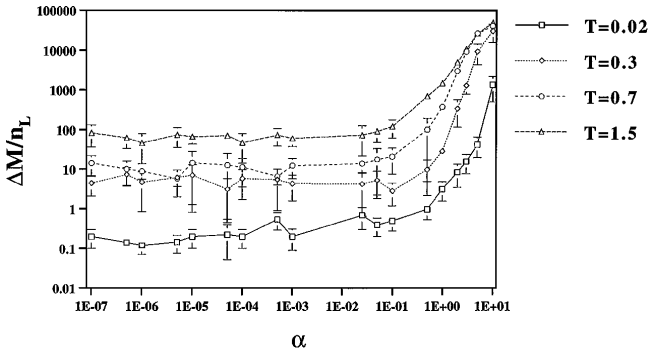

FIG. 4. Same as Fig. 2 but for $U_0 = 3J$, and α varies from 10^{-7} and 10.

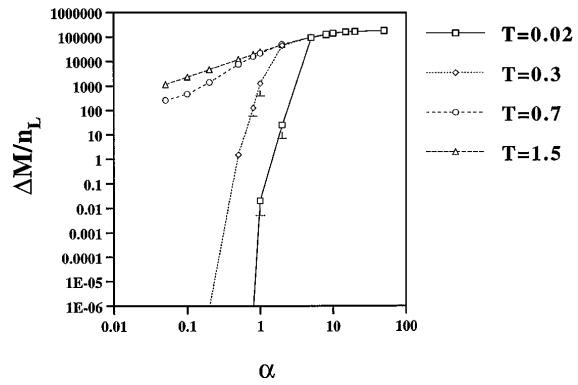

FIG. 5. Same as Fig. 2 but for 25 correlated defects along the c axis, with $U_0 = 10J$.

Our results are in good agreement with these observations as well as with the functional renormalization group analysis performed by Moore and Newman [20] (see also Ref. [21]).

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