Structure and Phase Transition of Josephson Vortices in Anisotropic High-T_c Superconductors

Xiao Hu and Masashi Tachiki
National Research Institute for Metals, Tsukuba 305, Japan
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Monte Carlo simulation is performed on high-T_c superconductors in a magnetic field $\perp \hat{\mathbf{c}}$. By monitoring the temperature dependence of the helicity modulus and the specific heat, we have demonstrated a second-order phase transition, in the universality class of the 3D *XY* model, between phases of finite resistivity and of zero *ab*-plane resistivity. Josephson-vortex lattice, glass, and chains waving along the *c* axis are obtained at lower temperatures depending on the anisotropy and the magnetic field. These results are discussed in consistency with experimental observations. [S0031-9007(98)05984-5]

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According to the pioneering work of Abrikosov [1], under an external magnetic field between the lower and upper critical fields, vortex lines penetrate into a type-II superconductor, and arrange themselves into a regular-triangle lattice in a cross section perpendicular to the field. Although it has been successful in describing the mixed state of conventional superconductors, this theory becomes insufficient for high-T_c superconductors, where the upper critical field disappears. It is now well accepted that the lattice of pancake vortex lines induced by the external magnetic field along the *c* axis is melted into vortex liquid via a first-order thermodynamic phase transition in these anisotropic superconductors [2–5]. The instability of the pancake vortex lattice is caused by thermal fluctuations. The anisotropy of the high-T_c superconductors enhances the effect of thermal fluctuations, and makes the phase transition first-order. When the external magnetic field is applied parallel to the *ab* plane, the effect of anisotropy to the flux state of a high-T_c superconductor is multiple, and thus more complicated. In high-T_c superconductors the superconducting order parameter is finite only in the very vicinity of the CuO_2 layers. When an external magnetic field above the lower critical field is applied parallel to the *ab* plane, the fluxons, Josephson vortices, penetrate the sample through the blocking layers in order to reduce the loss of superconducting cohesive energy. The layer structure of the high-T_c superconductor crystal itself works as natural pinning centers, as first discussed by Tachiki and Takahashi [6]. In the presence of the intrinsic pinning, the instability of the conventional triangular flux lattice comes from the anisotropy, the competition between intervortex forces and the layer structure, as well as thermal fluctuations. Therefore, to clarify the temperature and magnetic field dependence of the mixed state in the external magnetic field parallel to the *ab* plane is very important in a viewpoint of the theory for the mixed state of type-II superconductors. This physics situation has been investigated experimentally and theoretically [7–10]. Comparing with the much more studied case of the external magnetic field applied along the *c* axis, there are many aspects to be explored for the mixed state in the external magnetic field parallel to the *ab* plane. In this Letter, we present for the first time the results of a systematic Monte Carlo (MC) simulation for this problem. We have found that there is a thermodynamic, second-order phase transition between a high-temperature phase of finite resistivity in all of the directions and a low-temperature phase of zero resistivity in the *ab* plane. The ground state of the Josephson-vortex system takes an ordered flux lattice for certain ranges of the anisotropy, whereas a glass and an ensemble of waving chains are taken for other ranges of anisotropy. These phenomena can be well understood from the intrinsic pinning effect of the layered structure.

In order to describe the mixed state of a high-T_c superconductor to the strongly layered limit, we use the following 3D anisotropic, frustrated *XY* model [11,12]:

$$H = -J\Bigg[\sum_{\langle i,j\rangle \| x\text{-axis}} \cos\left(\varphi_i - \varphi_j - \frac{2\pi}{\phi_0}\int_i^j A_x dr_x\right) + \sum_{\langle i,j\rangle \| y\text{-axis}} \cos(\varphi_i - \varphi_j) + \frac{1}{\Gamma^2}\sum_{\langle i,j\rangle \| c\text{-axis}} \cos\left(\varphi_i - \varphi_j - \frac{2\pi}{\phi_0}\int_i^j A_c dr_c\right)\Bigg],$$

which can be derived from the Ginzburg-Landau Lawrence-Doniach free-energy functional [13,14]. The *y* direction is along the external magnetic field, and $\hat{\mathbf{y}} \perp \hat{\mathbf{c}} \perp \hat{\mathbf{x}}$. The lattice spacing along the *c* axis corresponds to the distance between the nearest neighboring CuO_2 planes in a cuprate, and thus in our model Hamiltonian the discreteness along the *c* axis is intrinsic. The underlying square lattice in the *x* and *y* directions, which are parallel to the *ab* plane, are introduced merely for implementing simulation. The effect of the fictitious pinnings in the

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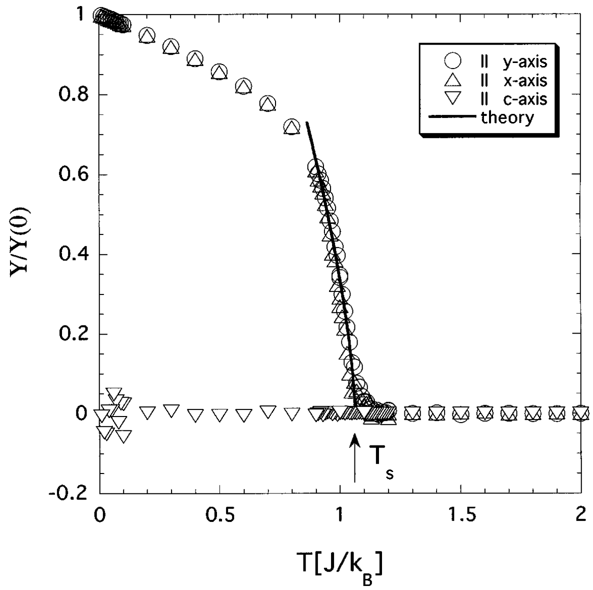

FIG. 1. Temperature dependence of the helicity moduli for $\Gamma = 10$. The solid curve is given by an index $\upsilon = 2/3$, which is expected to be the critical exponent of the 3D classical *XY* model. The system size is $L_x \times L_y \times L_c = 48 \times 40 \times 48$.

x and y directions can be made very small by using a low filling of flux lines such as $f = 1/24$ in the present Letter. The anisotropy constant Γ is a parameter controlling the ratio between the couplings in the ab plane and along the c axis. For small Γ the system should behave similar to a 3D anisotropic, continuous superconductor. However, for large Γ the effect of the layer structure in the c direction is much enhanced and comes to play an important role in determining the vortex structure. Therefore, the system of a large anisotropy constant is expected to be a good model of high-T_c superconductors. The system size is $L_x \times L_y \times L_c = 48 \times 40 \times 48$. We have checked the system-size dependence of the simulation results, adopting $L_x \times L_y \times L_c = 96 \times 40 \times 96$ and $L_x \times L_y \times L_c = 48 \times 80 \times 48$. The number of MC sweeps per degree of freedom and per temperature is 50 000 for equilibration and 100 000 for sampling. MC sweeps are taken up to two million for the system of $L_x \times L_y \times L_c = 48 \times 40 \times 48$ around the transition temperature. See Ref. [12] for more detailed conditions in simulation. We investigate both the thermodynamic behavior of the system upon sweeping the temperature, and the low-temperature phases of the Josephson-vortex system for various values of anisotropy.

Figure 1 shows the temperature dependence of the helicity moduli [15,16] for the system of the anisotropy constant $\Gamma = 10$. Above the critical temperature $T_s \simeq 1.06 J/k_B$, there is no long-range order in all of the directions, characteristic of the liquid of Josephson vortices. Upon cooling across the critical temperature T_s, the helicity modulus along the field and that along the x axis grow simultaneously. The superconductivity in a mixed state of a type-II superconductor is destroyed by a current perpendicular to flux lines if there is no pinning. The helicity modulus perpendicular to the external magnetic field should vanish in such a case. Therefore, the finiteness of the helicity modulus along the x direction is nothing but the result of the intrinsic pinning effect of the layer structure along the c direction, because of the property of the Lorentz force. The zero helicity modulus along the c axis shows very clear evidence that the flux lines are free of pinning along the x direction, as it should be. We have also monitored the specific heat and observed a peak around T_s, as shown in Fig. 2. Therefore, at T_s the system experiences a thermodynamic phase transition between the phase of finite resistivity, normal phase, and a phase of zero ab-plane resistivity, superconducting phase.

Let us pay attention to the nature of the phase transition at T_s. The continuous onset of the helicity moduli below T_s and the enhancement of thermal fluctuations around T_s signaled by the peak of the specific heat, a typical critical phenomenon, indicate clearly a second-order phase transition in the Josephson-vortex system. This fact is consistent with the transport experiment by Kwok *et al.* [9], in which the resistivity disappears continuously as the temperature approaches the critical point from above. The second-order phase transition in high-T_c superconductors in an external magnetic field parallel to the ab plane has been discussed theoretically by Balents and Nelson [10], and is attributed to the nematic-to-smectic transition. By constructing a model free energy and appealing to a renormalization-group analysis, the authors conclude that the phase transition is in the universality class of the 3D classical *XY* model.

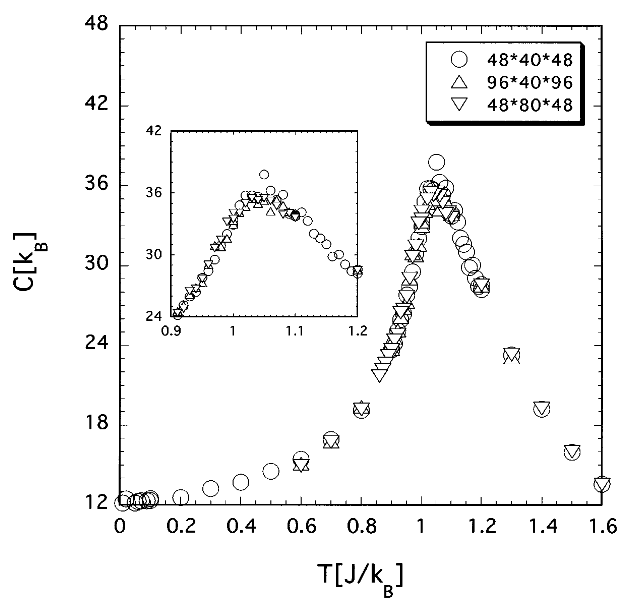

FIG. 2. Temperature dependence of the specific heat per fluxon per length of $d\gamma/\Gamma$ along the external magnetic field for $\Gamma = 10$. Results for different system sizes in simulation are denoted by $L_x \times L_y \times L_c$. The inset is for the vicinity around the critical point.

Our simulation results are consistent with this theoretical discussion presuming the critical exponent $v = 2/3$ for the helicity modulus: First, as shown in Fig. 1, our numerical results for the helicity moduli in the ab plane fit a single power function in the vicinity below the critical point $\Upsilon(T)/\Upsilon(0) \sim (1 - T/T_s)^v$ with $v = 2/3$; second, from the Josephson scaling law $v = 2 - \alpha - 2\nu$ and the hyperscaling relation $\alpha = 2 - D\nu$ [16,17] with D the spatial dimension and ν the exponent for the correlation length, one obtains $\alpha = 0$ for the specific heat from $D = 3$ and $v = 2/3$. This value of α is consistent with the data shown in Fig. 2 since the peak in the specific heat at T_s does not grow with the system size. It is, however, still difficult to estimate the critical exponents numerically from the present data.

It is worthwhile to notice that, in the system of the same anisotropy but with the external magnetic field applied along the c axis, the first-order melting transition occurs at a temperature $T_m \simeq 0.18J/k_B$ [18], much lower than $T_s \simeq 1.06J/k_B$. The relation $T_s(\mathbf{B}\perp\hat{\mathbf{c}}) > T_m(\mathbf{B} \parallel \hat{\mathbf{c}})$ establishes generally.

We then turn to see variations in the structure of Josephson vortices at low temperatures as the anisotropy is tuned. In the present study, flux lines are along the y direction where the external magnetic field is applied. The alignment of Josephson vortices in an xc plane normal to the field is the issue we address in what follows. Increasing the anisotropy constant Γ from unity up to $\Gamma_{c1} \simeq 1.6$, we obtain lattices of Josephson flux lines at sufficiently low temperatures. In Fig. 3(a) we display the structure factor $S(\mathbf{k}_{xc}, y = 0)$ for the case of $\Gamma = 1.6$. The Voronoi cell is a triangle elongated in the x direction. After a scaling of the x axis, namely, dividing the distance in the x direction with the anisotropy constant, the distorted-triangle lattice is transformed to the regular-triangle lattice up to the precision of unit mesh. Therefore, for $1 \le \Gamma \le \Gamma_{c1}$ the intrinsic pinning effect of the layer structure can be neglected. For $\Gamma_{c1} < \Gamma < \Gamma_{c2}$ with $\Gamma_{c2} \simeq 3.0$, no lattice of the Josephson flux lines can be observed, and the low-temperature phase of the system seems to be a glass. This is understood as the result of the frustration from the competition between the intervortex repulsive forces and the intrinsic pinning effect of the layer structure. For $\Gamma_{c2} \le \Gamma < \Gamma_{c3}$ with $\Gamma_{c3} \simeq 3.6$, the commensuration between the vortex alignment determined by the intervortex repulsive forces and the layer structure is achieved, and a lattice structure is recovered. Figure 3(b) is the structure factor $S(\mathbf{k}_{xc}, y = 0)$ for $\Gamma = 3$. For these values of anisotropy, however, the scaling of the distance according to the anisotropy constant is broken. This fact indicates clearly that in this region of anisotropy the intrinsic pinning effect of the layer structure plays an important role in determining the alignment of the Josephson vortices. For $\Gamma_{c3} \le \Gamma < \Gamma_{c4}$ with $\Gamma_{c4} \simeq 5.0$, the low-temperature phase is glass again. Note that the values of the critical anisotropies are up to a precision of 0.1. The above variations of the Josephson-vortex system at low temperatures with the anisotropy is similar to those with the magnetic field proposed by Balents and Nelson [10]. We notice that the magnetic field and the anisotropy constant in simulation can be related to each other by $B = f\phi_0\Gamma/d^2\gamma$, with d the distance between the nearest-neighboring superconducting layers, and $\gamma = \lambda_c/\lambda_{ab}$, with λ_c and λ_{ab} being the penetration depths parallel to the c axis and the ab plane. The transformation of the system to the solid phases seems to be a crossover, since no anomaly in the specific heat can be observed below the critical temperature T_s as in Fig. 2.

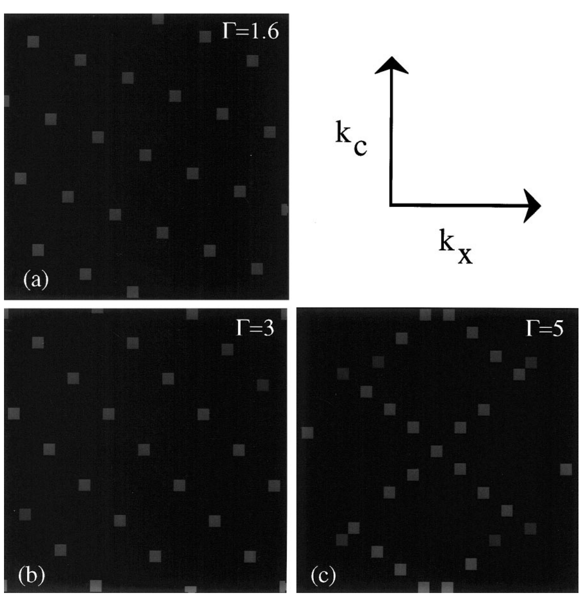

FIG. 3. Structure factors $S(\mathbf{k}_{xc}, y = 0)$ for the Josephson vortices at low temperatures.

As mentioned above, the structure factor in the range $1 \le \Gamma \le \Gamma_{c1}$ can be well understood in terms of an anisotropic, continuum superconducting system, in which the underlying lattice is not important. As Γ increases, the distance among the vortices in the x direction becomes larger, whereas that along the c axis becomes smaller. The fictitious pinning effect along the x direction becomes less, and the intrinsic pinning effect along the c direction becomes more important. Therefore, the possibility of the fictitious pinning effect in the ab plane on the structure of the Josephson vortex system can be excluded. We conclude that the variations of the low-temperature state obtained in the present study are the result of the competition between the anisotropic, repulsive force among the vortices and the intrinsic pinning effect of the layer structure.

When we increase the anisotropy constant further, a drastic change takes place in the structure of the Josephson-vortex system at low temperatures. Figure 3(c) is the structure factor $S(\mathbf{k}_{xc}, y = 0)$ of Josephson vortices at a low temperature for $\Gamma = 5$. While Bragg peaks associated with the local, distorted-hexagonal Voronoi

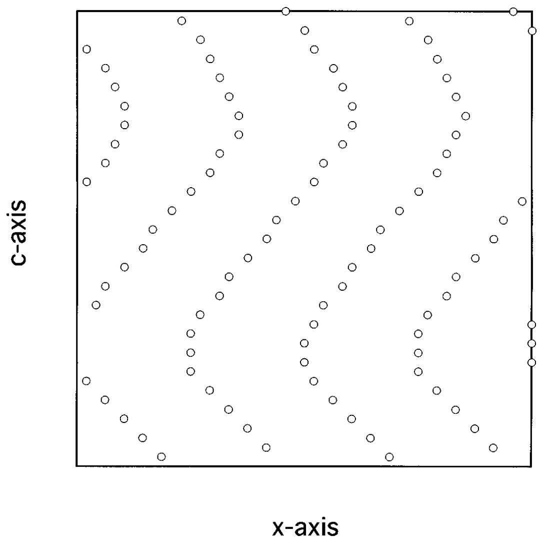

FIG. 4. Real-space distribution of Josephson vortices for Fig. 3(c).

cells are observed, the overall structure is characteristic of one dimension. The distribution of Josephson vortices in real space is shown in Fig. 4. The vortices are much nearer to each other in the c direction than in the ab plane, and thus manifest themselves as chains of flux lines [19]. The chains separate from each other with equal distance in the x direction. In detail, the vortices sit in every other layer in each individual chain, and shift by one layer in the neighboring chains. These properties can be understood by the anisotropy of interactions. If these chains were to stretch in a fixed direction, a sheared triangular lattice would be formed. However, the vortex chains wave along the c axis as in Fig. 4, and the uniform triangular lattice is broken. Although we cannot completely exclude the possibility of a triangular lattice at zero temperature, it is safe to say that the shear modulus for the triangular lattice would be very small [20], so that it is unstable against thermal fluctuations. Waving chains of Josephson vortices are observed at low temperatures for the anisotropy $\Gamma \geq \Gamma_{c4}$ in the present simulation.

The waving of the vortex chains along the c axis is consistent with the Bitter-pattern observation by Dolan *et al.* [7]. This phenomenon was discussed by Ivlev and Campbell in terms of a London model, and the mechanism of the instability of the Abrikosov lattice was attributed to the existence of a twin boundary [8]. In contrast, our simulation results indicate that the waving of the vortex chains exists without any twins. As revealed by the present MC simulation, thermal fluctuations enhance the instability of the triangular lattice and make the waving chains of vortex more favorable thermodynamically at finite temperatures.

In summary, by using the MC simulation, we have observed a second-order phase transition between phases of finite resistivity and of zero ab-plane resistivity. The simulation data are consistent with that of the phase transition belonging to the universality class of the 3D classical XY model. We have obtained Josephson-vortex lattice as the ground state in certain ranges of anisotropy, while we have obtained a glass for other ranges. Chains waving along the c axis are obtained for large anisotropy.

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