Phase transitions in a two-dimensional vortex lattice with defects: Monte Carlo simulation

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Abstract

Phase diagrams and phase transitions in a two-dimensional vortex lattice with defects have been investigated by Monte Carlo (MC) simulation techniques. It was found that in the presence of defects, the melting of the vortex lattice proceeds in two stages. First, the ideal triangular lattice transforms at low temperature into islands, which are pinned to the defects and rotate around them (‘‘rotating lattice’’ phase). Then, at a higher temperature, the boundaries of the ‘‘vortex lattice islands’’ become smeared and the system transforms into a vortex liquid. The dependencies of phase transition temperatures on pinning potential have been obtained. The visual pictures of the flux lattice structures have been calculated. The current–voltage characteristics (IVC) of the vortex structures with defects in forms of points, lines and squares were simulated at different temperatures and defects concentration. We have found that the point defects are more efficient than the other type of defects with equivalent specific concentration. It was shown that the dependencies of critical current on temperature and defects’ concentration are directly associated with the phase state of the vortex system. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

In recent years, considerable attention is paid to phase transformations and their dynamics in vortex lattice of HTSC. Wide application of numerical methods (especially the Monte Carlo (MC) method, see the review in Ref. [1]) has made it possible to simulate the phase states and phase transitions in various vortex systems, and to demonstrate the peculiarities of the vortex lattice melting dynamics in the presence of the pinning centers [2,3]. The MC method was used also for simulation of I–V characteristics (IVC) of model superconductors [4–8]. IVC were calculated in the presence of a large number of defects with different potential energies (relative to the number of vortices) [5]. The results on various phase modes of current flow, obtained recently from an analysis of IVC of HTSC, deserve special attention (see Ref. [8] as well as Refs. [9–11]). The modes of fixed vortex glass, plastic flow of vortex liquid, and moving vortex glass were observed. These phase states of the Abrikosov vortex, as well as transitions between them, are close to the phase

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transitions between the states of "rotating lattice" and "vortex liquid" [2,3]. IVC of layered superconductors have been calculated at different temperature and defects' concentration [4].

In this paper, we report the picture of phase transformation of two-dimensional vortex lattice and results of calculations of IVC and critical current of layered superconductors. We shall demonstrate the influences of temperature; type of defects and defects’ concentration on IVC are associated with the phase states of vortex lattice.

2. Model and computational method

Let us consider a two-dimensional vortex lattice simulating a superconducting HTSC layer on a periodic rectangular grid under the assumption of weak coupling between filaments in a direction perpendicular to the ab-plane and in the presence of pinning centers. The effective Hamiltonian of such a system has the form [12] (without the account of interaction between vortices and external field $B$):

$$ H = 0.5 \sum_{i \neq j}^{N} H(r_i, r_j) n_i n_j + \sum_{i=1}^{N} U_{ij}(r_i) n_i, $$

$$ H(r_i, r_j) = \left( \phi_0^2 d / 2 \pi \lambda^2(T) \mu_0 \right) K_0(|r_i - r_j|/\lambda(T)) $$

$$ = U_0(T) K_0(|r_i - r_j|/\lambda(T)). $$

Here $U_{ij}(r_i)$ is the energy of interaction between a vortex and a defect at the $i$th lattice site, $n_i$ the occupation numbers of vortices (0 or 1) at the $i$th site of the spatial grid with the total number of nodes $N$, $\phi_0$ the magnetic flux quantum, $K_0$ Bessel’s function of the imaginary argument, $d$ the superconducting layer thickness, $\lambda(T) = \lambda(0) / (1 - (T/T_c)^2)^{0.5}$ the depth of magnetic field penetration (we used $n = 3.3$ from data of $\mu^+$SR measurement [13]), and $\mu_0 = 4\pi \times 10^{-7}$ H/m. The energy of interaction of a vortex with a pinning center was chosen in the form $U_{ij}(T) = -U_0(T)$. We have used for simulation the parameters of HTSC Bi$_2$Sr$_2$CaCu$_2$O$_y$ [13]: $d = 0.27$ nm; $\lambda(0) = 180$ nm; $T_c = 84$ K and external magnetic field $B = 0.1$ T.

We have analysed various types of defects, but main calculations have been made for point defects occupying a single cell of the spatial grid. The range of two-dimensional concentrations of defects was from $10^{12}$ to $3 \times 10^{14}$ m$^{-2}$ (from 1 to 100 defects corresponded to 150 vortices in the system under investigation).

Dynamic processes have been investigated by an external transport current applied to the system. In this case, the Hamiltonian of the system was supplemented with the added term responsible for the action of the Lorentz force on each vortex. In the case of elementary motion of a vortex, the term $\delta U = \phi_0 J \Delta_s$ was subtracted from the total energy if the direction of vortex movement coincided with the direction of the Lorentz force exerted to it and added if the vortex moved against the Lorentz force. Critical current was defined from IVC as a current at fixed voltage (as in the experiment). The calculations were carried out on a square grid under periodic boundary conditions with the help of the classical MC by using the Metropolis algorithm. Details of numerical simulation of vortex lattice and IVC were described elsewhere [2–4].

3. Results and discussion

3.1. Phases states and phase transitions

Fig. 1 displays the vortex density distribution obtained by summing the instantaneous states of the vortex lattice (instantaneous vortex density) every 100 MC steps. Ordinarily, $10^4$ MC steps were required to thermalize the system and $10^4$ MC steps were made for calculation. A practically ideal triangular lattice is reproduced at $T = 1$ K (Fig. 1a). Not all defects are occupied by vortices. This fact testifies for the benefit of the stiffness of the vortex lattice at such temperatures. Defects would have been occupied by vortices if the correspondence between the arrangement of defect and the centers of the triangular lattice were ideal. At a temperature of 3 K, all defects are occupied by vortices, which rigidly hold the lattice around themselves. On account of the irregularity of their arrangement, the defects seemingly pull the lattice apart, breaking it up at locations that are (still) far away from defects. The boundaries between the coherent regions are melted and the lattice loses stiffness. As the tempera-
Fig. 1. Dynamics of melting of the vortex lattice with five-point defects ($U_{5}(T-2\,K) = -3.52\,\text{meV}$) marked as circles: (a) $T = 1\,\text{K}$; (b) $T = 5\,\text{K}$; (c) $T = 35\,\text{K}$.

ture increases further (up to 5 K, Fig. 1b), “islands” of the triangular lattice, which are kept around the defects and which move relative to the defects as an axis of rotation, seemingly rotate, smear the vortex density in concentric circles with maximum on coordination spheres exactly. A vortex-depleted region forms around the defects themselves at a distance of one coordination sphere. A coordination sphere is equal to the period of the ideal triangular lattice since a stationary pinned vortex prevents other vortices from approaching closer. In this new phase (the transition temperature is estimated to be $T_{m} = 3\,\text{K}$),
which we shall call a ‘‘rotating lattice,’’ a long-range order still is present within the coherent regions, which are much larger than the average distance between the vortices and are rigidly coupled to the pinning centers. As the temperature increases further, the vortices begin to detach from defects, coherent regions break up, and at $T = 35$ K, for example, a completely melted vortex liquid is observed (Fig. 1c).

Therefore, the process of melting of the lattice in the presence of pinning centers proceeds in the phases: triangular lattice $\rightarrow$ rotating lattice $\rightarrow$ vortex liquid.

As the pinning potential increases, the temperatures of both phase transitions shift: The temperature of the point ‘‘triangular lattice $\rightarrow$ rotating lattice’’ decreases slightly and the temperature of phase transition ‘‘rotating lattice $\rightarrow$ vortex liquid’’ increases substantially. So strong pinning increases the temperature range of the rotating phase.

For a quantitative investigation of the phase points on melting of vortex lattice, either a structure factor $S(q)$, for estimating the degree of a long-range order, or a hexagonal parameter $S_0$ [14,15], for analyzing the short-range correlations, is ordinarily calculated.

The alternative method is to calculate the specific heat $C(T)$ of the system as ($k_B = 1$):

$$C(T) = \langle \Delta E^2 \rangle / T^2.$$

Our $C(T)$ calculations show two clear peaks in the function $C(T)$, which correspond to phase transitions: triangular lattice $\rightarrow$ rotating lattice $\rightarrow$ vortex liquid. The dependency of temperature rotating lattice $\rightarrow$ vortex liquid on defect potential is presented in Fig. 2.

### 3.2. Current-voltage characteristics and critical current

We have calculated IVC for systems containing $N_d = 1 \div 100$ defects at temperatures 10, 20, 30, 40 K, etc. (up to $\sim 83$ K). In the vicinity of the critical temperature, the characteristics were calculated with an interval of $\sim 1$ K up to the critical region. In Fig. 3, the typical IVC are presented at various temperatures ($N_d = 100$, $U_p(T = 2$ K) = $-100$ meV). The actual scale of electric field strength, $E_p = 5 \times 10^{-2}$ V/m, has been determined by comparison of theoretical with experimental IVC of Bi$_2$Sr$_2$CaCu$_2$O$_8$ film [16,17].

Our results of calculation of the motion of a vortex system in the field of defects in the presence of current demonstrate different modes of IVC be-
haviour, depending on the phase state of the system. Fig. 3 shows two groups of curves conditionally divided by the temperature boundary \((T_m \approx 70 \text{ K})\), the temperature of transition from a rotating lattice to a vortex liquid. A visual analysis of the density of vortex distribution shows that a rotating lattice is observed at \(T < T_m\) and a vortex glass at \(T > T_m\). In the vortex lattice phase, IVC change slowly upon heating, which can be explained by a still strong interaction with pinning centers. On the contrary, at \(T > T_m\), we observe a strong influence of temperature (a virtually equidistant increase in voltage upon an increase in temperature by only \(2^\circ\) up to the critical region. Thus, the observed difference in the temperature behaviour of IVC of a real HTSC can be attributed to different states of the vortex system.

We have simulated also IVC for defects in the forms of line and square and compare IVC of vortex systems with different defects. For this purpose, we introduce the defects to the system by three different ways: (a) 90-point randomly distributed defects; (b) 10 clusters per nine-point defect in the form of square; c) 10 clusters per nine-point defect in the form of line. So, in all cases, there are the exactly equal specific concentration of point defects. Then, we calculate IVC at different temperatures for all types of defects and defined the temperature dependencies of critical current. The results of these calculations are presented in Fig. 4. We can see that at low and high temperatures, there are small differences between current and voltage characteristics. At intermediate temperatures, we have found that point defects are more efficient than other types of defects with equivalent density.

We have calculated the dependencies of critical current on concentration of point defects at different temperatures and found that the increase of concentration of point defects results in an increased critical current. These dependencies are presented in Fig. 5 for \(N_d\) = 20, 40, 60, 100. The most interesting result is that the degree of increase depends on temperature. Fig. 5 shows both \(J_c(T)\) dependencies for \(N_d\) = 20, 40, 60, 100 and the dependence of value \((J_{c100} - J_{c20})/J_{c20}\) on temperature (here, \(J_{c100}\) and \(J_{c20}\) — critical currents for \(N_d\) = 100 and 20, subsequently). It is seen that the \(J_c\) increase has a maximum in vicinity 40 K.

This result can be understood qualitatively according to the phase state of vortex system. At low temperature, the vortex lattice is cruel and increase of defects’ concentration does not result in additional pinning. At high temperature, when the vortex system is liquid, additional defect cannot pin all vortex. But, at intermediate temperature where there are the islands of rotating lattice, additional defects increase the number of islands that result in the stabilisation of the vortex system.

The observed result indicates that the increase of critical current by means of irradiation should de-
pend on temperature. It may be tested by irradiation experiments on perfect Bi-type single crystal. The resembling experimental data have been observed, for example, in Refs. [18,19].

4. Conclusions

We have presented the results of numerical simulation phase states and dynamic of a two-dimensional vortex lattice with defects. It was found that there are three main vortex states: triangular lattice—rotating lattice—vortex liquid. The $I-V$ characteristics (IVC) have been calculated over a wide range of temperature for different types and concentrations of defects. It was shown that the phase states of vortex lattice determine the dynamic characteristics of system such as IVC and critical current.

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