

Nature of the 45° vortex lattice reorientation in tetragonal superconductors

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The transformation of the vortex lattice in a tetragonal superconductor which consists of the 45° reorientation relative to the crystal axes is studied using the nonlocal London model. It is shown that the reorientation occurs as two successive second order (continuous) phase transitions. The transition magnetic fields are calculated for a range of parameters relevant for borocarbide superconductors in which the reorientation has been observed.

Properties of the vortex matter have recently attracted great attention due to the diversity of phases and phenomena associated with them. One of the main research goals is the determination of the phase diagram. In high-temperature superconductors the vortex matter phases include the vortex liquid and various vortex solids which exist due to the competition of intervortex interactions with fluctuations both thermal and those due to the quenched disorder.¹ On the other hand, in borocarbide superconductors a rich variety of quite perfect vortex crystals has been observed. The experimental information comes from such different measurements as neutron diffraction, decoration, and scanning tunneling microscopy.²⁻⁴ For these near isotropic materials the entropy contribution to the free energy is small and phase transitions in the vortex lattice are governed by competition between intervortex interactions of different symmetry.

The borocarbitides are materials of the tetragonal symmetry. Interactions of this symmetry should exist for any physical subsystem of the crystal. In particular, in the mixed state with the field along the fourfold tetragonal axis they would favor a square vortex lattice. However, the standard magnetic repulsion of vortices is isotropic in this case. The isotropic interaction becomes dominant when the intervortex distance is large enough and a sparse lattice is close to hexagonal, the most closely packed two-dimensional lattice. One, therefore, expects that the interplay of the interactions of different symmetries may result in structural transformations of the vortex lattices, observed in borocarbitides.

For the applied magnetic field along the fourfold symmetry axis, these transformations are as follows. With decreasing magnetic field, the lattice undergoes a second order phase transition, at which the square structure loses stability and becomes a rhombic (distorted hexagonal) vortex lattice.^{3,4} As the field further decreases, the rhombic lattice changes the orientation relative to underlying crystal by 45°,

which has been classified as the first order transition.^{5,2,6} For the field along the twofold axis, the 90° reorientation has been reported.⁷

In this paper we study in detail the 45° reorientation and clarify its nature. We show that this reorientation proceeds as two successive second order (continuous) transitions and not as an abrupt first order transition, the scenario assumed before. Instead of considering a limited class of rhombic lattices,⁶ we study the general class of arbitrary lattices. We find that in the field region between the two second order phase transitions, the lattice with the lowest possible symmetry is realized (with the inversion being the only symmetry element). This intermediate region is quite narrow and the structural evolution in this field domain might be difficult to discern experimentally. However, the thermodynamic characteristics of the superconductor are different for the two scenarios, and this can be tested. In particular, no latent heat is expected during the lattice reorientation. We also predict a peak in the critical current in the transition region if the pinning is of a weak collective type. Below we describe the London model with nonlocal corrections relevant for the mixed state of borocarbitides. Then, the numerical procedure is outlined and the results are presented.

A fruitful approach to the problem of the vortex lattice phases is the extended London model. We start here with London equations corrected for nonlocality^{8,6}

$$\begin{aligned} \frac{4\pi}{c} j_i(\mathbf{k}) &= -\frac{1}{\lambda^2} q_{ij}(\mathbf{k}) a_j(\mathbf{k}) \\ &= -\frac{1}{\lambda^2} (m_{ij}^{-1} - \lambda^2 n_{ijlm} k_l k_m) a_j(\mathbf{k}). \end{aligned} \quad (1)$$

Here $a_j = A_j + (\Phi_0/2\pi) \partial_j \theta$, A_j is the vector potential, θ is the order parameter phase, and Φ_0 is the flux quantum. The

nonlocal response kernel $q_{ij}(\mathbf{k})$ is expanded up to the second order terms in the wave vector \mathbf{k} . The tensor $n_{ijklm} \propto \langle v_i v_j v_l v_m \rangle \gamma(T, l)$ where \mathbf{v} is the Fermi velocity and the function γ decreases somewhat with temperature and drops fast for short mean-free paths l .⁹ It is difficult to accurately estimate the components of \hat{n} because of uncertainties in determination of Fermi velocities and, in particular, of the mean-free path. At low temperatures, $\hat{n} \sim \gamma/\kappa^2$, where κ is the Ginzburg-Landau parameter. Since good crystals of borocarbides are clean materials with $\kappa = 10-15$, one expects the components of \hat{n} to be of the order 10^{-2} . Note also that for the problem of vortex lattices in fields well under the upper critical field, the correction $\lambda^2 \hat{n} k^2 \sim \xi_0^2 k^2 \ll 1$ (ξ_0 is the zero- T coherence length). Therefore, for strong type-II superconductors, the corrections to the standard London equations and the truncation in expansion (1) are well justified.

For the tetragonal symmetry, the tensor \hat{n} in the crystal frame has four independent components n_{xxxx} , n_{xxyy} , n_{zzzz} , and n_{xxzz} . The inverse mass tensor has two different components $m_{xx}^{-1} = m_{yy}^{-1}$ and m_{zz}^{-1} . The London free energy functional corresponding to Eq. (1) reads

$$F = \frac{1}{8\pi} \int \frac{d\mathbf{k}}{4\pi^2} (|\mathbf{h}|^2 - \lambda^2 \epsilon_{ijk} \epsilon_{lmn} k_j k_m q_{ln}^{-1} h_n h_i), \quad (2)$$

where $\mathbf{h}(\mathbf{k})$ is the magnetic field and ϵ_{ijk} is the unit antisymmetric tensor. The nonlocal corrections preserve linearity of the London equations and do not change the standard London result that the interaction of two vortices is proportional to the field of one of them at the location of the other.⁹ As usual, the free energy density of a vortex lattice is given by $F = (B^2/8\pi\Phi_0) \sum_{\mathbf{g}} h_z(\mathbf{g})$ where B is the magnetic induction, \mathbf{g} is a vector of the reciprocal lattice, and h_z is the component of the single vortex field along the vortex axes. We are interested in the field along the fourfold symmetry axis z . Solving Eq. (1) for a single vortex one can bring the free energy density to the form⁶

$$F = \sum_{\mathbf{g}} \frac{B^2/8\pi}{1 + \lambda^2 g^2 + \lambda^4 (n g^4 + d g_x^2 g_y^2)}, \quad (3)$$

where $n = n_{xxyy}$ and $d = 2(n_{xxxx} - 3n_{xxyy})$. The free energy $F(B, T)$ is the thermodynamic potential, which is minimum in equilibrium of a superconducting slab in a perpendicular applied field. The temperature enters $F(B, T)$ via T dependent parameters $\lambda(T)$, $n(T)$, and $d(T)$ that can, in principle, be calculated using a microscopic model. Note that besides the factor B^2 , the induction enters via the area of the primitive lattice cell. We determine the stable lattice by numerical minimization of $F(B, T; \mathbf{g})$ with respect to the lattice structure specified by a given set of \mathbf{g} 's.

The vortex lattice is completely defined by the basis vectors \mathbf{a}_1 and \mathbf{a}_2 , i.e., by four parameters. Since a unit cell accommodates one flux quantum, $a_1 a_2 \sin \beta = \Phi_0/B$, three parameters suffice. Following Ref. 10 we choose α , $\rho \equiv (a_2/a_1) \cos \beta$, and $\sigma \equiv (a_2/a_1) \sin \beta$ as the needed three (see Fig. 1 for definitions of α and β). The parameters ρ and σ are convenient because one can select a domain of their variation, each point of which corresponds to a lattice with

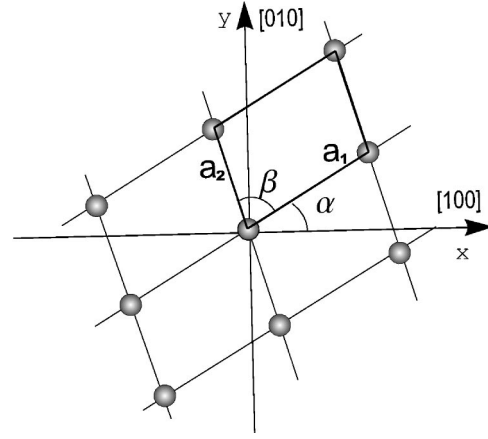


FIG. 1. General vortex lattice and its orientation relative to the crystal.

various equivalent choices of the basis vectors $\mathbf{a}_{1,2}$. Thus, the minimization of F is done at fixed B , n , and d with respect to ρ , σ , and α for $0 < \alpha < \pi$, $0 \leq \rho \leq 0.5$, and $\rho^2 + \sigma^2 \geq 1$.¹⁰ The minima of F are often located on the boundaries of this domain; we use the ‘‘Amoeba’’ numerical routine convenient in such circumstances.¹¹ The cutoff factor $\exp(-\xi^2 g^2)$ was introduced inside the sum (3) to properly account for the failure of the London model in the vortex core. Changing parameters B and n, d we obtain the phase diagram.

The main finding of this work is that the reorientation of the lattice proceeds as two steps. Figure 2 shows the transition lines on the B, d plane for a fixed $n = 0.015$. The equilibrium lattices both before and after the reorientation have the rhombic symmetry D_{2h} .¹² Their symmetry axes, which coincide with the diagonals of a rhombic unit cell (with the appropriate choice of such a cell, see Fig. 2), are aligned with $[110]$ and $[1\bar{1}0]$ at lower magnetic inductions, whereas the symmetry axes are at $[100]$ and $[0\bar{1}0]$ for higher B 's. This result is in accordance with data for $\text{YNi}_2\text{B}_2\text{C}$.⁵ In a narrow region between the two rhombic phases, a less symmetric lattice is stable. Here, the unit cell is a general parallelogram. All in-plane symmetry elements disappear except the inversion, and the symmetry group reduces to C_{2h} .

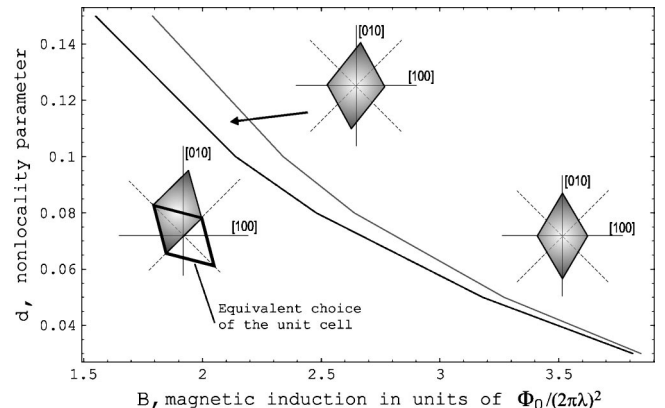


FIG. 2. Phase diagram of the vortex lattice in the region of the reorientation for $n = 0.015$. Nonlocal parameters n and d are defined in the text. The magnetic induction b is in units of $\Phi_0/2\pi\lambda^2$.

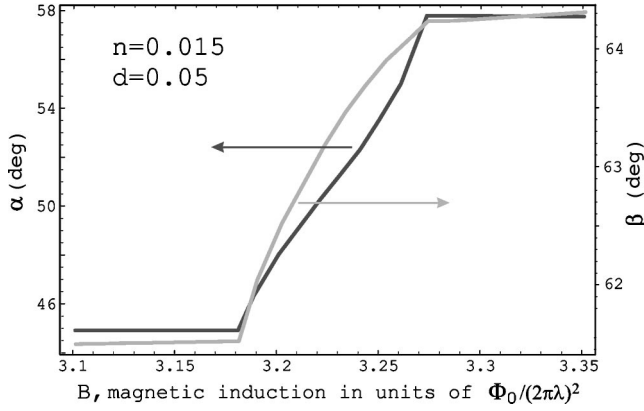


FIG. 3. Evolution of angles α and β (defined in Fig. 1) with field $b = 2\pi\lambda^2 B/\Phi_0$ during reorientation.

One could describe the reorientation process as a gradual rotation of the unit cell accompanied by a slight deformation. Figure 3 shows how the angles α and β change when B increases in the vicinity of the reorientation (for $d=0.05$ and $n=0.015$). The transitions at $B \approx 3.18 \Phi_0/(2\pi\lambda)^2$ and $B \approx 3.27 \Phi_0/(2\pi\lambda)^2$ are seen clearly. The angles α , β , and the other lattice parameters are continuous at the two transition fields. We conclude that both phase transitions that occur during the reorientation are of the second order. The sequence of symmetry changes with the field decreasing is $D_{2h} \rightarrow C_{2h} \rightarrow D_{2h}$. While at the first step of the reorientation, the symmetry becomes lower, at the second step the symme-

try increases. Correspondingly, the ground state is double degenerate in both D_{2h} phases; the degenerate vacua (two equilibrium structures of the same energy) are related by rotations over 90° . The structure becomes four times degenerate in the intermediate C_{2h} phase (rotations over $\pm 45^\circ$ and 90°). Practically, this may lead to apparently increased disorder in the C_{2h} phase.

It is worth noting that the relative energy differences between the equilibrium C_{2h} lattice and the rhombic ones is exceedingly small. As an example, we provide this figure for $d=0.05$ and $n=0.015$: the relative difference between energies of the rhombic lattice at the transition point and the lattice in the middle of the field domain of C_{2h} structure is of the order 10^{-7} . This is much smaller than 10^{-2} for the relative energy differences usually cited for triangular and square lattices within the standard London or Ginzburg-Landau models.

The location of the phase transition lines is sensitive to both n [the isotropic correction in Eq. (3)] and d (the fourfold symmetric correction). Figure 4 shows the phase diagram of the vortex lattice on B, d and B, n planes in the region of the reorientation process. The region of stability of the monoclinic lattice is broader for smaller n 's and larger d 's. Still, as is seen at Fig. 4, this field region is narrow for values of n and d adopted in our simulations. For example, for $\text{LuNi}_2\text{B}_2\text{C}$ with $\lambda \approx 710 \text{ \AA}$, the field unit $\Phi_0/(2\pi\lambda)^2$ is about 100 G.

The new scenario of the lattice reorientation in a tetragonal superconductor which is found this paper has implica-

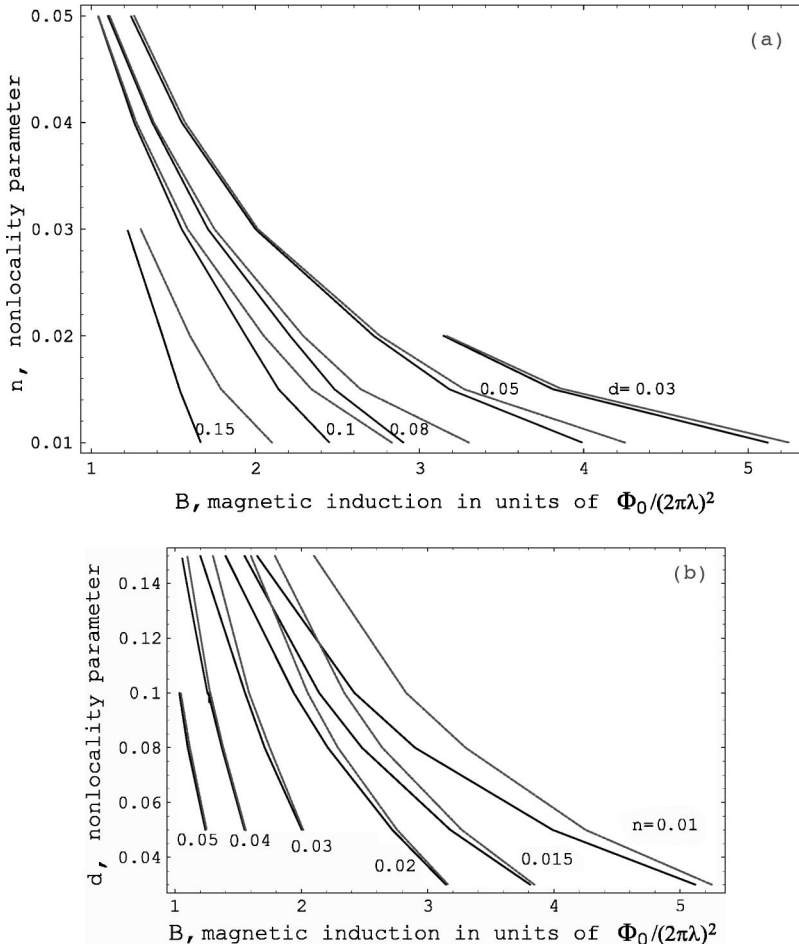


FIG. 4. Phase diagram of the reorientation transformation (a) in the n, b plane for a set of d 's indicated and (b) in the d, b plane for a set of n 's indicated.

tions for thermodynamic characteristics of the vortex lattice and its dynamic behavior. We have found, and this is our main result, that the reorientation proceeds as two successive phase transitions of the second order when the applied field or temperature vary. Therefore, continuous variation of the entropy (i.e., no latent heat) and of the reversible magnetization are expected during reorientation. In contrast, the old scenario of the first order transition implied discontinuous jumps of the above quantities.

As is seen at Fig. 4, for small values of n and d , the domain of monoclinic phase shrinks. Then, it would be difficult to distinguish experimentally this situation from first order transition, because the entropy would change fast with B during the reorientation (for the B sweep at a fixed T). Still, one should not observe hysteresis, characteristic of the first order transitions. If the sequence of transitions we suggest here is found, it would be of interest to suppress n and d by making the mean-free path shorter and to see how the transition evolves [as has been done with doping Lu-based borocarbide crystals with Co (Refs. 13 and 14)].

Both the upper and lower phase transitions ($D_{2h} \leftrightarrow C_{2h}$) of the reorientation process cause uniform spontaneous deformations of the vortex lattice. As a result, a particular com-

ination of the elastic lattice moduli vanishes at the transitions. It has been recently shown that a change of elastic properties of this type leads generally to peculiarities in the critical current, provided a weak collective pinning operates in the material.¹⁵ Therefore, the reorientation of the vortex lattice in borocarbides may lead to a peak in the critical current.

Finally, we would like to point to other possible applications of our results. The London model we employed reflects properly the symmetry of the system. It was originally derived for an anisotropic Fermi surface and isotropic superconducting pairing.⁸ However, the d -wave type of pairing also leads to a similar effective London model¹⁶ (for not very low temperature where the effects of the order parameter nodes become essential). The reorientation of the vortex lattice has indeed been found theoretically, and characterized as the first order transition.¹⁷ It would be of interest to check whether or not our scenario of the reorientation applies to this case as well.

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¹²To avoid misunderstanding we point out that in all cases we speak about the symmetry of gauge invariant quantities.

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