Anisotropic Peak Effect due to Structural Phase Transition in the Vortex Lattice

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It is shown that the recently observed new peak effect in YBCO could be explained by the softening of the vortex lattice due to a structural phase transition in the vortex lattice. At this transition square lattice transforms into a distorted hexagonal one. While conventional peak effect is associated with the softening of shear modes (elastic modulus c_{66} vanishes) at melting, in this case the relevant mode is "squash" mode ($c_{11} + c_{22} - 2c_{12}$ vanishes).

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The conventional peak effect, a sudden increase of the critical current, has been observed in great variety of both low- [1] and high-T_c [2] superconductors. In conventional superconductors the peak effect was theoretically explained a long time ago by Larkin and Ovchinnikov [3], while in high-T_c superconductors like untwinned $YBa_2Cu_3O_{7-\delta}$ (YBCO) it is generally believed that the peak is due to the softening of the shear mode just before the first order melting transition of the vortex lattice (VL) takes place [4]. Recently however another peak in the critical current in YBCO has been discovered on a line almost parallel to the T axis starting from the melting line at $H \sim 9$ T and continuing to lower temperatures (Fig. 1). First it appeared only as a "fishtail" in magnetization hysteresis loops [5], but recently a direct measurement of the critical current [6] clearly established a line presumably corresponding to some transition in the vortex matter (circles in Fig. 1).

Independently from these findings recent theoretical advances indicate that in YBCO there could exist a structural phase transition (SPT) in the VL. Starting from certain microscopic models Ginzburg-Landau (GL) theory for the $d + s$ wave superconductor on a square crystal lattice was constructed and the VL solution was studied [7]. The theory was simplified [8,9] so that it included just one, critical, order parameter and allowed easier derivation of essential VL properties. In all cases analysis of the mixed state shows that a "distorted" hexagonal VL stable at lower magnetic fields transforms into a square VL oriented at the angle $\vartheta = 45°$ relative to the crystallographic $[100]$ axis at higher fields. Experimentally, only a significantly distorted hexagonal phase has been observed in YBCO so far by means of scanning tunneling microscopy (STM) [10] and small-angle neutron scattering (SANS) [11,12]. Measurements, however, were performed at relatively low magnetic fields. A possible location of the SPT line can be inferred using the known theoretical dependence of the VL shape on a magnetic field [9]. In borocarbide superconductors, an analogous SPT was firmly established by SANS and STM experiments [13] and the GL formalism had been proven adequate [14,15].

In this note we show that SPT in the VL manifests itself as an anisotropic peak in the critical current. Thus we propose that the second line of peaks in the critical current of untwinned YBCO [6] could be explained by the softening of the "squash" elastic mode of VL (using terminology of [16]) on the line of SPT. We find that the characteristic size of vortex bundles depends on the orientation and we predict that the peak current oriented along $[100]$ and $[010]$ axes is larger than that oriented along $[110]$ and $[1\bar{1}0]$ by a factor of $\sqrt{2}$. These features can distinguish our scenario from another one in which a transition (or crossover) from the topologically ordered (Bragg) glass to vortex glass or pinned liquid was proposed [17].

We start with a description of SPT in VL and an estimate of its location on the phase diagram of untwinned YBCO. Qualitatively, anisotropy of the gap functions in both the d-wave (the dominant component) and the s-wave channels leads to an asymmetric four lobe shape of vortex cores [7]. This, in turn, causes VL to prefer the square arrangement. We employ a simple one field (d-wave) formulation of GL theory for fourfold symmetric

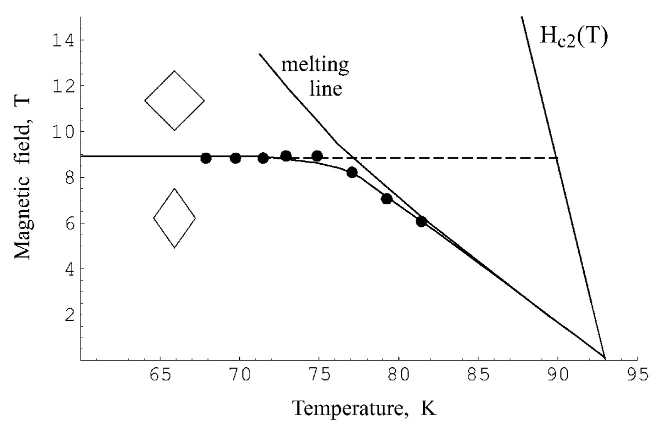

FIG. 1. Phase diagram of untwinned YBCO after Ref. [6] with solid circles being positions of the additional peak in the critical current. The dashed line is a possible location of the phase transition line from the distorted hexagonal lattice to the square lattice. Taking account of fluctuations would transform the phase transition line, as shown by the solid line.

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superconductors [8,9],

$$F[\psi] = \frac{\hbar^2}{2m_{ab}} |\mathcal{D}\psi|^2 + \frac{\hbar^2}{2m_c} |\nabla_z \psi|^2 - \alpha|\psi|^2 + \frac{\beta}{2} |\psi|^4 + \varepsilon|(\mathcal{D}_y^2 - \mathcal{D}_x^2)\psi|^2. \quad (1)$$

Here $\mathcal{D}_i \equiv \nabla_i - i(e^*/c)A_i$, $i = x, y$ is the covariant derivative, and e^* is the charge of the Cooper pair. The material parameter ε quantifies deviations from the exact rotational symmetry. We assume that the magnetic field is in the c direction and is constant (far enough from H_{c1}, this is a good approximation since $\kappa \gg 1$). At a certain value of ε there is a phase transition from distorted hexagonal (point symmetry group D_{2h}) to a more symmetric square lattice (D_{4h}). It is important for the calculation of the elastic moduli to consider the VL of a most general form (see inset in Fig. 2). An elementary cell is specified by vectors **a** and **b** with an angle ϑ between them. Angle φ defines the orientation of VL relative to the crystallographic [100] axis. Because of the flux quantization condition the relation $ab \sin\vartheta = 2\pi$ holds. One solves the linearized GL equation perturbatively in the dimensionless anisotropy parameter $\eta \equiv \varepsilon m_{ab} e^* H$ and obtains

$$F(\rho, \sigma, \varphi) = -[H - H_{c2}(T)]^2 / 2\beta(\rho, \sigma, \varphi), \quad (2)$$

$$\beta(\rho, \sigma, \varphi) = \beta_A(\rho, \sigma) + \eta[e^{4i\varphi}\delta(\rho, \sigma) + \text{c.c.}], \quad (3)$$

$$\beta_A = \sqrt{\sigma} \sum e^{2\pi i \rho(n^2 - m^2) - 2\pi\sigma(n^2 + m^2)},$$

$$\delta = \sqrt{\sigma} \sum (8\pi^2\sigma^2 n^4 - 6\pi\sigma n^2 + 3/8) \times e^{2\pi i \rho(n^2 - m^2) - 2\pi\sigma(n^2 + m^2)},$$

where $\beta \equiv \langle|\psi|^4\rangle / \langle|\psi|^2\rangle^2$ is the generalized Abrikosov geometrical parameter, $\rho \equiv (b/a)\cos\vartheta$ and $\sigma \equiv (b/a)\sin\vartheta$. The summation runs over all the integers or half integers m and n. To find the VL structure the energy of Eq. (2) is minimized analytically over φ and numerically over ρ and σ. At the minima ρ always equals to $1/2$ while the value of σ depends on η and we denote it as $\bar{\sigma}$ below. It was established [9,14] that the transition occurs at $\eta_c = 0.0238$. For every $\eta < \eta_c$ there are two degenerate minima (one of them has $\varphi = 0$) which correspond to VL related by the $\pi/2$ rotation around the c axis. On the mean field level the phase transition is of the second order with mean field critical exponents. For example, we calculated the dependence of the angle $\vartheta = \arctan(2\bar{\sigma})$ on η close to the transition point and found that $\vartheta = 3.3(\eta_c - \eta)^{1/2}$. These analytical results were corroborated and extended by numerical simulations [15]. This is in agreement with the general result that perturbation theory in the GL model is valid far beyond its naive range of validity extending as far as to $H_{c2}/10$ [18].

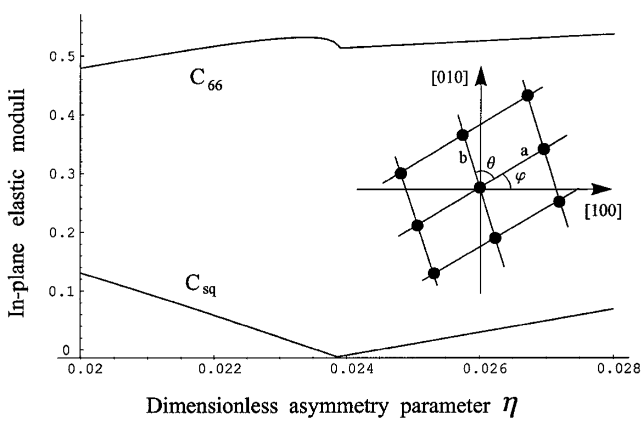

FIG. 2. Dependence of shear modulus c_{66} and squash modulus $c_{sq} = c_{11} + c_{22} - 2c_{12}$ on parameter η which controls the strength of the fourfold symmetric term in the free energy. Squash modulus vanishes at the phase transition point. Inset: Most general form of VL.

The line of STP in VL (dashed line in Fig. 1) is parallel to the T axis and goes at certain $H_{\mathrm{SPT}} = \eta_c/(\varepsilon m_{ab} e^*)$. Using $\vartheta = 53.5 \pm .5°$ at $H = 2$ T from Ref. [11] we estimate that for the sample of Ref. [6] $H_{\mathrm{SPT}} \simeq 6$ T. Since the SANS experiment sample had twinning planes which prefer the square lattice, the actual line in an untwinned sample is roughly at the correct place and we just fit the data with a straight line at 9 T. Although a convincing estimate can be made only after similar measurements are performed on the same sample, the order of magnitude is correct. In some theoretical works the SPT line is slightly tilted (in a positive or negative direction) [9,14,15]. This is the effect of yet another four derivative term $\varepsilon'|(\mathcal{D}_x^2 + \mathcal{D}_y^2)\psi|^2$. This term is rotationally symmetric and simply modifies H_{c2}. The tilt angle is very small, of the order of $\eta_c \sim 10^{-2}$.

Using thermodynamic arguments we calculate all the relevant nondispersive elastic moduli from Eqs. (2) and (3). The dispersive tilt modulus c_{44} [19] is not changed significantly compared to the usual case without the asymmetry term, the last term of Eq. (1). In order to obtain all "in-plane" elastic moduli of the flux line lattice we first choose a particular form of distortion and then express the excess free energy corresponding to this distortion in terms of elastic moduli. Distortions of the lattice can be described by the displacement vector u_i with $i, j = x, y$. Symmetric combinations of derivatives are denoted by $u_{ij} \equiv (1/2)(\partial_j u_i + \partial_i u_j)$, while the antisymmetric one describing rigid rotations around the c direction is $\omega_{xy} \equiv (1/2)(\partial_y u_x - \partial_x u_y)$. The distortion energy of a deformed two dimensional lattice is $F_{\mathrm{dist}} = F_{\mathrm{el}} + F_{\mathrm{rot}}$ with $F_{\mathrm{rot}} = \zeta u_{xy}\omega_{xy} + (1/2)\zeta'\omega_{xy}^2$ and

$$F_{\mathrm{el}} = \frac{c_{11}}{2} u_{xx}^2 + \frac{c_{22}}{2} u_{yy}^2 + c_{12} u_{xx} u_{yy} + 2c_{66} u_{xy}^2. \quad (4)$$

Since the compression modulus is very large near the phase transition compared to all others and will not play a role in what follows, we assume that the magnetic flux through the elementary cell of the lattice is constant. This means that the area of the unit cell has to remain fixed: $u_{xx} + u_{yy} = 0$. Subject to this restriction it is possible to obtain the following two combinations of the four elastic moduli: the shear c_{66} and the squash $c_{\rm sq} \equiv c_{11} + c_{22} - 2c_{12}$ in addition to ζ and ζ'. We used the following infinitesimal displacements: $\mathbf{u} = \mu(\pm y\hat{\mathbf{e}}_x + x\hat{\mathbf{e}}_y)$, $\mathbf{u} = \mu(x\hat{\mathbf{e}}_x - y\hat{\mathbf{e}}_y)$, $\mathbf{u} = \mu y\hat{\mathbf{e}}_x$, $\mathbf{u} = \mu x\hat{\mathbf{e}}_y$, and obtained $c_{\rm sq} = F'\beta_{\sigma\sigma}(2\sigma)^2$, $c_{66} = F'\beta_{\rho\rho}\sigma^2 + \zeta/4$, and $\zeta = \zeta' = 32\eta F'|\delta|$, where $F' = dF/d\beta$ and subscripts of β denote partial derivatives. The right-hand sides of the above equations are evaluated at equilibrium values $\sigma = \bar{\sigma}$ and $\rho = 1/2$ on both sides of the SPT line.

Note that the rotation modulus ζ is proportional to the anisotropy parameter η. Calculated shear and squash moduli are presented in Fig. 2. The dependence of shear modulus on anisotropy is weak. On the other hand, the squash modulus vanishes on the SPT line linearly in $|\eta - \eta_c|$ but with different coefficients above and below the transition point,

$$c_{\rm sq} = \begin{cases} 8.7|1 - \frac{\eta}{\eta_c}|[H - H_{c2}(T)]^2, & \eta_c < \eta\,, \\ 5.5|1 - \frac{\eta}{\eta_c}|[H - H_{c2}(T)]^2, & \eta_c > \eta\,. \end{cases} \quad (5)$$

This is similar to the behavior of the soft moduli at structural phase transitions in solids.

The softening of the VL due to the vanishing of the squash modulus should lead to some peculiarities of those properties of the superconductor that depend on the elasticity of the VL. Below we argue that a peak in the critical current should appear once one crosses the transition line. To determine critical current $\mathbf{j}_c$ we follow the "dynamical approach" [19,20] and write down the equation of motion for VL,

$$\frac{\sigma B^2}{c^2}\frac{\partial \mathbf{u}}{\partial t} = -\frac{\delta F_{\rm el}}{\delta \mathbf{u}} - \frac{\delta F_{\rm pin}}{\delta \mathbf{u}} + \frac{1}{c}\,\mathbf{j}\times\mathbf{B}\,, \quad (6)$$

where $F_{\rm el}$ is given by Eq. (4) and σ is the normal state conductivity. Equation (6) is solved perturbatively in the pinning energy $F_{\rm pin} = \int d^3r\, \varepsilon(\mathbf{r})$. The change of energy due to pinning $\varepsilon(\mathbf{r})$ depends on both the disorder potential and the vortex form factor; see [19]. One estimates its correlator as $\int d^3r\,\langle\varepsilon(\mathbf{r})\varepsilon(\mathbf{0})\rangle e^{i\mathbf{K}\cdot\mathbf{r}} = (2\pi\Phi_0/B)e^{-\xi^2K^2} \equiv (2\pi\Phi_0/B)W(\mathbf{K})$ [4], where $\mathbf{K}$ is a reciprocal lattice vector. The second order correction to the flux flow velocity $\mathbf{v}_0 = (c/\sigma B^2)\mathbf{j}\times\mathbf{B}$ is

$$-\frac{\Delta\mathbf{v}}{\mathbf{v}_0} = \frac{\pi B}{\Phi_0}\sum_{\mathbf{K}}\int\frac{d^3k}{(2\pi)^3}\frac{W(\mathbf{K})K^2K_\parallel^2}{P(\mathbf{k})^2 + (\frac{jBK_\parallel}{c})^2}\,, \quad (7)$$

$$P(\mathbf{k}) \equiv c_{44}k_z^2 + \frac{c_{66}(k_x^2 - k_y^2)^2 + c_{\rm sq}k_x^2k_y^2}{k_x^2 + k_y^2}\,, \quad (8)$$

where $K_\parallel = \mathbf{K}\cdot\mathbf{v}_0/v_0$. In Eqs. (7) and (8) the fact that the compression modulus is much larger than the other moduli was used. Let the current $\mathbf{j}$ flow at an angle θ relative to the [100] axis. Since $K\xi \sim 1$ and $W(\mathbf{K})$ falls off exponentially we retain in the sum only the nearest neighbors in the square lattice with $K_\parallel = \cos(\theta \pm \pi/4)$,

$$-\frac{\Delta\mathbf{v}}{\mathbf{v}_0} = 2W(0)\left(\frac{2\pi B}{\Phi_0}\right)^{7/4}(jBc_{44}c_{66}c_{\rm sq}/c)^{-1/2}f(\theta)\,,$$
$$f(\theta) = |\cos(\theta + \pi/4)|^{3/2} + |\cos(\theta - \pi/4)|^{3/2}. \quad (9)$$

The angular dependence is fourfold symmetric. To evaluate the critical current the condition $\Delta\mathbf{v} = -\mathbf{v}_0$ is used,

$$j_c(\theta) = \frac{4cW(0)^2(\frac{2\pi B}{\Phi_0})^{7/2}}{Bc_{44}c_{66}c_{\rm sq}}f(\theta)^2. \quad (10)$$

Therefore the critical current along the crystallographic [100] or [010] axes is larger by a factor of $\sqrt{2}$ compared to the one along [110] or [1$\bar{1}$0]. For untwinned YBCO one estimates [4] $W(0) = U_0^2B\xi^2n_p$, where n_p is point pinning centers density and U_0 is the depth of an individual pinning potential. As in the melting peak effect [20] the effect of thermal depinning can be taken into account by an additional factor $(1 + T/T_{\rm dp})^{-11/2}$ where $T_{\rm dp}$ is the depinning temperature. The case of "small bundles" where the dispersion of c_{44} is important can be treated analogously [4,19]. Because of different slopes of the moduli $c_{\rm sq}$ as a function of $\eta - \eta_c$ [see Eq. (5)] the peak shape is asymmetric provided the general $1/B$ trend is eliminated,

$$j_cB \sim \begin{cases} \frac{1}{8.7(B - B_{\rm str})}\,, & B < B_{\rm str}\,, \\ \frac{1}{5.5(B_{\rm str} - B)}\,, & B > B_{\rm str}\,. \end{cases} \quad (11)$$

Of course the cutoff is understood when the characteristic size of the correlation volume (the Larkin domain) is no longer large compared to the distance between vortices. In this case the elasticity theory becomes inapplicable. To determine the applicability region of the elasticity theory we calculate the correlation length which is the most important characteristic of the mixed state in the collective pinning theory. It is deduced from the displacement correlator $\langle u^2(\mathbf{r})\rangle \equiv \langle[\mathbf{u}(\mathbf{r}) - \mathbf{u}(\mathbf{0})]^2\rangle = 2W(0)\int\frac{d^3k}{(2\pi)^3}[1 - \cos(\mathbf{k}\cdot\mathbf{r})]G_{ij}(\mathbf{k})G_{ij}(-\mathbf{k})$ [19] where $G_{ij}(\mathbf{k})$ is the elastic Green's function. In the present case we have $\langle u^2(\mathbf{r})\rangle = 2W(0)\int\frac{d^3k}{(2\pi)^3}[1 - \cos(\mathbf{k}\cdot\mathbf{r})]P(\mathbf{k})^{-2}$ where $P(\mathbf{k})$ is defined in Eq. (8). To determine the correlation length in a certain direction of $\hat{\mathbf{n}}$ within the collective pinning theory one writes $\langle u^2(R_{\hat{\mathbf{n}}}\hat{\mathbf{n}})\rangle = \xi^2$. The correlator in the c direction does not change compared to the case of the hexagonal lattice, $\langle u^2(R_c)\rangle = 2W(0)R_c/(\pi^{3/2}c_{66}c_{44})$, while in the a-b plane it depends on the angle ϕ that $\hat{\mathbf{n}}$ makes with the crystallographic direction [100]: $\langle u^2(R_\phi)\rangle = [W(0)R_\phi/\pi^2c_{\rm sq}c_{66}^{1/2}c_{44}^{1/2}]\tilde{f}(\phi)$. The function $\tilde{f}(\phi)$ calculated numerically is close to that of Eq. (9). The results are significantly different compared to the case of the peak effect associated with the VL melting where c_{66} vanishes and $\langle u^2(R_{ab})\rangle = W(0)R_{ab}/(2\pi^2c_{66}^{3/2}c_{44}^{1/2})$. We see that $1/c_{\rm sq}$ replaces $1/c_{66}$. In the present situation the Larkin domain is not only asymmetric with respect to a, b versus c directions. Because of the particular orientation of the soft modes destroying the square lattice the correlation length becomes asymmetric within the a-b plane as well,

$$R_c = \frac{\pi^{3/2} c_{66} c_{44} \xi^2}{2W(0)}, \qquad R_\phi = \frac{c_{\rm sq} c_{66}^{1/2} c_{44}^{1/2} \xi^2}{W(0) f(\phi)}.$$

Now we supplement the dynamical approach calculation of j_c with a simpler and more intuitive derivation from the correlation volume. The critical current in the certain direction θ with respect to the crystal is determined by equating the Lorentz force to the pinning force. The pinning energy for the relaxed lattice is linked to the in-plane elastic energy due to the displacement of the order ξ in the direction $\theta + \pi/2$ caused by the Lorentz force [19]. The elastic energy is $U_c(\theta) \sim c_{\rm sq}(\xi/R_{\theta+\pi/2})^2 V_c$ where V_c is the correlation volume. Therefore the critical current obtained from the balance of the Lorentz force and the pinning force is $j_c(\theta) = (c/B)U_c(\theta)/(\xi V_c) \sim c_{\rm sq} j_0 (\xi/R_a)^2 f(\theta + \pi/2)^2$ where $j_0 = cH_c/(3\sqrt{6}\,\pi\lambda)$ is the depairing current. This agrees with the dynamical approach result.

There are two types of excitations near the transition. The first one is highly anisotropic: soft modes which are transverse waves propagating in $[110]$ and $[1\bar{1}0]$ directions. The second one is domain walls similar to those in Ising magnets. The transition in our case is of the group—subgroup type. Such transitions are generally continuous (second order). One can use the standard methods [21] to write the GL theory in terms of the order parameter $\Phi \equiv \vartheta - \pi/4$. Using the expression for the energy as a function of an angle Eq. (2) we obtain

$$F = [-a(\eta - \eta_c)\Phi^2 + (b/2)\Phi^4][H - H_{c2}(T)]^2$$

with $a = 7.0$ and $b = 1.2$. It would be very interesting to directly observe the soft modes by excitation using ac current or other means.

Near the melting line the fluctuations become important. Experimental results [6] show that near the melting line the second peak line sharply turns down. On the basis of the present considerations it can be qualitatively understood. The reason is the symmetry breaking pattern. Liquid is a state in which both the continuous translation symmetry and the fourfold symmetry are unbroken. In the solid the translation symmetry is spontaneously broken down to its discrete subgroup, while the fourfold symmetry is still intact. Finally in the distorted hexagonal phase both symmetries are broken. The thermal fluctuations favor the square lattice, so first the fourfold symmetry is restored. On the basis of symmetry considerations alone it is impossible to determine whether the line should follow the melting line; see the solid line in Fig. 1 or that there exists a triple point. The phenomenon is somewhat reminiscent of that of Alexander and McTague's [22] in solids.

To summarize the structural phase transition in the vortex lattice of YBCO or borocarbide superconductors leads to an anisotropic peak effect via the vanishing of squash elastic modulus. We calculated the value of the peak in the critical current and its shape. The second order transition is accompanied by soft modes.

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