Subsurface bending and reorientation of tilted vortex lattices in the bulk due to Coulomb-like repulsion at the surface

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We study vortex lattices (VLs) in superconducting weak-pinning platelet-like crystals of $\beta$-Bi$_2$Pd in tilted fields with a Scanning Tunneling Microscope. We show that vortices exit the sample perpendicular to the surface and are thus bent beneath the surface. The structure and orientation of tilted VL in the bulk are, for large tilt angles, strongly affected by Coulomb-type intervortex repulsion at the surface due to stray fields.

Vortices in superconductors are predicted to bend in order to orient perpendicular to boundaries between superconducting and normal areas or to the interface with vacuum [1, 2]. Physically, the bending is due to the vortex supercurrent loops which, on one hand, should be parallel to the surface, while on the other, tend to be in plane perpendicular to the vortex axis (in isotropic materials). To the best of our knowledge, such bending has never been verified experimentally. We provide Scanning Tunneling Microscopy (STM) data that cannot be interpreted in any other way—vortices exit the sample perpendicular to the surface. Our data also show that in weak-pinning crystals the VL structure and orientation are affected not only by the intervortex interactions in the bulk, but also by interactions at the sample surface.

We study vortex lattices (VLs) at the plane surface of platelet-like single crystals of $\beta$-Bi$_2$Pd with $T_c = 5$ K [3, 4]. The crystal is tetragonal, although the Fermi surface has sheets of mixed orbital character that lead to a near-isotropic macroscopic behavior [5–7]. Upper critical fields along the basal plane and perpendicular to it differ by barely 25% from $H_{c2,ab} = 0.7$ T to $H_{c2,c} = 0.53$ T (at low temperatures), leading to coherence lengths $\xi_a = 19$ nm and $\xi_b = 24$ nm [8, 9]. Estimates of the penetration depths from the data on the lower critical field give $\lambda_a = 105$ nm and $\lambda_c = 132$ nm [8].

We use a home-built STM/S attached to the dilution refrigerator inserted in a three axis vector magnet reaching 5 T in the z direction and 1.2 T for x and y [10, 11]. $\beta$-Bi$_2$Pd crystals ($3 \times 3 \times 0.5$ mm$^3$) are mounted with the c-axis along the z direction of the magnet. The other two crystalline orientations with respect to x and y of the magnet are found by scanning the surface with atomic resolution to find the square Bi lattice as outlined in [9], where the crystal growth is also described. The surface consists of large atomically flat areas of several hundreds nm in size, separated by step edges [9]. We use an Au tip cleaned and atomically sharpened in-situ by repeated indentations onto Au sample [12]. VL images are obtained by mapping the zero-bias conductance normalized to voltages above the superconducting gap [13]. All measurements are done at $T = 150$ mK. Data are usually taken within field-cooled protocol, although, due to weak vortex pinning of this material, we find the same results when changing the magnetic field at low temperatures. No filtering or image treatment is applied to the conductance maps shown below.

VLs in fields along c are hexagonal up to $H_{c2}$ with one of the VL vectors along a or b of the tetragonal crystal [9]. This gives a two-fold degeneracy in the VL orientation [14]. Hence we observe domains of differently oriented VLs; the spatial distribution of domains is random and determined by the pinning landscape. In some tetragonal materials in fields along c, the four-fold-symmetric nonlocal corrections to the London theory modify the isotropic repulsion and lead to two degenerate rhombic VLs which at large fields transform to the square VL [15, 16]. One of the requirements for the nonlocal corrections to work is a large Ginzburg-Landau parameter $\kappa$ [17]. In our crystals, $\kappa \sim 4$ and we do not observe VL transitions.

Let us consider the vortex core shapes at the surface. At $H \parallel c$, the cores have a circular shape of a size $\xi_{ab} \approx 24$ nm at 0.3 T (see discussions [9, 18]) shown in Fig. 1 as a white circle. If the vortex in a tilted field would have arrived to the surface being straight without any bending, the expected core shape at the surface would be an ellipse with the minor and major semiaxes of 24 nm and $24/\cos \theta$ nm ($\theta$ is the angle between $H$ and c). For $\theta = 80^\circ$ we would obtain the white ellipse shown in the right panel of Fig. 1. Instead we find the vortex core of the same shape and size as for $H$ normal to the surface as shown by the circle at the right panel of Fig. 1. Thus, our
images show that vortices must bend under the surface to exit the sample being perpendicular to the surface.

Vortex bending is expected to occur over a length of the order of the penetration depth $\lambda \approx 100 \text{ nm} \ [1, 2]$, which is large relative to the core size of 24 nm. Hence, we do not expect that the electronic density of states at the surface is influenced by the bent part of the vortex deep underneath.

The surface VLs are shown in Fig. 2(a) for a few tilts $\theta$. The panel 2(b) shows that the density of vortices at the surface goes as $\cos \theta$, as expected.

As mentioned, the material of our interest is nearly isotropic. The model we offer to describe VLs in tilted fields is isotropic. The model predictions, by and large, agree with the STM data. Within this model, the VL in the vortex frame of an infinite sample is hexagonal and degenerate: the angle $\alpha$ shown on the left of Fig. 2(c) can be taken as the degeneracy parameter. The circle where all nearest neighbors are situated has a radius $a$ fixed by the flux quantization, $a^2 = 2\phi_0/\sqrt{3}H$. We use the vortex coordinate frame $(x, y, z)$ with $z$ along the vortex direction and the $x$ axis in the tilt plane. For a given $\alpha$, the VL unit cell vectors (in units of $a$) are

$$
\mathbf{u}_1 = [\cos \alpha, \sin \alpha], \quad \mathbf{u}_2 = \left[ \cos \left( \alpha + \frac{\pi}{3} \right), \sin \left( \alpha + \frac{\pi}{3} \right) \right].
$$

(1)

In a sample much thicker than $\lambda$, the VL structure in the bulk is dominated by the bulk interactions, i.e. the VL is still hexagonal. However, the degeneracy is removed in tilted fields by the surface contribution to the interaction.

To evaluate this contribution, we note that due to subsurface bending the point of vortex exit is shifted relative to the exit point of a straight vortex. In small fields when the vortices are well separated, each one will experience the same shift. We assume that shifts are the same also in fields of our interest. In particular, this implies that the density of bent vortices at the surface is the same as if vortices were straight; this is consistent with the macroscopic boundary condition for the normal component of the magnetic induction $\dot{H} \cos \theta$. Hence, the arrangement of vortices at the surface is just shifted relative to the VL which would have been there without subsurface bending. Then, considering the VL structure, one can disregard the bending and the bulk nearest neighbors will be situated at the cross-section of a circular cylinder of radius $a$ with the flat surface, i.e. at the ellipse with semi-axes $a/\cos \theta$ and $a$, the right panel of Fig. 2c. Taking again the $x$ axis of the surface frame in the tilt plane, one obtains new unit cell vectors at the surface (in units of $a$):

$$
\mathbf{v}_1 = \left[ \cos \alpha \frac{\cos \alpha}{\cos \theta}, \sin \alpha \frac{\cos \alpha}{\cos \theta} \right], \quad \mathbf{v}_2 = \left[ \cos \left( \alpha + \frac{\pi}{3} \right), \sin \left( \alpha + \frac{\pi}{3} \right) \right].
$$

(2)
In particular, the angle $\alpha s$ between $v_1$ and $\hat{x}$ is related to the parameter $\alpha$ by $\tan \alpha s = \tan \alpha \cos \theta$. All vortex positions at the surface $R_{mn} = m v_1 + n v_2$ ($m,n$ are integers) can be expressed in terms of $\theta$ and $\alpha$ (or $\alpha s$).

Interaction of vortices at the surface is due to stray fields out of the sample, which can be approximated by point “monopoles” producing the magnetic flux $\Phi_0$ in the free space within the solid angle $2\pi$. The interaction energy of the vortex at the origin with the rest is

$$\frac{\phi_0^2}{4\pi^2} \sum_{m,n}^\prime \frac{1}{R_{mn}},$$

where $\sum^\prime$ is over all $m,n$ except $m = n = 0$. The surface vortex density is $H \cos \theta/\phi_0$, so that surface interaction per cm$^2$ is

$$F_s = \frac{\phi_0 H \cos \theta}{4\pi^2} \sum_{m,n}^\prime \frac{1}{R_{mn}} \frac{3^{1/4} \phi_0^{1/2} H^{3/2}}{4\sqrt{2\pi} n^2} S(\alpha, \theta),$$

$$S = \cos^2 \theta \sum_{m,n} \left\{ (m \cos \alpha + n \cos(\alpha + \pi/3))^2 + \cos^2 \theta [m \sin \alpha + n \sin(\alpha + \pi/3)]^2 \right\}^{-1/2}.$$  

It is readily checked that $\partial S/\partial \alpha = 0$ at $\alpha = -\pi/6$ and $\pi/3$. The corresponding structures in the vortex frame are hexagons, called hereafter $A$ and $A'$; in $A$ two out of six nearest neighbors are at $y$ axis, in $A'$ they are at $x$.

The sum $S$ is divergent and as such depends on the summation domain. We, however, are interested only in the angular dependence of $S(\alpha)$, because of its role in removing the VL degeneracy in the bulk. The angular dependence arises mostly due to vortices in the vicinity of the central one, because the number of far-away vortices grows with the distance and their contribution to the interaction is nearly isotropic. Our strategy for evaluation of $S(\alpha)$ is based on the fact that the Coulomb interaction out of the sample is isotropic and therefore we can do the summation within a circle $R_{mn} < L$, where $L$ is large enough to include a few “nearest-neighbor shells” of vortices surrounding the one at the origin. To provide a smooth truncation we add a factor $e^{-R_{mn}/L^2}$ to the summand of Eq. (5).

Results of these calculations are given in Fig. 3 for $\theta = 80^\circ, 70^\circ$ and $60^\circ$; smaller tilt angles are discussed in the supplemental material. Clearly, the structure $A$ ($\alpha = -\pi/6$) is unstable. The minimum energy for $\theta = 70^\circ$ and $60^\circ$ is at $\alpha = 0$, so that the preferred structure is $A'$. For $\theta = 80^\circ$ the minimum is shifted to $\alpha \approx -0.1$. These qualitative conclusions do not change if one takes a larger radius $L$ of the summation domain, notwithstanding the increase of the calculated surface energy $F_s$.

To show that our model describes the data well, and in particular to check again that the bulk hexagonal VL projects onto the surface as if the vortices were straight, one can follow the bulk nearest neighbors and their surface projections. The six nearest neighbors in the vortex frame correspond to the pairs $(m,n)$:

$$(0,1), \ (1,0), \ (0,-1), \ (-1,0), \ (-1,1), \ (1,1).$$

At the surface, these pairs mark six vortex positions situated at $\pm v_1, \pm v_2$, and $\pm (v_1 - v_2)$, see the sketch in Fig. 2c. These positions at the surface are not necessarily nearest, because at large tilt angles, they form a strongly stretched hexagon, whereas the position $(1,1)$ moves closer to the center.

Let us consider $\theta = 80^\circ$ for which according to Fig. 3 $\alpha \approx -0.1$ and evaluate distances $d_1 = |v_1|$, $d_2 = |v_2|$, and $d_3 = |v_1 - v_2|$. Skipping algebra, we provide formulas for these distances in the supplemental material. In units of $a$ we obtain $(d_1, d_2, d_3) = (5.68, 3.56, 2.63)$. Direct measurements at the corresponding image at Fig. 1 give $(d_1, d_2, d_3) \approx (6, 3.4, 2.4)$ in a good agreement with calculated values. Hence, the nearly degenerate hexagonal VL in the bulk bends as a whole when reaching the surface, just shifting the geometric projection of the tilted hexagonal bulk VL onto the surface.

In Fig. 4a we show results for a fixed polar angle (tilt) $\theta = 80^\circ$ and several azimuthal angles $\varphi$ of the field $B$. Interestingly, the surface vortex lattice shows different arrangements depending on $\varphi$. For $\varphi = 72^\circ$, the surface VL is a nearly perfect square, whereas for $\varphi = 317^\circ$ it is nearly hexagonal. As we show in the supplementary material, the $\theta$ and $\varphi$ where we expect such a square vortex lattice within our model are close to what we observe experimentally.

In Fig. 4b we show $\alpha$ for experiments changing the azimuthal angle $\varphi$ (for a polar angle of $\theta = 80^\circ$). We observe that $\alpha$ varies around the orientation $A'$. The
variations might be caused by the tetragonal symmetry, not included in our model or by weak pinning.

0.5 1.0 1.5 2.0
x (µm)

FIG. 4. VLs for a fixed tilt \( \theta = 80^\circ \) but different azimuthal angles \( \varphi \) of the applied field. For \( \varphi = 72^\circ \) the lattice appears at the surface as a square (confirmed by the Fourier transform in the red inset), whereas for \( \varphi = 317^\circ \) it is nearly hexagonal. Note also that VLs of vortices strongly bent under the surface at high tilts \( \theta \) are still very well ordered.

In summary, we have studied VLs in tilted fields in \( \beta-\text{Bi}_2\text{Pd} \), a nearly isotropic superconductor. We demonstrate that vortices exit the sample being perpendicular to the surface, that necessitates the subsurface bending of vortex lines. We find that intervortex Coulomb-like repulsion at the surface due to stray fields removes the degeneracy of the bulk hexagonal VLs thus fixing the bulk VL orientation. It is quite surprising to have a highly ordered VLs at the surface whereas under the surface all vortices are bent.

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Supplemental material for "Subsurface bending and reorientation of the tilted vortex lattice in the bulk due to Coulomb-like repulsion at the surface"

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We provide additional data for low tilt angles and explicit expressions for the intervortex distances. The nearest neighbor intervortex distances at the surface are equal or larger than the bulk intervortex distance.

S1. VORTEX LATTICES AT THE SURFACE

Within the isotropic model, the VL in the vortex frame of an infinite sample is hexagonal and degenerate: the angle $\alpha$ shown in the upper panel of Fig. 2(c) of the main text can be taken as the degeneracy parameter. For a given $\alpha$, the VL unit cell vectors (in units of $a$) are given by the Eq. (1).

Positions of the nearest neighbors are $\pm u_1, \pm u_2$, and $\pm (u_1 - u_2)$, all of them at the same distance $d = 1$ from the vortex at the origin.

It is argued in the main text that considering the VL structure, one can disregard the vortex bending. Then, the bulk nearest neighbors will be situated at the cross-section of a circular cylinder of radius $a$ with the surface plane, i.e. at the ellipse with semi-axes $a/\cos \theta$ and $a$ (right panel of Fig. 2c). Taking the $x$ axis of the surface frame in the tilt plane, one obtains new unit cell vectors at the surface (in units of $a$) given by Eq. (2).

The positions corresponding to the bulk nearest neighbors are $\pm v_1, \pm v_2$, and $\pm (v_1 - v_2)$. These positions at the surface are not necessarily the nearest. Their distances from the vortex at the origin are $d_1 = |v_1|$, $d_2 = |v_2|$, and $d_3 = |v_1 - v_2|$. For these distances one has:

\begin{align}
  d_1^2 &= \frac{\cos^2 \alpha + \cos^2 \theta \sin^2 \alpha}{\cos^2 \theta}, \\
  d_2^2 &= \frac{\cos^2 (\alpha + \pi/3) + \cos^2 \theta \sin^2 (\alpha + \pi/3)}{\cos^2 \theta}, \\
  d_3^2 &= \frac{[\cos (\alpha + \pi/3) - \cos \alpha]^2}{\cos^2 \theta} + \left[ \sin \left( \frac{\alpha + \pi/3}{3} \right) - \sin \alpha \right]^2.
\end{align}

Consider now the case $\alpha = \pi/3$ (which is equivalent to $\alpha = 0$, the structure $A'$), see Fig. 2c. With increasing tilt $\theta$, the position $(v_1 + v_2)$, which at small $\theta$ does not belong to the nearest neighbors, approaches the origin, whereas the distance to $(v_1 + v_2)$ increases. The two distances become equal when $(v_1 + v_2)^2 = (v_1 - v_2)^2$, in other words when $v_1 \cdot v_2 = 0$, i.e. $v_1 \perp v_2$. Since in this case by symmetry $|v_1| = |v_2|$, the surface VL will appear as having the square unit cell. A simple algebra yields for the tilt $\theta^*$ at which this happens: $\cos^2 \theta^* = -\cot(2\pi/3)/\sqrt{3}$ which corresponds to $\theta^* = 70.5^\circ$. We observe the square VL at angles that are close to that, namely $\theta = 80^\circ$ and $\alpha = 25^\circ$.

S2. LOW POLAR ANGLES

From Fig. 3 of the publication, one can see that the structure $A$ ($\alpha = -\pi/6$) is unstable since the energy has a maximum at this configuration. Moreover, this feature clearly does not depend on the number of neighbors included in the summation. Hence, we expect that for relatively small tilts, minimum energy shown in Fig. 3 corresponds to small $\alpha$ (along with $\alpha_S$) i.e., the VL structure is close to $A'$. For $\theta = 0.5 \approx 28.6^\circ$, the distances $d_i$ are 1.14, 1.04, 1.04, all three are larger than 1, as expected because of the Coulomb repulsion. Note that for the lattice $A$, there will be one of the $d_i$ equal to 1. Thus, even the smallest intervortex distance at the surface exceeds the bulk intervortex distance $d_0$.

We examine the situation for a polar angle $\theta = 20^\circ$. The result of the experiment is shown in Fig.S1a. Here, the vortex lattice remains practically undistorted. In Fig.S1b we show $\alpha$ for $\theta = 20^\circ$ and different azimuthal angles $\phi$. As we see in Fig.S1, the angle $\alpha$ corresponds to a structure different from $A$ and $A'$. We believe that this difference might be due to pinning. This question should be further studied.
FIG. S1. (Color online). As in Fig. 4 of the main text, VLs for a fixed tilt $\theta = 20^\circ$ but different azimuthal angles $\varphi$ of the applied field. White ellipses are drawn according to Fig. 2c and enclose the nearest neighbor positions (circles) of the surface vortex lattice. White arrows represent the in-plane magnetic field projection.