Probing the anisotropic vortex lattice in the Fe-based superconductor KFe_2As_2 using small-angle neutron scattering

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Using small angle neutron scattering, the anisotropy of the magnetic vortex lattice (VL), in the heavily hole-doped pnictide superconductor KFe_2As_2 , was studied. Well-ordered VL scattering patterns were measured with fields applied in directions between $\mathbf{B} \parallel \mathbf{c}$ and the basal plane, rotating either towards $[100]$ or $[110]$. Slightly distorted hexagonal patterns were observed when $\mathbf{B} \parallel \mathbf{c}$. However, the scattering pattern distorted more strongly as the field was rotated away from the $\mathbf{c}$ axis. At low field, the arrangement of vortices is affected by the anisotropy of penetration depth in the plane perpendicular to the field. By fitting the distortion with the anisotropic London model, we obtain an estimate of ~ 3.4 for the anisotropy factor γ between the in-plane and $\mathbf{c}$ -axis penetration depths at the lowest temperature studied. The results further reveal VL phase transitions as a function of field direction. We discuss these transitions using the “hairy ball” theorem.

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I. INTRODUCTION

Since the discovery of the iron-based superconductors by Hosono and his collaborators in 2008,¹ there has been an intense drive to search for the mechanism from which superconductivity originates in these materials. Iron-arsenide materials are multiband superconductors and it has been theorized that superconductivity arises from magnetic interactions resulting in repulsive forces between holes on Fermi surface (FS) sheets centered at the Brillouin zone center Γ and electrons on the other FS sheets at the corners.² This could give rise to an order parameter Δ with different signs on different Fermi surfaces. Such an order parameter can take on one of two symmetries: either s -wave, where it is rotationally invariant through a 90° rotation, or d -wave, which undergoes a sign

change. These symmetries can have many different structures, such as $s_{\pm}$, extended s , and $d_{x^2-y^2}$. For $s_{\pm}$, the phase of Δ is opposite between the hole and electron sheets. The d -wave symmetry has vertical nodes in the gap that lie along the hole Fermi surface. For the extended s -wave structure, the order parameter has what are called “accidental nodes” due to the fact their positions maintain the crystal symmetry, and are not determined by the gap symmetry but by features of the pairing interaction. Nodes can be vertical such as in the d -wave case on the electron pockets, or horizontal on the hole Fermi surface, or even in general positions satisfying the crystal symmetry.³⁻⁶

Many of the iron arsenides such as optimally doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$,⁷ $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$,⁸ and LiFeAs ⁹ have properties that indicate a gap structure having no nodes. There are some notable exceptions, such as $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$,¹⁰

LaFePO,¹¹ LiFeP, FeSe,¹² and KFe₂As₂,¹³ which show clear indications of nodes in the superconducting gap structure. This question is still under investigation for many of the iron-based superconductors. The focus of this paper is KFe₂As₂, which is the end member of the hole-doped 122 iron pnictide superconductor (Ba,K)Fe₂As₂ with Ba completely replaced by K and which has a reduced T_c below 4 K, compared with 39 K at optimal doping.¹⁴

In previous small angle neutron scattering (SANS) measurements on KFe₂As₂, where $\mathbf{B} \parallel \mathbf{c}$,¹⁵ a slightly distorted hexagonal vortex lattice (VL) was seen under all (B, T) conditions studied, even up to a high field region $\sim 2/3 H_{c2}$. In this region, the gap structure strongly affects the VL structure and tetragonal superconductors that are known to have a d -wave gap symmetry such as CeCoIn₅¹⁶ usually show changes in the VL symmetry as the field is increased, even at a small fraction of H_{c2} . With $\mathbf{B} \parallel \mathbf{c}$, namely, parallel to the nodal lines in CeCoIn₅, the VL structure changes from distorted hexagonal through rhombic to square. The absence of this effect in KFe₂As₂ indicates that it has no strong fourfold anisotropy in its gap structure within the ab plane. In contrast, the temperature dependence of the SANS signal shows a nodal type behavior of the superfluid density. Hence it appears that KFe₂As₂ has nodes in the gap structure, whereas optimally doped Ba_{1-x}K_xFe₂As₂ shows full gap behavior. In Ba_{1-x}K_xFe₂As₂, T_c changes monotonically with hole doping,¹⁴ suggesting that the superconducting symmetry is the same over the whole doping range. From these facts, we deduce that KFe₂As₂ has the same $s \pm$ symmetry as the optimally doped material but with accidental nodes that develop as the hole doping is increased. We have suggested that these nodes are horizontal,¹⁵ whereas laser-ARPES measurements suggest a more complicated s -gap structure, with accidental node positions, showing a variation around the $\mathbf{c}$ axis.¹⁷ Other authors^{18–20} accept the evidence for nodes in the gap but argue for a d -wave symmetry; however, if the gap were d -wave, vertical line nodes would be present in KFe₂As₂ on *all* the Fermi surface hole sheets, and this is in disagreement with the ARPES results¹⁷ and our earlier VL observations.¹⁵ Furthermore, optimally doped Ba_{1-x}K_xFe₂As₂ has no nodes, so there would need to be a smooth change of symmetry as a function of doping, which could only occur by forming a time-reversal-symmetry-breaking ($s \pm id$) mixture, for which there is no evidence at present.

The VL structure is determined by the interactions between the vortices and can be affected by anisotropy in the carrier effective mass, m^* , Fermi velocity and superconducting gap around the “ $B_\perp$ ” plane, perpendicular to the field. These in turn can lead to a (temperature-dependent) anisotropy of the penetration depth, λ . At low fields, where the coherence length, $\xi \ll a$ (the distance between vortices), the VL anisotropy is more affected by the anisotropy of λ in the $B_\perp$ plane than by the behavior of ξ .

The simplest model to describe the situation with anisotropic penetration depth is the anisotropic London model.²¹ In the basic London theory, $1/\lambda^2 = ne^2\mu_0/m^*$,²² while in the anisotropic London model, $1/m^*$ becomes $(1/m^*)_{ij}$. This is a second-rank tensor, so one can assume an elliptical cross-section for a single vortex in the $B_\perp(x, y)$ plane, except for the case that the field is applied

FIG. 1. (Color online) Schematic of the penetration depth in the anisotropic London model²¹ in the $B_\perp(x, y)$ plane for (a) isotropic and (b) anisotropic superconductors. Here, the horizontal and vertical axes are referred to as x and y . Note the definitions of λ_x and λ_y are given in the text. (c) Vortex lattice structure in an anisotropic superconductor for both real and reciprocal space. The anisotropy factor γ is given by the ellipse axial ratio $\frac{y}{x} = \frac{y^*}{x^*}$, which is equal to the ratio of penetration depths.

along a threefold or higher symmetry axis, where the vortex would have an isotropic cross section within this theory. However, if the field is applied in another direction (for instance perpendicular to $\mathbf{c}$ in a tetragonal crystal), then λ will be anisotropic. In London theory, the most logical way to label anisotropic penetration depths is by the direction of the screening supercurrents, since this results in a labeling of λ , which is independent of field direction. Thus, for an applied field along the $\mathbf{z}$ direction, the penetration depth along $\mathbf{x}$ is determined by supercurrents along $\mathbf{y}$. We therefore label this penetration depth as λ_y , and similarly, the variation of the field along $\mathbf{y}$ depends on the quantity labeled λ_x . Figure 1 shows the difference in the shape of the vortices for (a) isotropic, (b) anisotropic penetration depths within this picture, and (c) the resultant vortex structure expected from this anisotropy. If the penetration depth in the $B_\perp(x, y)$ plane is anisotropic, this changes the interaction between the vortices, which results in a lowering of the symmetry of the VL structure in real space. Within isotropic London theory, the screening currents of a single vortex lie on an ellipse with axial ratio equal to the ratio λ_x to λ_y , which corresponds to the anisotropy, γ in Fig. 1. SANS measurements probe this ratio by imaging the VL structure in reciprocal space which represents a 90° rotation of the real space structure. Then the anisotropy, γ , can be obtained from the axial ratio of the ellipse passing through the first-order VL scattering pattern.

The overall focus of this paper is to probe the anisotropy of the VL structure in KFe₂As₂ between the in-plane and out-of-plane directions by rotating the field direction away from the $\mathbf{c}$ axis. We find that even with $\mathbf{B} \parallel \mathbf{c}$, there are small distortions of the VL away from the exact isotropy given by London theory. As demonstrated in our earlier

work,¹⁵ these distortions increase with field, which may be understood as an increasing effect of the vortex core structure, as the cores are pushed closer together. This gives rise to higher-order anisotropy, additional to any arising from the effective mass, which reflects the variation of Fermi velocity and superconducting gap over the Fermi surface. Such effects, which occur when the scale of spatial variation is comparable to the core size $\sim \xi$ are referred to as “nonlocal,” because they may be described as departures from the local relationship between supercurrent and magnetic vector potential that gives rise to the London equation.^{23,24} They may also be implicated in the alignment of the VL to the underlying crystal lattice and any VL phase changes that represent a change of that alignment. We shall first describe the experimental setup for these measurements, followed by the results and discussion.

II. EXPERIMENT

The present SANS experiments on KFe_2As_2 were performed using the SANS-I instrument at the Swiss Spallation Neutron Source (SINQ), Paul Scherrer Institut (PSI), Switzerland and the GP-SANS instrument at the High Flux Isotope Reactor (HFIR), Oak Ridge National Laboratory, USA. The instruments at both facilities were run at a neutron wavelength of $\lambda_n = 10 \text{ \AA}$ with a spread $\frac{\Delta\lambda_n}{\lambda_n}$ of 0.1 and 0.15, respectively. The two samples measured were made up of a mosaic of crystals which were mounted with their $\mathbf{c}$ axes horizontal on a series of aluminum plates. In one mosaic, the crystals also had their $[100]$ axes horizontal on the instrument; the other mosaic had $[110]$ horizontal. Hereafter, they will be referred to as the $[h0l]$ and $[hhl]$ settings, respectively. To study the vortex structure, a magnetic field was applied by either a 11 T horizontal magnet with a dilution refrigerator insert capable of going down to 50 mK at PSI or a 4.5 T horizontal cryomagnet with a base temperature of 2 K at HFIR. For both experiments, the magnetic field was applied almost parallel to the incoming neutron beam. The resultant scattering patterns were collected on a 2D position-sensitive detector set at 18 m (PSI) and 19 m (HFIR) from the sample. To obtain these patterns, the sample and magnet were rotated together using fine angular steps on a goniometer to allow all measurable VL reflections to satisfy

the Bragg condition. To probe the anisotropy in KFe_2As_2 , we rotated the magnetic field away from the $\mathbf{c}$ axis towards either the $[100]$ or the $[110]$ direction depending on the setting being investigated. Hereafter, we denote α as the angle of the rotation of the applied magnetic field away from the crystallographic $\mathbf{c}$ axis towards $[100]$ or $[110]$.

As described above, the London model leads to an isotropic penetration depth within the tetragonal ab plane. Hence, the ratio of any in-plane penetration depths, e.g., $\lambda_{010}/\lambda_{\bar{1}10}$ would be equal to 1. Similarly, the anisotropic London model predicts that the ratio $\lambda_{001}/\lambda_{010}$ is equal to $\lambda_{001}/\lambda_{\bar{1}10}$. Thus the VL distortion γ at $\alpha = 90^\circ$ would be equal for $\mathbf{B} \parallel [100]$ and $\mathbf{B} \parallel [110]$. However, the data show that particularly for the $[hhl]$ setting the situation is more complex than this.

III. RESULTS

A. VL diffraction patterns

Figures 2(a)–2(j) show the diffraction patterns obtained from the VL at $T = 2 \text{ K}$. These represent a weighted average of data taken with the VL at various angles to the field. The weightings are calculated by Bayesian methods²⁵ to emphasize data from regions of the detector satisfying the Bragg condition for each VL angle. For both settings at $\alpha \sim 0$, the diffraction patterns show the superposition of signals from two VL domains, which arise from the two degenerate orientations that a hexagonal lattice can take relative to the underlying square crystalline structure. However, as shown in Figs. 2(a)–2(e), this degeneracy is suppressed for the $[h0l]$ setting as the field is rotated toward the $[100]$ axis. Also, the VL symmetry remains distorted-hexagonal for all measured angles α without a change of the VL orientation. The single VL domain observed at large α respects the symmetry of the underlying crystal lattice, which is the $[h0l]$ mirror plane, which is horizontal in Figs. 2(a)–2(e). In contrast, for the $[hhl]$ setting as shown in Figs. 2(f)–2(j), we find that the degeneracy between the two VL domains remains up to higher angles and that the VL domains change their orientation as a function of α . Namely, at $\mathbf{B} \parallel \mathbf{c}$, the VL structures have diagonal $[h0l]$ mirror planes, but as α is increased, the VLs rotate and distort and have no mirror planes at all, until they become one VL domain aligned

FIG. 2. (Color online) VL diffraction patterns at $T = 2 \text{ K}$ and $B = 0.2 \text{ T}$ for both $[h0l]$ (a)–(e) and $[hhl]$ (f)–(j) settings. The panels have an area of $(q = 0.030 \text{ \AA}^{-1})^2$. The angle α between $\mathbf{B}$ and $\mathbf{c}$ is marked for each panel, and the angle β between two VL reciprocal vectors and the misalignment angle η are defined in (a) and (f), respectively.

FIG. 3. (Color online) The opening angle of the VL, β , in the $[h0l]$ setting as function of α . The data show a steady decrease in β for a variety of fields and temperatures. The line is a guide to the eye.

with the mirror $[hhl]$ plane at $\alpha \sim 45^\circ$. We note that if two VL domains are present, the individual domains do not respect the symmetry of the underlying crystal; however, the total diffraction pattern does, because of the degeneracy of the two VL domains imposed by the crystal symmetry.

B. Distortion of the VL

From the results, we may obtain a quantitative measure of the distortion of the VL as a function of α for both settings. For the $[h0l]$ setting, this may be represented by the opening angle β , which lies between two basis vectors of the VL primitive cell in a single domain, as illustrated in Fig. 2(a). As shown in Fig. 3, β continuously decreases with increasing α . The legend in Fig. 3 shows that the data were taken at many different fields and temperatures, and so the present results indicate that β for this setting is almost field and temperature independent. On the other hand, for the $[hhl]$ setting, the evolution of the VL as a function of α may be quantified by the misalignment angle η , which is defined in Fig. 2(h), and the result is plotted in Fig. 4. We see that η shows a rapid variation near $\alpha \sim 45^\circ$, followed

FIG. 4. (Color online) The misalignment angle η of the VL as a function of α for the $[hhl]$ setting at $T = 2$ K and $B = 0.2$ T. The definition of η is shown in Fig. 2(f). The line is a guide to the eye.

(b)

FIG. 5. (Color online) (a) Schematics of the variation of VL structure with field angle. We have only measured over two angle scans, but simple continuity allows us to fill in the behavior for all field directions between them. (b) shows schematically some typical diffraction patterns arising from the behavior in (a).

by a constant value of zero, suggestive of a second-order phase transition.

We can systematize the presence and absence of VL phase transitions as a function of field direction, by making use of considerations arising from the “hairy ball” (HB) theorem.²⁶ It shows that there *must* be discontinuities in VL structure and orientation as the field direction is varied. The VL structure may spontaneously break the underlying crystal symmetry and give multiple VL domains; however, the resultant diffraction pattern will respect the crystal symmetries about the axis **B**. The application of the HB theorem to our 2-K data is laid out in Fig. 5. In Fig. 5(a), we show schematically the VL diffraction patterns from KFe_2As_2 at 0.2 and 2 K as a function of field direction in an octant of solid angle, with the field directions projected onto a circle. The diagonal blue lines represent loci across which the equilibrium VL

FIG. 6. (Color online) VL diffraction patterns for the low temperature region with $T < 0.35$ K and $B = 0.2$ T for both $[h0l]$ (a)–(e) and $[hhl]$ (f)–(j) settings. The angle α between $\mathbf{B}$ and $\mathbf{c}$ is marked for each panel. The angle β between two VL reciprocal vectors and the misalignment angles 2η and 2ϕ are defined in (a), (f), and (i), respectively.

orientation changes discontinuously. Everywhere else, the VL distortion and orientation change smoothly as a function of field direction. On the blue lines, two VL domains are degenerate and present in approximately equal proportions, but on moving away from these loci, the lower-energy VL will predominate. The yellow lines interconnecting spots and the center in some patterns are guides to the eye, to show how the VL orientation rotates on changing field direction from near $[h0l]$ to near $[hhl]$. Weaker spots are represented by smaller symbols. In Fig. 1(b), the VL structures are represented schematically by the resulting diffraction patterns as a function of α . The situation for the $[h0l]$ rotation is the simpler: on leaving $[001]$ where the blue lines cross, one VL orientation is strongly favored, and this retains its orientation and merely distorts as α is increased. For $[hhl]$ rotation at small α , the field direction remains on the blue line, so that two VL domains are present. This remains the case until the VL locks to the axis. Another change also takes place at the same point: two of the six spots become weaker. The four strong spots are bisected by the $[hhl]$ direction, just like four of the six spots for rotation along the $[h0l]$ direction.

In Figs. 6(a)–6(j), we show diffraction patterns obtained as a function of α at dilution refrigerator temperatures. For the $[h0l]$ (a)–(e) setting, we find that the preferred single domain is already selected at smaller values of α , but otherwise the behavior is qualitatively similar to that seen at $T = 2$ K. However, for the $[hhl]$ (f)–(j) setting, two VL domains remain for all angles measured. As may be seen in Fig. 6(a), it is difficult to quantify the misalignment by the angle η [plotted in Fig. 7(a)], because the relevant diffraction spots become very weak at large α and are close to the horizontal axis. However, we can use another angle ϕ , defined in Fig. 6(i), which will be zero for a single domain VL aligned with the horizontal axis. As we see in Fig. 7(b), ϕ remains nonzero for all angles in a $[hhl]$ scan and is likely to remain so to $\alpha = 90^\circ$. This implies that the blue lines in Fig. 1(a)—denoting coexisting VL's and discontinuous orientation change—extend to the $[hk0]$ plane. If so, they will extend a short distance around this plane away from $[110]$. We were unable to measure under these conditions (neutron beam almost parallel to the crystal plates) but we may predict that the total diffraction

pattern will always respect the crystal symmetry, and on the blue lines, this will be assured by the coexistence of two VL domains with orientations related by the relevant mirror symmetry planes of the underlying crystal as shown in Fig. 8. The temperature-dependence of the behavior of the VL in KFe_2As_2 is reminiscent of that for niobium,²⁷ which also shows additional spontaneous breaking of the crystal lattice symmetry by the VL at lower temperatures.

FIG. 7. (Color online) The VL angles (a) η and (b) ϕ as a function of α for the $[hhl]$ angle scan at low temperature below $T = 0.25$ K, together with lines as a guide to the eye.

FIG. 8. (Color online) The predicted behavior of the VL diffraction patterns from KFe_2As_2 at $B = 0.2$ T and $T < 0.35$ K as a function of field direction in the region of solid angle centered on the $[110]$ direction. The conventions used in this figure are as in Fig. 5(a).

C. Superconducting anisotropy of KFe_2As_2 from the VL distortion

As discussed in the introduction, the anisotropy factor γ for KFe_2As_2 at a given angle of rotation α can be obtained by fitting an ellipse to the diffraction patterns and taking the ratio of the major (x^*) to minor (y^*) axes. This can only give smooth change with angle if the VL symmetry remains the same for all α , so we use this approach only for results from the $[h0l]$ setting. The anisotropic London model²¹ gives

$$\gamma(\alpha) = \left(\frac{1}{\gamma_{\alpha=90^\circ}^2} \sin^2 \alpha + \frac{1}{\gamma_{\alpha=0^\circ}^2} \cos^2 \alpha \right)^{-1/2}.$$

For tetragonal KFe_2As_2 , London theory gives $\gamma_{\alpha=0^\circ} = 1$, but the VL shows a slight distortion even at $\alpha = 0^\circ$, so we used the following formula to fit the data:

$$\gamma(\alpha) = A \left(\frac{1}{\gamma'^2} \sin^2 \alpha + \cos^2 \alpha \right)^{-1/2}.$$

The curves in Fig. 9 show the results of fits to the $[h0l]$ data taken at 2 K and <0.35 K, where we obtained the following fitting parameters: $A = 1.03 \pm 0.03$, $\gamma' = 3.24 \pm 0.21$ (2 K), and $A = 1.06 \pm 0.003$, $\gamma' = 3.35 \pm 0.03$ (<0.35 K). The present results indicate that the anisotropy between the **a**- and **c**-axis penetration depths in KFe_2As_2 is a factor of ~ 3.3 . This is somewhat smaller than the anisotropy of the upper critical field obtained from heat capacity measurements:²⁸ $\gamma = (H_{c2}^{\text{ab}}/H_{c2}^{\text{c}}) = 4.5$ extrapolated to $T = 0$. In contrast, resistivity measurements²⁹ gave an anisotropy of 3.52 at $T = 0$, which is in relatively good agreement with our results.

IV. ANGLE-DEPENDENCE OF FORM FACTOR

The effect of uniaxial crystal anisotropy on the components of the spatially varying magnetic field within anisotropic London theory was described some years ago by Kogan.²¹ Some misprints in this paper were corrected and the model

FIG. 9. (Color online) Anisotropy factor γ for the $[h0l]$ setting at 2 K (triangles) and <0.35 K (circles) as a function of the rotation angle α with a fit to the data that gives $\gamma' = 3.24 \pm 0.21$ (2 K) and 3.35 ± 0.03 (<0.35 K).

was extended to calculate SANS signals as a function of field direction for the case of biaxial anisotropy in Ref. 30. The theory may be further extended to include anisotropic core effects as in Ref. 31. In the current case, there are two effects on the SANS signal if the field is rotated away from **c**. The first is that the longer penetration depth for currents in the **c** direction reduces the form factor for the four spots on the left and right of Figs. 2 and 6(c)–6(d). However, the form factor for the two top and bottom spots is mainly controlled by currents in the basal plane and does not fall for small rotations of the field direction away from **c**. The other effect on the form factors is that rotation away from **c** at constant B causes a reduction in the core overlap effects, because B_{c2} increases as the field is rotated towards the basal plane, and hence a fixed value of B becomes a smaller fraction of B_{c2} . The core overlap factor has the same value for all the diffraction spots. The net effect is that the form factor for the top and bottom spots of Figs. 2 and 6 should increase on rotation away from **c** and become stronger than the other four spots which decrease in intensity. This qualitative behavior is clearly observed. A more detailed study of form factor versus angle was carried out at low temperature below $T = 0.35$ K for field rotation in the $[h0l]$ plane up to 45° from **c**. The results, along with a theoretical curve are shown in Fig. 10. This shows that the expected behavior can be well accounted for by the extended London model. We note that a peak in form factor versus angle for top and bottom spots has recently been observed in the far more anisotropic material strontium ruthenate.³²

V. DISCUSSION

The most striking result is that the degree of basal plane anisotropy, seen in KFe_2As_2 by VL measurements, depends strongly on the direction of the applied field. With the field parallel to **c**, the VL structure remains a weakly distorted hexagon under all B and T conditions studied,¹⁵ and there is no sign of a transition to a square VL favored by fourfold anisotropy terms. On the other hand, when the field is applied in the basal plane, we find distinctly different behavior for

FIG. 10. (Color online) Form factor for the two top and bottom diffraction spots and the four left/right spots versus field direction for rotation of a 0.2-T field away from $\mathbf{c}$ in the $[h0l]$ plane at low temperature below $T = 0.35$ K. The form factors are normalized to their values for $\mathbf{B} \parallel \mathbf{c}$. The theoretical lines are calculated using the values of λ , ξ , the coefficient c in $\exp(-cq^2\xi^2)$ in the core correction factor used in our earlier publication,¹⁵ and the value 3.35 for γ .

the field along the $[100]$ compared with the $[110]$ direction, particularly at low temperatures. Fourfold anisotropy cannot arise from London theory but appears in nonlocal extensions to this theory, which reflect anisotropy of Fermi velocity and gap.^{23,24} Hence the observed behavior cannot arise from nonlocal effects in a simple model of cylindrically symmetric Fermi surface sheets with purely horizontal line nodes in the gap. In any case, band structure calculations³³ and ARPES data¹⁷ indicate that the situation in KFe_2As_2 is more complicated than this.

It is important to note that with the field along $\mathbf{c}$, supercurrents and hence the London penetration depth $\lambda_a = \lambda_b$ will be determined by the basal-plane component of the Fermi velocity of the gapped electrons/holes, and the vortex core structure will be determined by the basal plane anisotropy of gap and Fermi velocity of these same carriers. However, with the field applied in the basal plane, the shorter value of penetration depth will be again be λ_a , but the longer one is λ_c . The value of this will instead be controlled by the gapped electrons/holes that have a $\mathbf{c}$ -axis component of Fermi velocity. To explain our results, we are therefore looking for differences in $\mathbf{c}$ -axis warping (and gap value) between Fermi surface regions perpendicular to $[100]$ and $[110]$. This is most likely to be strong in the electronlike regions of Fermi surface near the Brillouin zone corners. The increase in the $[100]/[110]$ anisotropy at low temperatures probably reflects the fact that nonlocal effects are expected to increase as the temperature is reduced.

In KFe_2As_2 , λ_a is smaller than λ_c by a factor of ~ 3.4 at lowest temperature. In the simplest possible model, isotropic gap and single ellipsoidal FS, the anisotropy factors of λ and ξ are equal (both arising from the anisotropic effective mass). In this model, γ is equal to the axial ratio of the ellipsoidal FS. Given the complicated FS and gap structure in KFe_2As_2 , we cannot make numerical use of this model, but our value

of $\gamma \sim 3.4$ shows that the Fermi surface in KFe_2As_2 is not strongly two dimensional.

We note that the orientation of the VL when the field is not along a principal axis of the anisotropic effective mass m is predicted by London theory. It is the orientation observed for the $[h0l]$ setting. We can conclude that for the $[hhl]$ setting, nonlocal effects are sufficient to overcome the London-predicted orientation at least up to 45° at $T = 2$ K and up to 90° for $T < 0.35$ K. We note another difference between these two settings. For $\mathbf{B}$ close to $[100]$, the VL structure is distorted-hexagonal with all six spots of comparable intensity (as predicted by anisotropic London theory). In contrast, for $\mathbf{B}$ close to $[110]$, the VL structure has only four strong spots, so could be referred to as a “rhombic” VL. However, this can smoothly distort, with a continuous change in intensity of the weaker spots, into a stretched hexagonal VL as the field direction is rotated towards $[100]$.

VI. CONCLUSION

We have presented new results from SANS experiments at $B = 0.2$ T on the vortex lattice in KFe_2As_2 as a function of field direction. These show more complex behavior than given by anisotropic London theory, particularly for rotation of magnetic field direction between the $[001]$ and $[110]$ axes. However, the results can be systematized using the hairy ball theorem²⁶ and show signs of “nonlocal” effects. In particular, the VL phase diagram becomes more complex at low temperatures, and the difference between $[100]$ and $[110]$ directions may be related to the nodal structure of the gap. We find that the $a - c$ anisotropy factor increases at low temperatures towards a value ~ 3.4 . This value is close to those obtained from macroscopic measurements of H_{c2} anisotropy.^{28,29} In simple London theory, there would be one value of anisotropy factor for penetration depth, H_{c2} and effective mass. In our measurements in KFe_2As_2 , the applied field is sufficiently far below H_{c2} that London theory supplies a useful first approximation, but anisotropy of the gap and of the Fermi surface add important modifications.

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