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Image simulations of kinked vortices for transmission electron microscopy

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ABSTRACT

We present an improved model of kinked vortices in high-T_c superconductors suitable for the interpretation of Fresnel or holographic observations carried out with a transmission electron microscope. A kinked vortex is composed of two displaced half-vortices, perpendicular to the film plane, connected by a horizontal flux-line in the plane, resembling a connecting Josephson vortex (JV) segment. Such structures may arise when a magnetic field is applied almost in the plane, and the line tension of the fluxon breaks down under its influence. The existence of kinked vortices was hinted in earlier observations of high-T_c superconducting films, where the Fresnel contrast associated with some vortices showed a dumbbell like appearance. Here, we show that under suitable conditions the JV segment may reveal itself in Fresnel imaging or holographic phase mapping in a transmission electron microscope.

1. Introduction

Recent transmission electron microscopy (TEM) experiments carried out on YBaCuO thin films revealed some intriguing features in the Fresnel (out-of-focus) images of vortices: by increasing the applied field angle away from the sample perpendicular, the vortex image become first elongated as if its core was adapting to the direction of the field [1]. Then, when the field is applied almost in the film plane, sometimes vortices exhibit a dumbbell like appearance [2]. These observations hint towards something peculiar happening to the structure of the vortices. The physics of magnetically coupled layered superconductors suggests that the vortex line might become unstable at large angles of the applied field, and that an alternative kinked structure may be energetically favorable [3].

Aiming at interpreting these phenomena, we first developed an anisotropic model [4] and another with a simplified pancake structure of the vortices [5]. The latter was subsequently modified to increase the number of pancake vortices by resorting to a continuum approximation of the screening layers above and below the one containing the pancake vortex [6]. In this way, we could distribute a set of pancake vortices over suitable locations within the superconducting film, and build a kinked structure that was then used in support of our interpretation. The dumbbell appearance of vortices in Fresnel mode was well reproduced by two displaced stacks of pancake vortices.

However, pancake vortices are Josephson-decoupled, and represent a limiting case where the superconductor has infinite anisotropy (the penetration depth along the c axis is infinite, i.e. the material behaves like vacuum along the c axis) [7]. As a consequence, no Josephson vortex (JV) was present as a connection between the two separate stacks. Here, we re-examine the more representative continuous anisotropic model that was employed successfully in the interpretation of vortex images in the presence of columnar pinning sites [4]. By superimposing the magnetic fields associated to a tilted central core and to a couple of perpendicular cores located at the ends of the tilted core segment, we develop a more realistic description of a kinked vortex and we illustrate under which conditions (choice of the material and electron-optical set-up) both the JV segment and the two vertical half-vortices may be observed and investigated.

2. General considerations

Let us first briefly recall the main conventions regarding the coordinate systems and the basic formulas describing the interaction of the electron beam with the magnetic field associated to a vortex. Two coordinate systems have been introduced and described [5,6,8], namely: (i) the microscope coordinate system having the z axis parallel to the electron beam

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and aligned in the same direction, with (x,y) being the coordinates in the object plane, perpendicular to the optical axis z, and (ii) the specimen reference system (x_S,y_S,z_S), having its z_S axis, of unit vector $\mathbf{k}_S$, coincident with the specimen normal $\mathbf{n}$ and oriented in the opposite direction as z, the x_S axis, of unit vector $\mathbf{i}_S$, having initially the same direction as x, and the y_S axis determined by the requirement of left-handedness, i.e. opposite to y.

The specimen, assumed of constant thickness $t=2d$, can be inclined of an angle α with respect to the electron beam, around the tilt axis coincident with the y axis. The specimen can be also rotated of an azimuth angle β around its normal $\mathbf{n}$, coincident with the tilted z_S axis. A sketch of the sample, reference system, and geometrical parameters is shown in Fig. 1.

In order to describe the interaction between the electron beam and the magnetic field associated to the vortex, the standard high-energy or phase object approximation is used, according to which the vortex is a pure phase object [9,10], with the magnetic phase shift given by

$$\varphi(x,y) = -\frac{e}{\hbar}\int_l \mathbf{A}\cdot d\mathbf{l} = -\frac{\pi}{\phi_0}\int_{-\infty}^{+\infty} A_z(x,y,z)\,dz \tag{1}$$

where $\mathbf{A}$ is the vector potential, e and $\hbar$ are the absolute value of the electron charge and the reduced Planck constant, respectively, $\phi_0=2.07\times10^{-15}\,\mathrm{T\,m^2}$ is the flux quantum, and x and y are kept fixed since we consider an electron trajectory parallel and in the same direction as the z axis. This trajectory passes through the regions above, within and below the specimen, thus crossing separated space domains. For the calculation of the phase shift by means of Eq. (1), in order to avoid unwanted extra terms arising from contour integrals along the domain boundary, it is essential to choose a vector potential continuous in its components parallel to the boundaries [8].

In the specimen system, the above trajectory is characterized by the parametric equation

$$\mathbf{l} = (x_S - w\tan\alpha\cos\beta)\mathbf{i}_S + (y_S - w\tan\alpha\sin\beta)\mathbf{j}_S + w\mathbf{k}_S \tag{2}$$

where w ranges between $(+\infty,-\infty)$ due to the fact that $\mathbf{k}_S$ and $\mathbf{k}$ point in opposite directions. The correspondence between the coordinates of the intersection of the trajectory with the object plane (x,y) and with the specimen midplane (x_S,y_S) is given by

$$x_S = x\frac{\cos\beta}{\cos\alpha} + y\sin\beta, \quad y_S = x\frac{\sin\beta}{\cos\alpha} - y\cos\beta \tag{3}$$

Therefore, the phase shift equation (1) can be calculated in the specimen system according to the relation:

$$\varphi(x_S,y_S) = \frac{\pi}{\phi_0}\int_{+\infty}^{-\infty} \mathbf{A}(x_S - w\tan\alpha\cos\beta, y_S - w\tan\alpha\sin\beta, w) \cdot \begin{pmatrix} \tan\alpha\cos\beta \\ \tan\alpha\sin\beta \\ -1 \end{pmatrix} dw \tag{4}$$

and converted finally in the microscope reference system through the indicated coordinate transformations.

As regards the Fresnel phase contrast method, starting from the object phase the out-of-focus images in the observation plane, located at a distance Z from the object plane, can be calculated by means of the Kirchhoff–Fresnel integral [11]:

$$I(X,Y,Z) = \left|\frac{1}{\lambda_e Z}\iint e^{i\varphi(x,y)} e^{(i\pi/\lambda_e Z)[(x-X)^2+(y-Y)^2]}\,dx\,dy\right|^2 \tag{5}$$

where X and Y are the coordinates in the out-of-focus plane, Z is the defocus, and λ_e is the de Broglie wavelength of the incident electrons (~ 1 pm for 1 MeV electrons).

3. The kink model

The physical observable required to interpret TEM images is the electron-optical phase shift, proportional to the integrated magnetic vector potential along the electron trajectory. Hence, we aim at describing kink vortices via their vector potential. In order to do so, we first sketch its general structure inside and outside the superconducting film as a set of solutions to the appropriate differential equation valid in each of the five regions we divide space: (1) upper vacuum; (2) upper SC layer (with one half-vortex); (3) mid-SC layer (with the JV segment); (4) lower layer (with the second half-vortex); (5) lower vacuum. The mid-layer has thickness $2d_0$, while the total thickness is $2d$. The vortex core is vertical (perpendicular to the specimen surfaces) in the upper and lower layers, and tilted at an angle θ in the mid-layer. Then, we apply proper boundary conditions and determine the actual physical structure of a kinked vortex, where we allow a degree of freedom in the choice of JV tilt angle and thickness of the two half-vortices (assumed equal and symmetrically displaced). In regions (1) and (5), each Cartesian component of the vector potential satisfies Laplace equation $\nabla^2\mathbf{A}=0$. In regions (2)–(4), the vector potential satisfies the London equation $\mathbf{A}+\mathcal{L}(\nabla\times\nabla\times\mathbf{A})=\mathbf{\Phi}_L$, where

$$\mathbf{\Phi}_L = \frac{\phi_0}{2\pi}\frac{\mathbf{r}_F\times\mathbf{k}_F}{r_F^2} \tag{6}$$

is the London vector describing the elementary vector potential field associated to a quantized flux-line. In Eq. (6), $\mathbf{k}_F$ is the unit vector pointing in the direction of the vortex core, and $\mathbf{r}_F$ is a two-dimensional position vector perpendicular to $\mathbf{k}_F$. The anisotropic tensor $\mathcal{L}$ is represented by the matrix

$$\mathcal{L} = \lambda^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \gamma^2 \end{pmatrix} \tag{7}$$

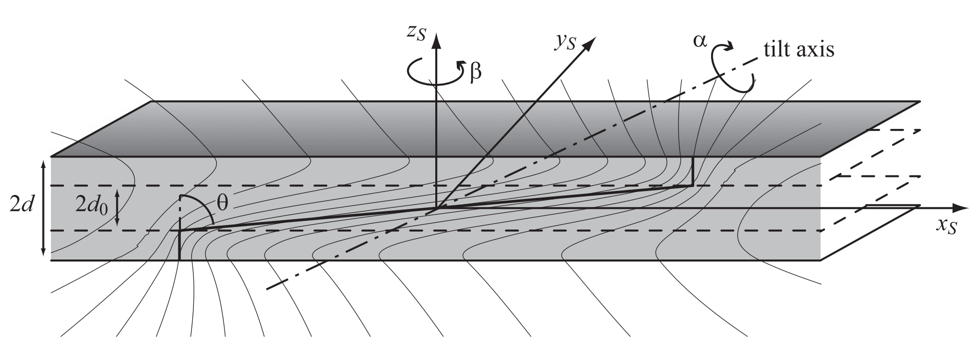

Fig. 1. Outline of a kinked vortex within a superconducting slab of thickness $2d$. The JV segment connecting the two half-vortices is confined in a thin layer of thickness $2d_0$, and is inclined at an angle θ. The specimen (x_S,y_S,z_S) reference system is also indicated, where α (tilt) and β (azimuth) are the angles of rotation relating the specimen and microscope coordinate systems. The tilt axis coincides with the y axis of the microscope reference frame.