Diamagnetic soliton at twin boundary

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(Submitted 18 January 1990)
Pis'ma Zh. Eksp. Teor. Fiz. **51**, No. 6, 310–314 (25 March 1990)

Near a twinning plane, the susceptibility blows up as $\chi \propto B^{-2}$ as $B \Rightarrow 0$. It follows that there is an induced surface diamagnetism, independent of the temperature, with a domain size ~100 Å and with a magnetic field ~10^6–10^7 Oe in the domain.

Diamagnetic domains in metals are a well-known effect.[1] The reason for it is that oscillations of the magnetic susceptibility χ (the de Haas-van Alphen effect) can lead to large values of χ, greater than $1/4\pi$. The system then becomes thermodynamically unstable, and diamagnetic domains appear. The amplitude of the oscillations in χ in the de Haas-van Alphen effect becomes infinite as $\mathbf{B} \to 0$ $(T = 0)$:

$$\chi = (v_F / c)^2 (\mu / \hbar\Omega)^{3/2} , \quad (1)$$

where $\Omega = eB/mc$ is the cyclotron frequency. As the temperature is raised, the amplitude of the χ oscillations falls off exponentially, $\propto \exp\{-2\pi^2 T/\hbar\Omega\}$. Diamagnetic domains thus occur only at temperatures low enough that this exponential factor is on the order of unity.

Let us examine the appearance of diamagnetism at the boundary of a bicrystal. This question is of considerable interest because of the observation of anomalies in the susceptibility in several simple metals through measurements of the Knight shift[2] and by the μSR method,[3] both of which detect the magnetic field distribution at the local level. It turns out that, in contrast with the bulk case, diamagnetism at the boundary of a bicrystal has a remarkable property: The effect is not limited to low temperatures and instead occurs at all real temperatures ($T \ll \mu$). Furthermore, this effect has an amplitude much larger than that in the bulk case. For clarity, we will be discussing the most symmetric case: that of a twined crystal. We assume that the magnetic induction vector B is directed along the z axis, which lies in the twinning plane. In a region of width $4r_L$ ($r_L = cp_F/eB$ is the electron Larmor radius), a magnetization current j then arises. This vector j is perpendicular to B and also lies in the twinning plane, along the y axis. The relationship between B and j is determined by Maxwell's equations, which in this case reduce to

$$-dB/dx = 4\pi/cj \cdot \tag{2}$$

The coordinate x runs perpendicular to the twinning plane. The reason why the magnetization current vanishes identically at distances greater than $2r_L$ from the twinning plane is that an electron does not collide with the twinning boundary, and a uniform bulk magnetization arises. In a band of width $4r_L$, on the other hand, there are electrons which collide with the twinning boundary. As a result, the magnetization M becomes spatially nonuniform, and the magnetization current nonzero. By virtue of the symmetry of the twins to the left and right of the twinning boundary, a given magnetic field leads to oppositely directed magnetization currents. This current is therefore an odd function of the coordinate x:

$$j(-x) = -j(x) \tag{3}$$

By virtue of Maxwell's equations (2), a symmetric distribution of the induction B arises at the twinning boundary.

Up to this point we have been discussing the magnetization near a twinning boundary in an external magnetic field. We have seen that in this case the magnetization unavoidably has a nonuniform spatial distribution. We now set the external magnetic field equal to zero. We will see that a necessary and sufficient condition for the appearance of a spontaneous magnetization near the twinning boundary is that the magnetization current density j behave in the following way as $B \Rightarrow 0$:

$$j \propto B^{\alpha} \qquad (0 \leqslant \alpha < 2)\,. \tag{4}$$

The limiting behavior in (4) as $B \Rightarrow 0$ corresponds to

$$j \propto ev_F p_F^{3}/\hbar^3(\hbar\Omega/\mu)^{\alpha}. \tag{4a}$$

From (4) and (4a) we easily find an estimate of the susceptibility. Since we have $\chi \propto \partial M/\partial B = c^{-1} j/dB/dx$, and since the derivative obeys $dB/dx \propto B/r_L$, we have $\chi \propto B^{\alpha-2}$ as $B \Rightarrow 0$. A joint solution of Eqs. (2) and (4a) yields the characteristic magnetic field,

$$\hbar\Omega \propto \mu(e^2/\hbar c\, v_F/c)^{1/(2-\alpha)}, \tag{5}$$

and, correspondingly, the Larmor radius,

$$r_L \propto \hbar/p_F (e^2/\hbar c . v_F/c)^{-1/(2-\alpha)} . \tag{5a}$$

The magnetic induction B found from (5) and the Larmor radius r_L given in (5a) depend strongly on the index α. In the bulk case, which corresponds to (1), we would have $\alpha = 1/2$. The minimum possible value of α corresponds to $\alpha = 0$. This result means that the magnetization is produced by all the conduction electrons, without any substantial cancellation among them. This situation is characteristic of a twinning boundary, as we will see below.

Let us consider a twinning boundary of the tilt type in an anisotropic metal. According to Ref. 4, its behavior in a magnetic field is described by the Hamiltonian.

$$H = -\ 1/2\partial/\partial x(m_{11}^{-1}(x)\partial/\partial x) + \frac{m_{11}(x)}{2m_1 m_2}(k_y - e/cA(x))^2 + k_z^2/2m_3 . \tag{6}$$

The mass $m_{11}(x)$ here can be expressed in the following way in terms of the masses m_1 and m_2 along the principal crystallographic axes, with respect to which the twinning boundary is tilted an angle φ:

$$m_{11}^{-1}(x) = m_1^{-1}\cos^2\varphi + m_2^{-1}\sin^2\varphi \qquad (m_1 < m_2). \tag{6a}$$

We assume that as a twinning boundary of width 2b is crossed, the angle φ changes from 0 to π. The effective potential energy which corresponds to this geometry, $U = [m_{11}(x)/m_1 m_2]k_y^2$, is a potential barrier of width 2b (Fig. 1). We assume that the radius of the electron orbit is much larger than the transition layer between the crystallites of the twin: $r_L \gg b$. We also assume that the barrier transmission $U(x)$ is small. This assumption corresponds to the case of the inequality $2p_F b(1 - m_1/m_2)^{1/2} \gg 1$. In this case, electrons with an energy lower than the height of the barrier near the twinning boundary are reflected from the barrier in a specular fashion, while those with an energy above the barrier height cross freely, without experiencing any above-barrier reflection. The electrons which do not collide with the surface have the usual spectrum

$$E_n(k_y, k_z) = \epsilon_n(k_y) + k_z^2/2m ,$$

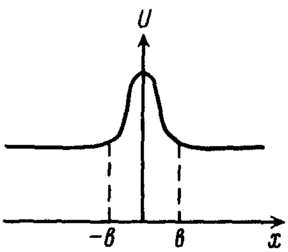

FIG. 1.

where $\epsilon_n = \Omega(n+1/2)$, and k_y satisfies one of the two conditions $k_y^2/2m_1 > \epsilon_n$ or $k_y^2/2m_2 < \epsilon_n, k_y > 0$. For the electrons which are reflected from the barrier in Fig. 1, with $\epsilon_n < k_y^2/2m_2$, the spectrum changes: $\epsilon_n = \pi\Omega(n+3/4)/\sigma(p), \sigma = \pi/2 + \arcsin p - p\sqrt{1-p^2}, p = k_y/\sqrt{2m\epsilon_n}$. Using this spectrum and the corresponding semiclassical wave functions, we find an expression for the magnetization current:

$$j(x) = 2e \int_0^\infty dE J(E,x)/(1+\exp(E-\mu)/T) \qquad X = x/a; \quad a = c\sqrt{2m_2\epsilon}/eB$$

$$J(E,x) = -\sqrt{m_1 m_3}/4(\pi\hbar)^3 \int_0^E \sqrt{\epsilon}/(E-\epsilon) d\epsilon \theta(X)\theta(2-X)$$

$$\times \int_{X-1}^{1} d\zeta \theta(\zeta^2 m_2/m_1 - 1) Q(\zeta, X) \tag{7}$$

$$Q(\zeta, X) = \zeta(1-\zeta^2)^{1/2}(\zeta - X)(\pi/2 + \arcsin\zeta)^{-1}(1-(\zeta-X)^2)^{-1/2}.$$

It can be seen from (7) that at $T=0$ we have $j(x) \equiv 0$ for all $x > 2r_L$. Near $x \approx 2r_L$, we can easily calculate $j(x)$:

$$j(x) = 8\sqrt{2}/15 j_0 \delta^{5/2}; \qquad j_0 = e\sqrt{m_1 m_3}\mu^2/(\pi\hbar)^3; \quad \delta = 1 - x/2r_L, \quad \delta \ll 1.$$

At the point $x=0$, $j(x)$ has the opposite sign:

$$j(0) = -\pi j_0/8 \int_0^\pi \phi^{-1} d\phi \sin\phi \cos^2\phi\, \theta(\cos^2\phi - m_1/m_2).$$

On the whole, the behavior of $j(x)$ along the coordinate is as shown in Fig. 2(a). The value of j depends on the ratio m_1/m_2, vanishing identically at $m_1 = m_2$. Using the explicit expression for the current in (7), we can easily show that the current component of the free energy is negative:

$$-\int M(x) B dx = -c^{-1} B \int x j(x) dx < 0. \tag{8}$$

Consequently, the appearance of nonvanishing values of B and j in (7) in the system is favored from the energy standpoint. Our estimates of the current $j(x) \propto j_0$ correspond to estimate (4a) with $\alpha = 0$. It follows that it is possible to construct a soliton with an

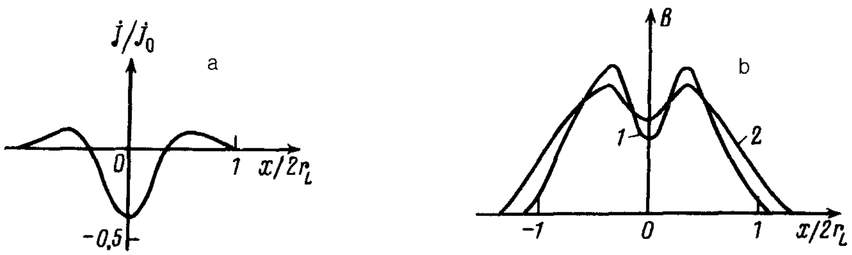

FIG. 2.

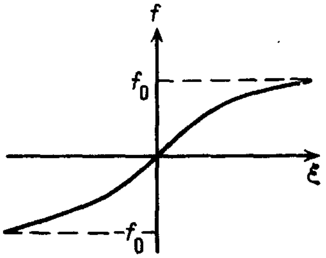

FIG. 3.

amplitude B and a size which agrees with (5) and (5a) in the case $\alpha = 0$. By virtue of condition (3), a soliton appears at the twinning boundary with a magnetic field distribution which is symmetric with respect to the twinning plane. To find the shape of the soliton, we need to supplement Maxwell's equation (2) with a constitutive equation which relates $j(x)$ to $B(x)$. The simplest way to close the system is to use a local approximation for the induction $B(x)$, namely $a = c\sqrt{2m_2\epsilon}/eB(x)$, in (7). This approximation gives us the induction distribution $B(x)$ in the soliton which is shown by curve 1 in Fig. 2(b). Note, however, that this way of closing the problem is not completely self-consistent. The reason is that the local approximation used in constructing a soliton is suitable if the length scale of the variations in $B(x)$ is much greater than r_L. Actually, it turns out that B varies over a distance on the order of r_L. This circumstance can be taken into account completely systematically in the semiclassical approximation. For this purpose it is convenient to put the equation in dimensionless form:

$$B(x) = B_0 f'(x/r_0), \tag{9}$$

where B_0 is the value of the induction at the center of the soliton, $r_0 = c\sqrt{2m_2\mu}/eB_0$, and $f(\zeta)$ is the vector potential in dimensionless variables. In a soliton, $f(\zeta)$ varies in a monotonic way between symmetric limits, from $-f_0$ to f_0 (Fig. 3). The function $f(\zeta)$ is conveniently written in differential form:

$$df/d\zeta = f_0^2 - f^2. \tag{9a}$$

The semiclassical spectrum of electrons and the analog of functional (7) for $j(f)$ can then be found explicitly. We can then find the shape of the soliton in a self-consistent way; see curve 2 in Fig. 2(b). The energy of this formation, as in (8), is lower than the energy of the system in the case $B(x) = 0$. A distinguishing feature of this soliton is that it exists at all temperatures, with the single restriction $T \ll \mu$. Furthermore, the amplitude of the induction B in this soliton is substantially larger than its values in bulk diamagnetic domains, by a factor $(c/v_F)^{1/3} > 1$, which would be ~ 5 in ordinary metals. From estimates (5) we find the amplitude of B to be 10^6–10^7 Oe, while r_L is ~ 100 Å. The diamagnetic soliton which we have constructed is not restricted to low temperatures, as we have already mentioned. However, as the temperature is lowered, the shape of this soliton changes, because at sufficiently low temperatures, $T \sim (2\pi^2)^{-1}\epsilon_F v_F/c$, the conditions for the de Haas-van Alphen effect for the magnetic field begin to hold in the volume, and this soliton induces near the twinning boundary a magnetic field distribution which varies with the temperature. This temperature can be several tens of degrees because of the large amplitude of B.

The effect which we have been discussing here could be observed directly by measuring the Knight shift, by the μSR method (cf. Refs. 2 and 3), or by a decoration method, which has been used successfully to observe a lattice of Abrikosov vortices in high-T_c superconductors.[5] The appearance of a spontaneous magnetic field causes changes in the properties of this system at the macroscopic level also. In the system as a whole, there is a breaking of time-reversal symmetry. This symmetry breaking gives rise to various macroscopic effects, similar to those which occur in systems lacking an inversion center.[6] In particular, Anderson's theorem is violated. There is the possibility that the exotic superconductivity predicted in Ref. 7 is stimulated.

We are indebted to the Scientific Council on the Problem of High-Temperature Superconductivity for support of this study, within the framework of Plan No. 174 of the State Program "High Temperature Superconductivity."

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Translated by Dave Parsons