

Kinematic localization of electronic states at the boundary of a bicrystal of an anisotropic metal

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The effect of the structure of a bicrystal of an anisotropic metal on the electron spectrum near a boundary is analyzed. It is predicted that discrete electronic states of a new type will exist at a twinning boundary. These states should lie in the conduction band.

Anomalous features have recently been found in a variety of physical properties in metal bicrystals, i.e., perfect crystals consisting of two single-crystal blocks.¹⁻³ One possible explanation for these anomalous features is the existence of particular features in the lattice properties and phonon spectra which arise at the boundary of bicrystals.

An alternative explanation is a change in the electron spectrum near the boundary of the bicrystal. In the present letter we work from elementary considerations to propose a new mechanism for the appearance of anomalous features in the electron spectrum near a bicrystal boundary. This new mechanism is of a general nature.

For an isotropic electron spectrum ($\epsilon = p^2/2m$), no particular features of any sort arise when electrons cross the bicrystal boundary. If the electron spectrum is anisotropic, the situation is radically different. In this case, some of the electrons are reflected because the conservation laws for the energy and for the quasimomentum component parallel to the boundary cannot be satisfied in other parts of the bicrystal. As a result, for a completely definite type of bicrystal boundary, specifically, a twinning plane (and only for it), discrete electronic levels arise. The primary distinguishing feature of these levels is that they lie entirely in the conduction band; they also contribute to the state density at the Fermi level.

For our study of the electron spectrum we assume a quadratic anisotropic dispersion law with masses m_1, m_2, m_3 along the principal crystallographic axes:

$$\hat{H} = -\frac{1}{2} \frac{\partial}{\partial x} \left(\frac{1}{m_{11}} \frac{\partial}{\partial x} \right) - \frac{1}{2} \left[\frac{\partial}{\partial x} \left(\frac{1}{m_{12}} \right) + \frac{1}{m_{12}} \frac{\partial}{\partial x} \right] \frac{\partial}{\partial y} - \frac{1}{2m_{22}} \frac{\partial^2}{\partial y^2} - \frac{1}{2m_3} \frac{\partial^2}{\partial z^2} \quad (1)$$

where x is the coordinate running normal to the surface of the bicrystal. The mass-tensor elements m_{ik}^{-1} are expressed in terms of m_1, m_2, m_3 as follows:

$$\begin{pmatrix} m_{11}^{-1} & m_{12}^{-1} \\ m_{21}^{-1} & m_{22}^{-1} \end{pmatrix} = \begin{pmatrix} m_1^{-1} \cos^2 \varphi + m_2^{-1} \sin^2 \varphi & (m_1^{-1} - m_2^{-1}) \sin \varphi \cos \varphi \\ (m_1^{-1} - m_2^{-1}) \sin \varphi \cos \varphi & m_1^{-1} \sin^2 \varphi + m_2^{-1} \cos^2 \varphi \end{pmatrix} \quad (2)$$

where $\varphi = \varphi(x)$ is the angle through which principal crystallographic axes 1 and 2 are rotated with respect to the spatial axes x and y . The angle $\varphi(x)$ is continuous at the bicrystal boundary, changing from the value φ_- in the left-hand half-space to the value of φ_+ in the right-hand half-space $\varphi_- \leq \varphi(x) \leq \varphi_+$ over a distance L which is characteristic of the change in the structure of the crystallographic axes near the boundary of the bicrystal from one single-crystal block to the other ($L \gg a$, where a is the distance between atoms). Since the variation of $\varphi(x)$ is smooth, we can use the effective-mass approximation in Hamiltonian (1). A particular case of a bicrystal is a twinned crystal, for which we have

$$\varphi_+ = -\varphi_- = \varphi_0. \quad (3)$$

To study the energy spectrum of Hamiltonian (1), we transform to Fourier components along the coordinates y and z along the surface of the bicrystal. We then perform a gauge transformation of the phase of the wave function $\psi(x)$:

$$\psi(x) = \tilde{\psi}(x) \exp \left\{ -ik_y \int_0^x dx' m_{11}(x') / m_{12}(x') \right\}.$$

In this case Hamiltonian (1) becomes

$$\hat{H} = -\frac{1}{2} \frac{d}{dx} \left(\frac{1}{m_{11}(x)} \frac{d}{dx} \right) + \frac{1}{2} \frac{m_{11}(x)}{m_1 m_2} k_y^2 + \frac{1}{2m_3} k_z^2, \quad (4)$$

where k_y and k_z are conserved components of the momentum along the surface of the bicrystal. The term with the kinetic energy $K(x) = (1/2)k_y^2 [m_{11}(x)/m_1 m_2]$ with the mass variable $m_{11}(x)$ is an effective potential energy $U(x)$ in which an electron moves. For an arbitrary bicrystal we have one of the three characteristic situations shown in Fig. 1 as plots of $U(x)$ and of the corresponding position of the Fermi surface in various spatial regions. When $|\varphi(x)|$ varies monotonically, $U(x)$ is as shown in Fig. 1a. If the momentum of the electron in the left-hand half-space exceeds k_{y0} ($|k_y| > k_{y0}$), it cannot penetrate into the right-hand half-space, since in the right-hand half-space there is no state with a momentum which would both conserve the energy and conserve the momentum components k_y and k_z along the bicrystal boundary. As a result, a potential barrier arises. This barrier is associated with the kinematics of the electron motion at the bicrystal boundary and is analogous in meaning to the centrifugal energy in a centrally symmetric field. This phenomenon is completely analogous to total internal reflection in optics. If $|\varphi(x)|$ instead varies in a nonmonotonic way, as it does, e.g., for the twinning plans [see Fig. (3)], then we will have either the situation shown in Fig. 1b or that in Fig. 1c, depending on the sign of the mass difference $m_1 - m_2$. If $m_1 < m_2$ (Fig. 1b), $U(x)$ is a potential well, and a discrete spectrum of electronic states arises because an electron with a momentum $|k_y| > k_{y0}$ cannot move off to either plus infinity or minus infinity. At a sharp boundary, with $L \sim a$, there will be a shallow symmetric well in which there is a single discrete level with a localization length much longer than the distance between atoms. If the boundary is instead gradual ($L \gg a$), the number of discrete levels increases to $\sim L/a$, and we can use the semiclassical approximation for an analysis of the spectrum. For a variable mass $m_{11}(x)$ the Bohr-Sommerfeld quantization rule gives us

$$\int \left[2m_{11}(x) \left(E_n - \frac{k_y^2}{2m_2} \frac{m_{11}(x)}{m_1} - \frac{k_z^2}{2m_3} \right) \right]^{1/2} dx = \pi(n + 1/2),$$

where the integration is carried out over the classically allowed region. The discrete

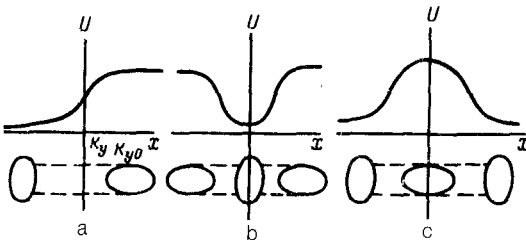


FIG. 1.

levels are found from the relation

$$E_n = \frac{k_y^2}{2m_2} (1 + \xi_n(k_y)) + \frac{k_z^2}{2m_3}, \quad (5)$$

where ξ_n satisfies the equation

$$\xi_n \int_0^1 dy \sqrt{1-y^2} \sqrt{1 + \xi_n y^2} = \frac{\pi}{2L} \frac{n+1/2}{|k_y|} (\rho m_2/m_1)^{1/2}.$$

The variable mass $m_{11}(x)$ differs from m_2 in a region of size L :

$$m_{11}(x) = m_1 [1 + \rho(x/L)^2], \quad |x| < L; \quad \rho = (m_2 - m_1)/m_1$$

In the limit of a weak anisotropy, $\rho \ll 1$, the spectrum is equidistant:

$$\xi_n = 2(n+1/2)(\rho m_2/m_1)^{1/2} / |k_y| L, \quad (5a)$$

and the distance between the levels in (5) is proportional to $|k_y|$. In the opposite limit, $\rho \gg 1$, which is characteristic of semimetals and semiconductors, the spectrum becomes nonequidistant:

$$\xi_n = \left(\frac{3\pi}{2L}\right)^{2/3} (n+1/2)^{2/3} |k_y|^{-2/3} (\rho m_2/m_1)^{1/3} \quad (5b)$$

Since the distance between the discrete levels in (5) depends smoothly on k_y , the state density of discrete levels, $\nu_d(E)$, has structural features only at the end points of the spectrum and at the Fermi level:

$$\nu_d(E) = \frac{S}{2\pi^2} L (2m_1 m_2 m_3 E)^{1/2} \alpha(\rho), \quad (6)$$

where E is the total energy of the electron, S is the area of the bicrystal boundary, and $\alpha(\rho)$ is a smooth function with $\alpha(\rho \rightarrow 0) = \rho^{1/2}$ and $\alpha(\infty) = 4/\pi$.

The number of levels below the Fermi surface is

$$N(\mu) = L(m_1 \mu \rho/2)^{1/2} \tilde{\alpha}(\rho); \quad \tilde{\alpha}(0) = 1, \quad \tilde{\alpha}(\infty) = 2/3\pi. \quad (7)$$

This analysis can be generalized to a nonquadratic anisotropic dispersion law. For metals with a Fermi surface which exceeds the Brillouin cell the electron spectrum is highly anisotropic, and there is a kinematic localization at twinning boundaries.

The structural features where the electrons cross the bicrystal boundary and the appearance of an effective potential $U(x)$ (Fig. 1) and of discrete spectrum lead to anomalies in the behavior of the system in a magnetic field and in the propagation of electromagnetic waves. In particular, because of the discrete levels, the magnetic susceptibility near the twinning boundary increases over a distance $\sim L$ to $\chi \sim \chi_0 N^2(\mu)$, where $\chi_0 \sim (v_F/c)^2$ is the diamagnetic susceptibility of the normal metal. Those anomalies which are observed experimentally specifically at twinning boundaries, not at

bicrystals of a general type,¹⁻³ may be due to the phenomenon described here.

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