Dislocations and localization effects in multivalley conductors

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In multivalley conductors with valleys that do not lie at the faces of the Brillouin zone, dislocations will disrupt the phase coherence and thereby prevent the localization of electrons. The corresponding contribution to the conductivity is estimated for the limiting cases of high and low dislocation densities.

The interference between two trajectories on which an electron moves in opposite directions and which return to the same point leads to a quantum correction to the conductivity which is a singular function of the temperature, the frequency, and the magnetic field.[1–3] Electrons undergo a common phase shift on these trajectories because of the symmetry under time reversal.

In multivalley semiconductors with long intervalley relaxation times $\tau_V \gg \tau_i$ (τ_i is the momentum relaxation time within a single valley), there is an approximate conservation of the particles in each valley. In this case, however, there is an identical phase shift in motion in opposite directions within a common valley only in the case of scattering by a static potential, in which the reference point for the momentum is inconsequential and can be shifted to the bottom of the band, so that the previous situation, with invariance under time reversal, can be restored.

This is not the case for arbitrary scatterers, and even purely elastic processes may disrupt the phase coherence within a single valley. In the present letter we show that dislocations in a crystal will cause an effect of this sort, and we estimate its magnitude. The Hamiltonian of an electron in a deformed crystal (see Ref. 4, for example) incorporates (1) the rising of the bottom of the valley, (2) corrections to the effective mass, and (3) a change in the position of the bottom of the valley in **k** space. The first effect corresponds to a scattering by a static potential, while the second is small by virtue of the assumed proximity of the momenta to the bottom of the valley. The most important effect is the third effect, where the dependence of the position of the bottom of the valley on the deformation serves in an obvious way as a vector potential. Below we assume a cubic symmetry, and we also assume that the vectors $\mathbf{k}^0$, which determine the positions of the bottom of the valley, have a symmetry axis of order higher than twofold. In this case the shift of the bottom of the valley due to the deformation is

$$k_n - k_n^0 = - w_{jn} k_j^0 + \gamma_1 (w_{nj} + w_{jn}) k_j^0 + \gamma_2 w_{jj} k_n^0 + \gamma_3 w_{jm} \frac{k_j^0 k_m^0}{(k^0)^2} k_n^0 , \qquad (1)$$

where $w_{jm} = (\partial u_j / \partial x_m)$ is the distortion tensor, and the phenomenological coefficients γ_i are on the order of 1. The first term describes the shift of the vector $\mathbf{k}^0$ for purely geometric reasons, while the last three terms describe a shift associated with a change in the interaction upon the deformation.[4] Guided by the qualitative results, we restrict the discussion to the case $\gamma_i = 0$, which corresponds to an exact analysis of screw dislocations parallel to $\mathbf{k}^0$ (in this case the coefficient of 1 in the first term must be replaced by $1 + \gamma_1$). In the effective-mass approximation, the Hamiltonian describing the interaction of the electrons with the dislocation is then

$$\hat{H} = \frac{1}{2m_\perp} \sum_{\mathbf{k}^0} (\hat{\mathbf{p}}_\perp - \mathbf{A}_\perp(\mathbf{k}^0))^2 + \frac{1}{2m_\parallel} \sum_{\mathbf{k}^0} (\hat{p}_\parallel - A_\parallel (\mathbf{k}^0))^2 + U(\mathbf{r}), \qquad (2)$$

$$A_j(\mathbf{k}^0) = - \mathbf{k}_n^0 w_{nj} \mathbf{k}_0 ,$$

where $\perp$ and $\parallel$ denote the components respectively perpendicular and parallel to $\mathbf{k}^0$, $U(\mathbf{r})$ is the potential created by impurities and dislocations, and the operator $\hat{p}_j$ represents the electron quasimomentum. Hamiltonian (2) is the same as the Hamiltonian of the "topological" interaction with dislocations.[5,6]

According to (2), the phase shift of an electron as it traverses a closed contour around a dislocation within a single valley depends on the direction of the motion and is determined by the circulation

$$\frac{\varphi_0(k^0)}{2} = \frac{1}{\hbar} \oint A_j (\mathbf{k}^0) dx_j = \frac{1}{\hbar} (k_j^0 b_j)(-1),$$

where b_j is the Burgers vector of the dislocation. The dislocation is therefore equivalent to a narrow solenoid with dimensions on the order of the inelastic center of the dislocation, where the effective "magnetic" field is concentrated (this point was noted in Ref. 7 for the case of screw dislocations). The "magnetic" flux in this solenoid is on the order of one quantum if $\mathbf{k}^0/\hbar$ is on the order of the size of the Brillouin zone.

A deviation of γ_i from zero in (1) leads to an analogous Hamiltonian, with the sole difference that the effective "magnetic field" exists everywhere not exclusively at the center of the dislocation. This distinction is of little importance for the discussion below. The quantum corrections to the conductivity break up into a contribution of diagrams with electron lines from one valley and a contribution of diagrams with electron lines from two valleys, of which the most important are the valleys with oppositely directed quasimomenta[3] (we are ignoring the electron-electron interaction). The relative contributions of these diagrams depend on the relation between the scale time for intervalley scattering and the scale time (τ_φ) for the loss of phase coherence due to inelastic processes.

Dislocations have little influence on the second of these contributions (because of its invariance under time reversal). The contribution of the single-valley diagrams to the conductivity depends strongly on the dislocations and is given by[3]

$$\delta\sigma_{ij}^{\mathrm{qu}} = -\frac{2e^2}{\pi\hbar}\sum_{\mathbf{k}^0} D_{ij}(\mathbf{k}_0)\tau_i C_{\mathbf{k}^0}(r,r), \tag{3}$$

where the cooperon $C_{\mathbf{k}^0}(r,r')$ obeys the equation

$$\left[\frac{1}{\tau_1} + D_\perp(\hat{\mathbf{p}}_\perp - 2A_\perp(k^0))^2 + D_\parallel(\hat{p}_\parallel - 2A_\parallel(k^0))^2\right] C_{\mathbf{k}^0}(r,r') = \frac{1}{\tau_i}\delta(\mathbf{r}-\mathbf{r}'). \tag{4}$$

Here $D_{ij}(k^0)$ is the diffusion tensor, and $1/\tau_1 = 1/\tau_v + 1/\tau_\varphi$. The distortion tensor in $A_j(\mathbf{k}^0)$ is determined by the sum of the deformations from the various dislocations, which we assume to be rectilinear, parallel, and distributed uniformly with a density N_D.

We begin with the case of a low dislocation density, in which we have $D_c N_D \sin\varphi_0(\mathbf{k}^0) \ll 1/\tau_1$, $(D_c^2 = D_\perp(D_\perp \cos^2\alpha(\mathbf{k}_0) + D_\parallel \sin^2\alpha(\mathbf{k}_0))$, and α is the angle between the direction of the dislocations and the vector $\mathbf{k}_0$. We assume that $\mathbf{k}^0/\hbar$ does not lie at the faces of the Brillouin zone, so that we have $\sin\varphi_0 \neq 0$. Deriving the correction to the cooperon for the presence of dislocations in the approximation linear in N_D reduces to a calculation of the Green's function in the Bohm-Aharonov effect and yields a conductivity correction

$$\Delta\sigma_{ij} = \frac{e^2}{2\pi\hbar} N_D \frac{\sqrt{\tau_1}}{D_a^{3/2}} \sum_{\mathbf{k}^0} D_c(\mathbf{k}^0) D_{ij}(\mathbf{k}_0) \frac{|\varphi_0(\mathbf{k}^0)|}{2\pi}\left(1 - \frac{|\varphi_0(\mathbf{k}^0)|}{2\pi}\right), \tag{5}$$

$$D_a = \sqrt[3]{D_\perp^2 D_\parallel}.$$

In the case of high density of dislocations, in which the phase coherence is disrupted primarily by dislocations, $D_c N_D \sin\varphi_0 \gg 1/\tau_1$, it is sufficient to replace τ_1 by $(D_c N_D)^{-1}$ (under the assumption $\sin\varphi_0 \sim 1$) in the expression for the single-valley cooperon, $C_{k^0}^0$, in order to find an estimate (by analogy with the case of a strong magnetic field[3]). We find

$$\delta\sigma_{ij}^{\mathrm{qu}} = \frac{e^2\sqrt{N_D}}{2\pi^2\hbar D_a^{3/2}} \sum_{\mathbf{k}^0} \sqrt{D_c(\mathbf{k}^0)}\, D_{ij}(\mathbf{k}^0). \tag{6}$$

The scattering by dislocations also changes the mean free path, giving rise to a correction to the conductivity $\Delta\sigma_1 \approx -(e^2/\hbar)n^{2/3}l^2 N_D\lambda$ (n is the density of electrons, l the mean free path, and λ the thickness of the dislocation).

It can be seen from expressions (5) and (6) that the quantum corrections may change the sign of the resultant contribution of dislocations to the conductivity. Using the characteristic values $n = 10^{18}$ cm^{-3}, $l = 10^{-5}$ cm, $N_D = 10^8$ cm^{-2}, $\lambda = 10^{-7}$ cm, and assuming $D_c N_D > 1/\tau_1$, we find the ratio $\Delta\sigma_1/\delta\sigma^{\mathrm{qu}} = -0.1$. We thus see that the quantum corrections for dislocations may be larger than the direct contribution to the mean free path. We also note that dislocations, like a magnetic field, prevent localization effects.

The same effect could occur at the surface of the crystal, where dislocations emerging at the surface from the interior could prevent the localization of corresponding two-dimensional electrons, under analogous assumptions regarding the multivalley spectrum.

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