Influence of electron-electron drag on piezoresistance of $n$-Si

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Abstract. Piezoresistance of $n$-Si is considered with due regard for inter-valley drag. It has been shown that inter-valley drag gains the piezocoefficient and diminishes the mobility. In the region of nondegenerate carriers, the effect of drag increases when the carrier concentration rises and temperature falls.

Keywords: silicon, balance equation, mobility, piezoresistance, inter-valley drag.

1. Introduction

In crystals with one and only simple band, the electron-electron scattering does not change the total momentum of carriers and therefore does not give a direct, independent contribution to the conductivity. Quite another situation we have for crystals with a composite band structure. There the conductivity of crystal can be essentially influenced by mutual drag of carriers that belong to different partial bands or valleys (see Refs. [1, 2]). In particular, the inter-valley drag can sufficiently diminish the electron mobility of $n$-Si and $n$-Ge at low temperatures. The reason of that is a principal difference between scattering of band electrons from some valley on fixed charged impurities or equilibrium phonons and scattering on nonequilibrium electrons from another valley, where divergence of equilibrium differs. Now, we have some right to hope that the inter-valley drag in multy-valley semiconductors can noticeably influence not only conductivity but piezoresistance as well. In this article, we again will pay the main attention to the region of low temperatures where Coulomb scattering is not damped by collisions of electrons with phonons. We restrict here our calculations by charged impurities and acoustic phonons as an external scattering system.

2. Balance equations

In Refs [1, 2], the set of balance equations obtained as a first momentum of quantum kinetic equations was presented:

$$
e E^{(a)} + \sum_{b=1}^{6} E^{(a,b)} = 0 \quad (a = 1, 2, \ldots, 6).$$  (1)

Here, the symbol $a$ numerates different valleys; $E^{(a)}$ is the applied electric field; the resistant force

$$E^{(a)} = -\frac{e^2}{(2\pi)^6 n} \int d^3k \int d^3\bar{q} \int d^3\bar{q}' \times$$

$$\times \int d\omega \delta(\hbar\omega - \varepsilon_k^{(a)} + \varepsilon_{k-\bar{q}}^{(a)} - \varepsilon_{k-\bar{q}'}^{(a)} + \varepsilon_{k-\bar{q}}^{(b)} + \varepsilon_{k-\bar{q}'}^{(b)}) \left[ f_k^{(a)} - f_{k-\bar{q}}^{(a)} + \frac{1}{2} (1 - f_k^{(a)}) + \frac{1}{2} (1 - f_{k-\bar{q}}^{(a)}) + f_{k-\bar{q}'}^{(a)} (1 - f_k^{(a)}) \right] \left[ \langle \varphi_1 \rangle_{\omega, \bar{q}} + \langle \varphi_{1(\text{ph})} \rangle_{\omega, \bar{q}} \right]$$  (2)

relates to interaction between drifting carriers from $a$- and $b$-valleys.

$$Y_{ab}(\bar{k}, \bar{k}', \bar{q}) = f_{\bar{k}}^{(a)} (1 - f_{\bar{k}}^{(b)}) f_{\bar{k}-\bar{q}'}^{(b)} (1 - f_{\bar{k}-\bar{q}}^{(b)})$$  (3)

relates to interaction between drifting carriers from $a$- and $b$-valleys.

Here, $n^{(a)}$ and $\varepsilon_k^{(a)}$ are the concentration and dispersion law for electrons from $a$-valley. For undeformed crystal of $n$-Si, we have (see Fig. 1):
\[ \varepsilon_k^{(a)} = \frac{h^2}{2} \left( \frac{k_x^2}{m_{xx}^{(a)}} + \frac{k_y^2}{m_{yy}^{(a)}} + \frac{k_z^2}{m_{zz}^{(a)}} \right). \] (4)

For two valleys \((a = 1, 4)\) \(m_{zz} = m_{xx} = m_{yy} = m_{\perp}\); for two valleys \((a = 2, 5)\) \(m_{xx} = m_{yy} = m_{\perp}\); and for two valleys \((a = 3, 6)\) \(m_{xy} = m_{\perp}\), \(m_{xx} = m_{zz} = m_{\perp}\). Therefore,

\[
\varepsilon_k^{(1,4)} = \frac{h^2}{2} \left( \frac{k_x^2 + k_y^2 + k_z^2}{m_{\perp}} \right); \quad \varepsilon_k^{(2,5)} = \frac{2}{2} \left( \frac{k_x^2 + k_y^2 + k_z^2}{m_{\perp}} \right); \quad \varepsilon_k^{(3,6)} = \frac{2}{2} \left( \frac{k_x^2 + k_y^2 + k_z^2}{m_{\perp}} \right).
\] (5)

The screening dielectric function for quasi-elastic collisions possesses the form

\[
\varepsilon(\omega, \mathbf{q}) = \varepsilon_L + \Delta \varepsilon(\omega = 0, \mathbf{q}),
\]

where \(\varepsilon_L\) is the dielectric constant of crystal lattice and \(\Delta \varepsilon(\omega = 0, \mathbf{q})\) is the contribution of band electrons to the total dielectric function. For convenience, we will use the following form:

\[
\Delta \varepsilon(0, \mathbf{q}) = \varepsilon_L q_0^2(\mathbf{q}) / q^2.
\]

Then,

\[
\langle \hat{\Phi}_{(t)}^2 \rangle_{\omega, \mathbf{q}} = \frac{32\pi^3 e^2 n_f}{\varepsilon_L [q^2 + q_0^2(\mathbf{q})]^2} \delta(\omega).
\]

\[
\langle \delta \Phi_{(ph)}^2 \rangle_{\omega, \mathbf{q}} = \varepsilon_D^2 \frac{2\pi^3 k_B^2 T}{e^2 \rho \delta^2} \delta(\omega).
\] (6)

Here, \(n_f\) is the concentration of charged impurities; \(\varepsilon_D = \varepsilon_d + (1/2)\varepsilon_u\), where \(\varepsilon_d\) and \(\varepsilon_u\) are dilation and shear deformation potential constants (see, for example, Refs. [6] and [7]). The form (7) corresponds to the approximation of quasi-elastic collisions.

The screening plays a significant, even appointing role in the area of small transferred vectors \(\mathbf{q}\); therefore, instead of \(q_0^2(\mathbf{q})\), we can use the following approximate expression (see Ref. [1]):

\[
q_0^2(\mathbf{q}) \rightarrow q_0^2(0) = \frac{12 e^2 m^{3/2} k_B^2 T}{h^3 L \sqrt{\pi \varepsilon_L}} F_{-1/2}(\eta). \] (7)

Here, the Fermi-integral

\[
F_\eta(\eta) = \frac{1}{\Gamma(r+1)} \int_0^\infty w^r dw.
\] (8)

\[
L = m_{\perp} / m_{\perp}, \quad \Gamma = \text{the gamma-function}, \quad \eta = \varepsilon_F / k_B T
\]

is the dimensionless Fermi-energy. The form (7) is valid for deformed crystal, if one uses linear approximation over deformation. For nondegenerate carriers

\[
q_0^2(0) = \frac{4\pi e^2 n}{\varepsilon_L k_B^2 T}.
\] (9)

To calculate drift velocities \(\mathbf{u}(\mathbf{q})\) of electrons from \(a\)-group, we accept the model of non-equilibrium distribution functions as Fermi functions with the argument containing shift of velocity \(\mathbf{v}(\mathbf{k}) = h^{-1}(\partial \varepsilon(\mathbf{k}) / \partial \mathbf{k})\) by the correspondent velocity \(\mathbf{v}_k(\mathbf{q})\):\n
\[
f_k(\mathbf{q}) = f^{0(\mathbf{q})}(\mathbf{v}_k(\mathbf{q}) - \mathbf{u}(\mathbf{q})), \quad (a = 1, 2, \ldots, 6). \] (10)

Here, \(f^{0(\mathbf{q})}(\mathbf{v}(\mathbf{q})) = f^{0(\mathbf{q})}(\mathbf{e})\) is the equilibrium distribution function for \(a\)-carriers. Drift velocities \(\mathbf{u}(\mathbf{q})\) are proportional to partial densities of currents \(j_q(\mathbf{q})\):

\[
\mathbf{u}(\mathbf{q}) = \frac{1}{e n(\mathbf{q})} j_q(\mathbf{q}). \] (11)

Here, \(n(\mathbf{q})\) is the concentration of electrons in the \(a\)-valley. The density of total current:

\[
j = \sum_{a=1}^6 j_q(\mathbf{q}). \] (12)

Using the forms (10) and carrying out linearization of forces in Eqs. (2) and (3) over drift velocities, we obtain:

\[
F_{\eta}(\mathbf{u}) = -e \beta(\mathbf{q}) \mathbf{u}(\mathbf{q}) ;
\]

\[
F_{\eta}(\mathbf{u}, \mathbf{v}) = -e \rho(\mathbf{q}, \mathbf{u}) \mathbf{u}(\mathbf{q}) - \mathbf{u}(\mathbf{q}). \] (13)

Here, components of tensors \(\beta(\mathbf{q})\) and \(\rho(\mathbf{q}, \mathbf{u})\) are (see [2, 3] and Eqs. (6) and (7)):

\[
\beta_{uv}(\mathbf{q}) = \chi_{uv}(\mathbf{q}) ; \quad \rho_{uv}(\mathbf{q}, \mathbf{u}) = \frac{3}{2(2\pi)^3 e n(\mathbf{q}) k_B T} \int d\mathbf{v} \times
\]

\[ \times \left[ \frac{q^2 d^3 \mathbf{q}}{\sinh \left[ (h_0 / k_B T) \right] \mathbf{q} \cdot \mathbf{u} \cdot \mathbf{v}} \right] q \cdot \mathbf{u} \cdot \mathbf{v} \cdot \mathbf{u} = \frac{e n_f}{2\pi^3 \rho \varepsilon_L} \int \left[ \frac{\left| \text{Im} \Delta \varepsilon(\mathbf{k}) / \mathbf{q} \cdot \mathbf{u} \cdot \mathbf{v} \right|}{q^2 + q_0^2(\mathbf{q})} \right] d^3 \mathbf{q}. \] (15)
\[\chi_{\omega}^{(a)} = \frac{\hbar}{2(2\pi)^3 n^{a0} k_B T} \int d\omega \times \]
\[\times \int \frac{q^2 d^3 q}{\sinh(h\omega/k_B T)} q_a q_l \text{Im} \Delta(\omega) \left(\begin{array}{c} q^2 \end{array}\right) = \]
\[\Xi^2 k_B T \frac{32\pi n^a}{e^2 n^{a0} k_B T} \int \frac{d\omega}{\sinh(h\omega/k_B T)} \times \]
\[\times \int \frac{q^2 d^3 q}{\left[q^2 + q^2_0(\omega)\right]^2} \text{Im} \Delta(\omega) \left(\begin{array}{c} q^2 \end{array}\right) \]
\[\lambda(\omega) = \frac{2\pi^2 m_1 m_2/3}{\gamma} \frac{q^2_0 q_l q_a}{\left[q^2 + q^2_0(\omega)\right]} d^3 q, \]
\[[1 + \exp\left\{\frac{\hbar^2}{8k_B T} \left(q^2_0 q_l q_a + q^2_0(\omega) - \eta_a\right)\right\}]^{-1} \]}
\[\lambda^{(a)}(\omega) = \frac{\eta_a}{2\pi^2 n^{a0} \epsilon^{l}} \int \lambda(\omega) d^3 q, \]
\[\lambda^{(a)} \left(\begin{array}{c} q^2 \end{array}\right) q_a^2 q_l d^3 q, \]
\[\gamma = \int \frac{w^2 dw}{\sinh^2 w} \approx 3.29. \]
\[\text{Note that} \]
\[n^{(a)}(a,b) = n^{(b)}(a,b) \]
\[\sum_{a=1}^{6} n^{(a)} = n_f = n \sum_{a=1}^{6} n^{(a)}. \]
\[\sum_{a=1}^{6} n^{(a)} = n = \frac{3 (2\pi k_B T)^{3/2} m_1^{1/2}}{2\pi^2 \hbar^3 L} F_{1/2}(\eta). \]

3. Populations of valleys in deformed crystal

Let a silicon crystal is mechanically compressed along the axis [001] (see Fig. 1), then the components of stress tensor are
\[X_{ab} = -\delta_{ab} \delta_{ac} X \] (here \(X > 0\)).

For this situation, the dispersion law for different valleys can be written in the following form (see Ref. [4]):
\[\varepsilon_{k}^{(a)}(X) = \varepsilon_{k}^{(a)}(X = 0) + \Delta \varepsilon^{(a)}(X) = \varepsilon_{k}^{(a)} + \Delta \varepsilon^{(a)}(X) \]
\[(a = 1, 2, \ldots, 6), \]
\[\Delta \varepsilon^{(a)}(X) = \frac{2}{3} \Xi u (s_{11} - s_{12}) X, \]
\[\Delta \varepsilon^{(a)}(X) = \frac{2}{3} \Xi u (s_{11} - s_{12}) X, \]
\[\Xi u \] is the shear deformation potential, \(s_{11}\) and \(s_{12}\) are the elastic constants.

The density of carriers in the \(a\)-valley is
\[n^{(a)}(X) = \frac{d^3 k}{4\pi^3} f_{0}^{(a)}(\varepsilon_{k}^{(a)}(X)) = \]
\[= \int \frac{d^3 k}{4\pi^3} f_{0}^{(a)}(\varepsilon_{k}^{(a)}(X)) = \]
\[\frac{1 + \exp\left[\varepsilon_{k}^{(a)}(X)/k_B T - \eta_a\right]}{1 + \exp\left(\varepsilon_{k}^{(a)} + \Delta \varepsilon^{(a)}(X)/k_B T - \eta_a\right)} \]
\[\sum_{a=1}^{6} n^{(a)}(X) = \frac{3 (2\pi k_B T)^{3/2} m_1^{1/2}}{2\pi^2 \hbar^3 L} F_{1/2}(\eta). \]

4. Kinetic coefficients for deformed silicon crystal

Consider the case when the electric field is applied along some fourfold \(l\)-axis, that is
\[\bar{E} - \bar{B}^{(a)} u^{(a)} - \sum_{b=1}^{6} \bar{z}^{(a,b)} (u^{(a)} - u^{(b)}) = 0 \]
\[(a = 1, 2, \ldots, 6). \]
Then, only \( l \)-components of drift velocities \( \vec{u}^{(a)} \) and diagonal components of the tensors \( \vec{\beta}^{(a)} \) and \( \vec{\xi}^{(a,b)} \) are distinct of zero (in the coordinate system related to fourfold axes), and then one can write the system of equations corresponding to the system (24) in the form
\[
E_l - \beta^{(a)}_{ll}(X)u^{(a)}_l = \sum_{b=1}^{6} \xi^{(a,b)}_{ll}(X)(\eta^{(a)}_l - u^{(b)}_l) = 0
\]
\((a = 1, 2, \ldots, 6)\).

Here, the expressions for \( \beta^{(a)}_{ll}(X) \) and \( \xi^{(a,b)}_{ll}(X) \) have the forms (14), (18)-(21) where the dimensionless Fermi energy \( \eta_a \) in the formulae (18) is shifted in the following manner:
\[
\eta_a \rightarrow \eta - \Delta \epsilon^{(a)}(X) \frac{k_B T}{\epsilon_0}.
\]

Below we assume the deformation to be small and linearize all the expressions over the stress \( X \).

In this paper, we consider only nondegenerate gas (see Fig. 2; there the solid line corresponds to the relation \( \epsilon_p(n, T) = 0 \)). Then, it follows from symmetry of the considered system for carriers:
\[
n^{(a)}(X) = (n/6) C_a(X); \quad C_4(X) = C_1(X); \quad C_3(X) = C_2(X) = C_6(X) = \frac{C_2(X)}{2},
\]
where (see Eqs. (29), (30))
\[
C_1(X) = 1 + \frac{2}{3k_B T} \Xi_n(s_{11} - s_{12})X; \quad C_2(X) = 1 - \frac{1}{3k_B T} \Xi_n(s_{11} - s_{12})X.
\]

Note that \( C_1(X) + 2C_2(X) = 3 \).

Also it follows:
\[
\beta^{(a)}_{ll}(X) = \beta^{(a)}_{ll}(X = 0) ; \quad \xi^{(a,b)}_{ll}(X = 0) = \xi^{(a,b)}_{ll}(X = 0) C_b(X).
\]

Consider now the case when the electric field is applied along \( z \)-axis, that is \( \vec{E} = E \hat{z} \).

Then, only \( z \)-components of drift velocities \( u^{(a)}_z \) and \( \xi^{(a,b)}_{zz} \) components of the tensors \( \beta^{(a)}_z \) and \( \xi^{(a,b)}_{zz} \) are distinct of zero, and one can write Eqs. (32) in the form
\[
E_z - \beta_a z^{(a)} u_z^{(a)} - \sum_{b=1}^{6} \xi^{(a,b)}_{zz}(X)(\eta^{(a)} - u_z^{(b)}) = 0
\]
\((a = 1, 2, \ldots, 6)\).

Here, \( \beta_a z = \beta^{(a)}_{zz}(X = 0) ; \quad \xi^{(a,b)}_{zz}(X = 0) = \xi^{(a,b)}_{zz}(X = 0). \)

It is evident that
\[
\xi^{(a,b)}_{zz}(X = 0) = \xi^{(a,b)}_{zz}(X = 0) \frac{\beta^2_{zz} + 2\xi^2_{zz} \beta^2_{zz} + 2\eta \xi_{zz}}{\beta^2_{zz} + 2\xi^2_{zz} \beta^2_{zz} + 2\eta \xi_{zz}}.
\]

One can write the resulting expression for total conductivity of deformed crystal in the following form:
\[
\sigma_{zz}(X; \xi) = \sigma_{zz}(X; \xi) = \frac{\sigma_{zz}(X; \xi)}{\Xi_n(s_{11} - s_{12})X} = \frac{\sigma_{zz}(X; \xi)}{\Xi_n(s_{11} - s_{12})X} \frac{\beta^2_{zz} + \beta^2_{zz} + 18\xi}{\beta^2_{zz} + \beta^2_{zz} + 18\xi}.
\]

Let us define the piezoresistance coefficient \( \pi_{kk}(\xi) \) by using the expression (see Refs. [5, 6])
\[
\pi_{kk}(\xi) = -\frac{1}{\sigma_{kk}(0; \xi)} \frac{d\sigma_{kk}(X; \xi)}{dX} \bigg|_{X=0}.
\]

If we direct the electrical field \( \vec{E} \) along \( x \)- and \( y \)-axes, for the case (25) we will obtain the relation
\[
\pi_{zz}(\xi) = -2\pi_{xx}(\xi) = -2\pi_{yy}(\xi).
\]

To investigate the dependence of conductivity and piezoresistance coefficient on the parameter of intervalley drag, we use the following formulae obtained from the Eqs. (35), (42), (43):
\[
\sigma_{zz}(0; \xi) = \mu(\xi) = \frac{\beta^2_{zz}(2\beta^2_{zz} + 2\xi^2_{zz} + 2\xi_{zz})}{(\beta^2_{zz} + 2\xi^2_{zz})(\beta^2_{zz} + 2\xi_{zz})};
\]
\[
\sigma_{zz}(0; \xi) = \mu(\xi) = \frac{\beta^2_{zz}(2\beta^2_{zz} + 2\xi^2_{zz} + 2\xi_{zz})}{(\beta^2_{zz} + 2\xi^2_{zz})(\beta^2_{zz} + 2\xi_{zz})};
\]
\[
\pi_{zz}(0; \xi) = \frac{\Xi_n(s_{11} - s_{12})}{3(\beta^2_{zz} + 2\xi^2_{zz})}(2\beta^2_{zz} - \beta^2_{zz});
\]
\[
\pi_{zz}(0; \xi) = \frac{\Xi_n(s_{11} - s_{12})}{3(\beta^2_{zz} + 2\xi^2_{zz})}(2\beta^2_{zz} - \beta^2_{zz});
\]
5. Results of numerical calculations

These results are shown in Figs 3 to 5. Here, Figs 3(a, b, c) show the absolute value of piezoresistance coefficients. In calculations, we use the following data (see Refs. [5, 6]):

\[ m_0 = 9.1066 \times 10^{-28} \text{g}, \]
\[ m_l = 8.342 \times 10^{-28} \text{g}; \]
\[ M = 6; \]
\[ L = 4.8; \]
\[ \varepsilon_L = 12; \]
\[ \Delta \varepsilon_s = 0.916; \]
\[ s_{11} - s_{12} = 9.82 \times 10^{-12} \text{Pa}^{-1}; \]
\[ \Xi_u = 8.6 \text{eV}; \]
\[ \varepsilon = 12, \]
\[ \rho s^2 = 1.66 \times 10^{10} \text{Pa}, \]
\[ \Xi = \Xi_u + (1/2)\Xi_s = -4.2 \text{eV}. \]

In Figs (a), (b), (c), solid lines represent the piezoresistance coefficient for crystal where band carriers are involved in drag. The dashed lines correspond to the calculations when inter-valley drag is ignored.

Figs 4 and 5 represent relative values. One can see that inter-valley drag gains the piezocoefficient and diminishes the mobility. Within the region of nondegenerate carriers, the drag effect becomes more pronounced when the carrier concentration grows and temperature falls.

References