Scattering of Carriers by Charged Dislocations in Semiconductors

Bhavtosh Bansal*, V. Venkataraman
Department of Physics, Indian Institute of Science, Bangalore 560 012, India
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The scattering of carriers by charged dislocations in semiconductors is examined within the framework of the Boltzmann transport theory. The ratios of quantum and transport scattering times are evaluated after averaging over the anisotropy in the relaxation time. A new approximate expression for the carrier mobility is proposed and the value of the Hall scattering factor is computed. Change in the resistivity when the dislocations are tilted with respect to the plane of transport is determined. Finally an expression for the relaxation time is derived when the dislocations are located within the sample with a uniform angular distribution.

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I. INTRODUCTION

Epitaxial growth of thin semiconductor films on substrates which have a large lattice constant mismatch results in the films being strained. Depending on the growth conditions and the films' thickness, this strain can either partially or fully relax through a formation of various possible kinds of lattice defects. Among these defects edge dislocations are prominent and have a pronounced effect on the mobility of carriers. While the theory for charged dislocation scattering was first formulated to explain the low temperature mobility of plastically deformed semiconductors[1], interest in dislocation scattering has revived in context of GaN [2, 3, 4, 5, 6, 7, 8]. Indeed it is important in all epitaxially grown materials [9] on mismatched substrates, as well as bulk crystals whose growth techniques have not yet been mastered [10].

An edge dislocation is a row of dangling bonds formed by an abruptly terminated plane somewhere inside the crystal[2]. This local departure from tetragonal coordination produces acceptor states in the energy gap, forming one dimensional lines of charge. The effective screened electrostatic potential energy, $U(x_\perp)$ is thus cylindrically symmetric if the extent of the edge dislocation is taken to be infinite[11, 12].

$$U(x_\perp) = \frac{Qe}{2\pi\epsilon} K_0(x_\perp/\lambda) \tag{1}$$

where Q is the charge per unit length, K_0 is the modified zeroth order Bessel function of the second kind, $\epsilon = \epsilon_0\epsilon_r$ is the dielectric constant, λ is the screening length and $x_\perp$ is the distance from the dislocation line in a perpendicular plane, $\mathbf{r} = f(x_\perp, \theta, z)$. These one dimensional lines of charge have detrimental effects on the transport properties of charge carriers.

*Present Address: Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai- 400005, India, Electronic Mail: bhavtosh@tifr.res.in

II. ISSUES ADDRESSED

(i) The scattering potential, due to its cylindrical symmetry, is highly anisotropic and the validity of the extension of the relaxation time approach to this problem has been questioned[2, 7, 13].
(ii) Pödör's [1] expression for the relaxation time

$$\tau = \frac{8\epsilon^2\, m^{*2}}{N_d e^2 Q^2 \lambda} \left(\frac{\hbar^2}{4m^{*2}\lambda^2} + v_\perp^2\right)^{3/2} \tag{2}$$

is *apparently* physically incorrect. $v_\perp$ is the component of electron velocity perpendicular to the dislocation axis and N_d is the number of dislocations per unit area, all assumed to be parallel and independent. Only the perpendicular component of the impinging electron's velocity contributes to scattering and the component parallel to the dislocation is unaffected. Equation 2 is finite when $v_\perp \to 0$, whereas in this limit, τ should diverge.
(iii) The method of energy averaging employed by Pödör has been questioned[4].
(iv) Due to (iii), the tensor nature of resistivity is not evident in the final expression. In particular if the dislocations are tilted at an angle with respect to the direction perpendicular to the plane of transport, it is difficult to give anything better than a rough estimate[8] in the present theory. Most often, the effect of dislocation orientation is disregarded and $\mu_\perp$ is replaced by a scalar number.
(v) Quantum and classical scattering times were calculated[14] without averaging out the anisotropy in the problem.
(vi) There are corrections to the measured Hall mobility due to the Hall scattering factor.
(vii)In general, dislocations may not be all parallel.

Points (i) and (ii) above were what led us to the reexamination of this problem. Nevertheless, a first principles treatment of the calculations shows that Pödör's 40-year old formula is indeed correct. The reasons for the apparent discrepancy are traced to the limits where the solution of the Boltzmann equation is invalid. This is discussed in the next section.

III. THEORETICAL FORMULATION

We start from the Boltzmann equation within the linear response regime[15]. Then upto first order in electric field, the perturbed distribution function may symbolically be written as $f_{\mathbf{k}} = f_{0k} + \phi_{\mathbf{k}}$, where $\phi_{\mathbf{k}}$ is deviation from an equilibrium distribution in presence of a perturbing external electric field $\mathbf{F}$. In absence of a thermal gradient and a magnetic field, the linearized Boltzmann equation for carriers described by spherical parabolic band reduces to

$$\frac{e\hbar}{m^*}\mathbf{F}\cdot\mathbf{k}\frac{\partial f_{0k}}{\partial E} = \sum_{\mathbf{k}'} W_{\mathbf{k}',\mathbf{k}}[\phi_{\mathbf{k}'} - \phi_{\mathbf{k}}] \tag{3}$$

$W_{\mathbf{k},\mathbf{k}'}$ is the transition rate between initial and final plane wave states, $\mathbf{k}$ and $\mathbf{k}'$, in presence of the scattering potential given by equation (1). For scattering from charged dislocations, the scattering rate is given by $W_{\mathbf{k},\mathbf{k}'} = \delta(k_z - k'_z)\delta(k - k')g(|\mathbf{k}'_\perp - \mathbf{k}_\perp|)$. $g(|\mathbf{k}'_\perp - \mathbf{k}_\perp|)$ is the part depending on only a function of in-plane momenta (shown below). Thus (a) collisions are elastic, (b) the components of the incident electron's momenta which are parallel and perpendicular to the dislocation line are separately conserved, (c) no electric field develops along the dislocation axis, i.e. $\mathbf{F}\cdot\mathbf{k} = \mathbf{F}_\perp\cdot\mathbf{k}_\perp$. This immediately implies that no relaxation time can be defined along the direction parallel to the dislocations' axis. In other words, for time independent electric field, there is no steady state solution to the Boltzmann equation if the collision term is zero. Nevertheless, one may physically argue that $1/\tau_z = 0$. The argument is clear within the variational formalism[15] where one defines the sample resistivity in terms of the Joule-heat dissipated due to a finite current. With constraints (a)-(c) in mind, we shall choose a $\phi_{\mathbf{k}}$ which solves the Boltzmann's equation *exactly*. Ansatz:

$$\phi_{\mathbf{k}} = -\frac{e\hbar}{m^*}\tau(k,k_\perp)\mathbf{F}_\perp\cdot\mathbf{k}_\perp\frac{\partial f_k}{\partial E} \tag{4}$$

Substituting $\phi_{\mathbf{k}}$ in equation(3) yields

$$\frac{\partial f_{0k}}{\partial E}\mathbf{F}_\perp\cdot\mathbf{k}_\perp = \mathbf{F}_\perp\cdot\sum_{\mathbf{k}'} W_{\mathbf{k},\mathbf{k}'} \times\left[\frac{\partial f_{0k'}}{\partial E}\tau(k',k'_\perp)\mathbf{k}'_\perp - \frac{\partial f_{0k}}{\partial E}\tau(k,k_\perp)\mathbf{k}_\perp\right] \tag{5}$$

From energy and perpendicular momentum conservation,

$$\frac{\partial f_{0k'}}{\partial E}\tau(k',k'_\perp) = \frac{\partial f_{0k}}{\partial E}\tau(k,k_\perp). \tag{6}$$

Thus the linearized Boltzmann equation is exactly solved if

$$\frac{1}{\tau(k,k_\perp)} = \sum_{\mathbf{k}'} W_{\mathbf{k},\mathbf{k}'}(1 - cos\,\theta) \tag{7}$$

Here θ is the angle between $\mathbf{k}_\perp, \mathbf{k}'_\perp$ which lie on a circle parallel to the xy-plane since k_z is independently conserved. The wave vectors in the summation in equation (7) are three dimensional.

Within the Born approximation

$$W_{\mathbf{k},\mathbf{k}'} = \frac{2\pi}{\hbar}[L_z\delta_{k_z,k'_z}]^2\delta(E_k - E_{k'}) \times\left[\frac{1}{L_xL_yL_z}\int d\mathbf{x}_\perp U(x_\perp)e^{i(\mathbf{k}_\perp - \mathbf{k}'_\perp)\cdot\mathbf{x}_\perp}\right]^2 \tag{8}$$

Here L_z, L_y and L_x are the crystal dimensions over which the plane wave electron states are normalized and the length of the 'infinite' dislocation has been limited to the size of the crystal along the z direction. The energy conserving delta function, $\delta(E_k - E_{k'}) = (\partial E/\partial k)^{-1}\delta(k - k') = (\hbar k/m^*)^{-1}(k/k_\perp)\delta(k_\perp - k'_\perp)$ due to δ_{k_z,k'_z} in the summation. Thus, as previously claimed, both the perpendicular and the parallel components of the electron momenta are separately conserved. Since, $\Sigma_{\mathbf{k}'_\perp} \to L_xL_y/(2\pi)^2\int d\mathbf{k}'_\perp$, an overall factor of area remains in the denominator after the primed momenta have been integrated over. This simply means that the scattering due to a single charged dislocation is ineffective in a large sample.[16] When there are many charged dislocations within this area which are all parallel, one can simply replace $(L_xL_y)^{-1}$ by N_d the dislocation density per unit area if the interference terms can be neglected. The Fourier transform in equation (8) can be approximately written as [4]

$$U(|\mathbf{k}'_\perp - \mathbf{k}_\perp|) \simeq \frac{Qe\lambda^2}{\epsilon(1 + |\mathbf{k}'_\perp - \mathbf{k}_\perp|^2\lambda^2)} \tag{9}$$

IV. RESULTS

A. Transport Lifetime

From equation(7), the relaxation time in the direction perpendicular to the dislocation axis is

$$\tau_\perp(k,k_\perp) = \frac{\hbar^3\epsilon^2}{Q^2e^2\lambda^4m^*N_d}[1 + (2k_\perp\lambda)^2]^{3/2} = \tau_\perp(k_\perp) \tag{10}$$

This is exactly what Pödör had derived (equation (2)) and $k_\perp = 0$ implies a finite $\tau_\perp$ even after our rederivation. While in three dimensions an electron with $k = 0$ is unphysical (there is no associated phase space), an electron with $k_\perp = 0$ and $k_z \neq 0$ corresponds to a physical situation. The inconsistency in the final formula results from the breakdown of the validity of the assumed solution, $\phi_{\mathbf{k}} = 0$ for $k_\perp = 0$ in equation (4). This condition is outside the scope of the present scheme of the solution, which is otherwise consistent.

The anisotropy in τ necessitates a further angular averaging for a comparison with any physical quantity associated with a measurement which involves a thermodynamic distribution of electrons. This transport scattering

time is directly connected to mobility, $\mu = (e/m)\langle\langle\tau\rangle\rangle$, where $\langle\langle\rangle\rangle$ denote an *energy* average, (see below) over a distribution function of appropriate degeneracy. In a fully degenerate system, using equation (13), this simplifies to $\langle\langle\tau_{tr}\rangle\rangle = (3/4)\int_0^\pi \sin^3\theta\tau_\perp\, d\theta$.

B. Quantum Scattering Time

A quantum scattering time, $\tau_\perp^q(k_\perp)$ is, by definition, equation (7), but without the $(1-\cos\theta)$ factor and may be calculated similarly. This was recently done by Jena and Mishra[14].

$$\tau_\perp^q(k_\perp) = \frac{\hbar^3\epsilon^2}{Q^2e^2\lambda^4m^*N_d}\frac{[1+(2k_\perp\lambda)^2]^{3/2}}{1+2(k_\perp\lambda)^2} \tag{11}$$

However, the angular dependence of $\tau_\perp^q$ must also to be averaged out. The meaningful quantity is $\langle 1/\tau^q\rangle = (2/\pi)\int_0^{\pi/2}[\tau^q(\theta)]^{-1}d\theta$ and is often connected to the finite amplitude and width of the Shubnikov-de Haas or de Haas-van Alphen oscillations. The quantum scattering time may be looked upon as an effective 'Dingle' temperature, $T_D \sim (\hbar/2\pi k_B)\langle 1/\tau^q\rangle$.

Nevertheless, while comparing Shubnikov amplitudes, the scattering rates are better calculated between Landau wave functions and with a density of states at the Fermi level modified by the magnetic field, as was done long back by Vinokur[17] for the essentially the same problem. Furthermore, literature on the connection between scattering times for dislocations' strain field and de Haas-van Alphen oscillation amplitudes in metals was a subject of lively debate sometime back. Many parallel interpretations for level broadening [18] have been suggested. Some semiclassical arguments even favour a small angle cutoff. This fact may be particularly important in two dimensions where it could rescue the quantum scattering time from a divergence [14] in a simple and physically meaningful way, the small angle cutoff θ_c (in radians) being inversely proportional to the Landau level index n, $\theta_c \simeq \pi/2n$ [19, 20].

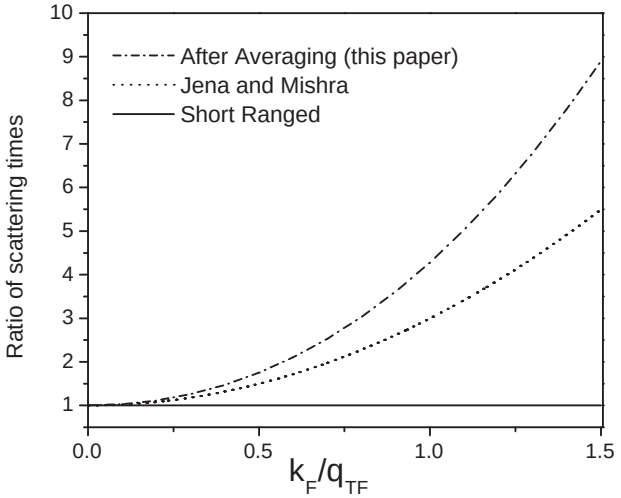

FIG. 1: *The ratio of dislocation scattering limited transport and quantum scattering times for a degenerate electron gas.*

Despite the preceding remarks, the concept of a quantum scattering time finds a widespread use in literature (for example, references [20, 21, 22]). Therefore we have plotted the suitably defined ratio $\langle 1/\tau^q\rangle\langle\langle\tau_{tr}\rangle\rangle$ of the transport and quantum scattering times for a three dimensional degenerate carrier gas in figure 1. The graph is plotted as a function of the dimensionless parameter, k_F/q_{TF}. q_{TF} is the simple wave vector independent Thomas-Fermi screening function. The largeness of this ratio is often regarded as a measure of 'anisotropy' of scattering. [23]. The real space anisotropy of the dislocation potential is different from the anisotropy in its Fourier transform, which is more a measure of the effective range of the potential. An additional averaging causes the transport to quantum scattering times ratio to be larger than what was calculated by in reference [14].

C. Mobility

In calculating mobility, the averaging procedure employed by Pödör has been called 'unspecified'[4] and hence it is worked out below. For dislocations along the z-axis, the current and electric field directions coincide as long as the measurement is done in the xy-plane. Then, $j_x = ne\langle\langle v_x\rangle\rangle$ and $\langle\langle v_x\rangle\rangle = \mu_\perp F_x$ where

$$\langle\langle v_x\rangle\rangle = \frac{\sum_{\mathbf{k}}(f_{0k}+\phi_{\mathbf{k}})v_x}{\sum_{\mathbf{k}}(f_0+\phi_{\mathbf{k}})} = \frac{\sum_{\mathbf{k}}\phi_{\mathbf{k}}v_x}{\sum_{\mathbf{k}}f_{0k}} \tag{12}$$

Or

$$\sigma_{xx} = \frac{e^2\hbar^2}{m^{*2}}\frac{2}{(2\pi)^3}\int k_x^2\left(-\frac{\partial f_0}{\partial E}\right)\tau_\perp(k,k_\perp)d^3k \tag{13}$$

Or

$$\sigma_{xx} = \frac{\hbar^5\epsilon^2}{4\pi^2m^{*3}Q^2N_d\lambda^4}\int_0^\pi d\theta\sin^2\theta \times\int_0^\infty dk k^4\left(-\frac{\partial f_0}{\partial E}\right)\left[1+(2k\lambda\sin\theta)^2\right]^{3/2} \tag{14}$$

The integrals must now be evaluated numerically. Equation (13) has the unpleasant feature of depending very strongly on screening length and thus at low temperatures turns out to be dependent on the model used for the temperature dependent of carrier concentration and screening. A simple analytic expression can be estimated by interpolating the two integrals ($\int d\theta$ and $\int dk$) between the two extremes cases, when the first term is much

smaller and when it is much larger than the second term in square brackets in equation (13). This is significantly better than Pödör's high temperature approximation[11] ($k\lambda \sin\theta \gg 1$). The relative percentage errors are plotted in figure 2 as a function of the dimensionless parameter $\frac{8m^* k_B T\lambda^2}{\hbar^2}$. It can be seen that this approximation of the integral never deviates from the numerically calculated exact answer by more than 5%.

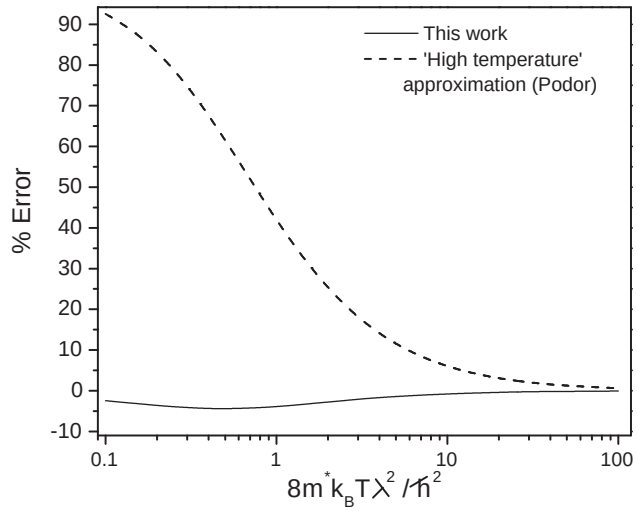

FIG. 2: *The relative percentage errors ($\frac{\mu_{exact}-\mu_{approx}}{\mu_{exact}} \times 100$) in our formula and Pödör's approximation with respect to the exact expression evaluated numerically. The graphs are plotted as a function of dimensionless parameter $\frac{8m^* k_B T\lambda^2}{\hbar^2}$.*

Assuming that the electrons are distributed according to Maxwell-Boltzmann distribution,

$$\mu_\perp \simeq \frac{4\pi^{1/2}\hbar^3\epsilon^2}{em^{*2}Q^2N_d\lambda^4}\left[\pi^{1/3}+\left(\frac{15\pi}{8}\right)^{2/3}\frac{8\lambda^2 m^* k_B T}{\pi\hbar^2}\right]^{3/2} \tag{15}$$

and when the carrier gas is fully degenerate

$$\mu_\perp^{\rm deg} \simeq \frac{3\hbar^5\epsilon^2}{4m^{*3}Q^2N_d\lambda_{TF}^4}\left[(4/3)^{2/3}+(5\pi/16)^{2/3}\,4k_F^2\lambda_{TF}^2\right]^{3/2} \tag{16}$$

D. Hall Factor

In most experiments it is not the drift but the Hall mobility which is measured. Under the assumption that the scattering rate does not alter in presence of a magnetic field, B and when the magnetic field is aligned with the dislocations' axis, only the in-plane relaxation time comes into the picture. Using the same line of arguments, it is easy to again establish its existence for arbitrarily strong non-quantizing magnetic fields. Then, if $j_x = \sigma_{xx}E_x + \sigma_{xy}E_y$, the Hall scattering factor r_H is defined as

$$r_H = n\,e\frac{\sigma_{xy}}{B\sigma_{xx}^2} \tag{17}$$

where the off-diagonal conductivity, σ_{xy}, for carriers with parabolic energy dispersion which are distributed along isotropic constant energy surfaces is

$$\sigma_{xy} = \frac{e^3B}{\hbar^2m^*}\int\frac{d^3k}{4\pi^3}\tau_\perp^2\frac{\partial f_0}{\partial E}\left(\frac{\partial E}{\partial k_x}\right)^2\left[1+\left(\frac{e\tau_\perp B}{m^*}\right)^2\right]^{-1} \tag{18}$$

From equations (13), (18) and (17) the Hall scattering factor for nondegenerate carriers at high temperatures (i. e. $\frac{8m^* k_B T\lambda^2}{\hbar^2} \gg 1$) approaches a value of 2.17, obtained by dropping the second term in square brackets in equation (13). At lower temperatures, its value is dependent on the model of carrier density and screening but always smaller. The anisotropy in scattering makes the value higher than the Hall factor for ionized impurity scattering which is 1.93.

E. Effect of Dislocation Tilt

Assume that dislocations are all parallel, but now at a longitude ϕ and latitude θ with respect to the z-axis while the measurement is being done in the xy-plane. A unit vector along this dislocation axis is $\hat{\mathbf{d}} = \hat{\mathbf{x}}\sin\theta\,\sin\phi + \hat{\mathbf{y}}\sin\theta\,\cos\phi + \hat{\mathbf{z}}\cos\theta$. Because the electric field is developed only along the direction perpendicular to the dislocations' axis, $\mathbf{F}_\perp = \rho\mathbf{j}_\perp = \rho[\mathbf{j} - (\mathbf{j}\cdot\hat{\mathbf{d}})\hat{\mathbf{d}}]$ which yields (with cos and sin abbreviated to c and s)

$$\rho' = \rho\begin{bmatrix} 1-\mathtt{s}^2\theta\mathtt{s}^2\phi & -\mathtt{s}^2\theta\mathtt{s}\phi\mathtt{c}\phi & -\mathtt{c}\theta\mathtt{s}\theta\mathtt{s}\phi \\ -\mathtt{s}^2\theta\mathtt{s}\phi\mathtt{c}\phi & 1-\mathtt{s}^2\theta\mathtt{c}^2\phi & -\mathtt{c}\theta\mathtt{s}\theta\mathtt{s}\phi \\ -\mathtt{c}\theta\mathtt{s}\theta\mathtt{s}\phi & -\mathtt{c}\theta\mathtt{s}\theta\mathtt{s}\phi & 1-\mathtt{c}^2\theta \end{bmatrix} \tag{19}$$

Negative sign in the off diagonals indicates the direction of the electric field developed.

F. Angular Distribution of Dislocations

Let us next consider the case when all the dislocations are not parallel to each other but are instead distributed with a uniform distribution of angles. One can, of course, average over the angles[24] appearing in equation (19). This averaging over the angles in the rotated resistivity tensor amounts the use of Matthiessen's rule and will not change the temperature dependence of mobility.

For a better approximation, we again start from the linearized Boltzmann equation, equation (3). In the present case, the relaxation time must be isotropic and therefore let the ansatz for the distribution function be

$$\phi(k) = -\frac{\hbar e}{m}\frac{\partial f_{0k}}{\partial E_k}\tau_{iso}(k)\mathbf{k}\cdot\mathbf{F} \tag{20}$$

We shall further assume incoherent scattering such the scattering rates due to different dislocation lines add. If the scattering rate due to an i^{th} dislocation is $W^i_{\mathbf{k},\mathbf{k}'}$, then the total rate is $\sum_i W^i_{\mathbf{k},\mathbf{k}'}$.

Without loss of generality, one can choose the electron wave vector $\mathbf{k}$ to be along the z-axis, $\mathbf{k} = k\hat{z}$. If the axis of the i^{th} dislocation, $\mathbf{d}^i$ is at an angle (θ, ϕ) with respect to the z-axis, then the unit vector along the dislocation axis is given by $\hat{d}^i = \sin\theta\sin\phi\hat{x} + \sin\theta\cos\phi\hat{y} + \cos\theta\hat{z}$. The component of the wave vector perpendicular to the dislocation axis is given by

$$\mathbf{k}^i_\perp = \mathbf{k} - (\mathbf{k}\cdot\mathbf{d^i})\hat{d}^{\,i}$$

Or

$$\mathbf{k}^i_\perp = k\left[(1-\cos^2\theta)\,\hat{z} - \cos\theta\sin\theta\cos\phi\,\hat{y} - \cos\theta\sin\theta\sin\phi\,\hat{x}\right] \quad (21)$$

Substituting back in the Boltzmann equation, we get

$$F_z k_z = -\tau_{iso}(k)\mathbf{F}\cdot\sum_i\left[-\mathbf{k}^i_\perp\frac{1}{\tau(k,k^i_\perp)}\right] \quad (22)$$

Converting the sum into an integral,

$$F_z k_z = \tau_{iso}(k)\,\frac{N_A}{4\pi}\mathbf{F}\cdot\int d\Omega\;\mathbf{k}^i_\perp\frac{1}{\tau(k,k^i_\perp)} \quad (23)$$

Here N_A is the dislocation density per unit solid angle.

Since the averaging over the dislocation orientations is equivalent to an averaging over the electron wave vectors, the expression for the relaxation time becomes

$$\frac{1}{\tau_{iso}(k)} = \frac{N_A}{4\pi}\frac{Q^2e^2\lambda^4m^*N_d}{\hbar^3\epsilon^2}\int_0^\pi d\theta\frac{sin\theta(1-\cos^2\theta)}{[1+k^2\lambda^2\sin^2\theta]^{3/2}} \quad (24)$$

where the ϕ integral has been performed and we have noted that $\int_0^{2\pi}\sin\phi d\phi = \int_0^{2\pi}\cos\phi d\phi = 0$. From here on, it is straightforward to calculate the isotropic mobility, although it must be done numerically [25].

V. SUMMARY

Within the framework of the conventional transport theory, we have shown that a relaxation time can be defined for scattering of carriers by charged dislocations. Difference between quantum and classical scattering times was discussed and it was pointed out that the anisotropy necessitates an appropriate angular averaging. A new approximate formula for mobility was derived and it was shown be within 5% of the exact result at all temperatures. The value of the Hall scattering factor and the effect of dislocation tilt on resistivity was determined. Finally we derived a new expression for the relaxation time when the angular orientation of dislocations is isotropic.

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[25] An explicit plot of the temperature dependence of the resulting mobility for an isotropic distribution of dislocations is not given here. This is because the screening length depends on the carrier density that has a strong non-universal temperature dependence, especially since the dislocations themselves act as trapping centres for charge carriers.