Intervalley-Scattering Induced Electron-Phonon Energy Relaxation in Many-Valley Semiconductors at Low Temperatures

M. Prunnila$^1$, P. Kivinen$^2$, A. Savin$^3$, P. Törnä$^2$, and J. Ahopelto$^1$

$^1$VTT Information Technology, P.O.Box 1208, FIN-02044 VTT, Espoo, Finland
$^2$NanoScience Center, Department of Physics, University of Jyväskylä, P.O.Box 35, FIN-40014 Jyväskylä, Finland and
$^3$Low Temperature Laboratory, Helsinki University of Technology, P.O.Box 2200, FIN-02015 HUT, Finland

(Dated: March 23, 2022)

We report on the effect of elastic intervalley scattering on the energy transport between electrons and phonons in many-valley semiconductors. We derive a general expression for the electron-phonon energy flow rate at the limit where elastic intervalley scattering dominates over diffusion. Electron heating experiments on heavily doped n-type Si samples with electron concentration in the range 3.5 – 16.0 × 10^{25} m^{-3} are performed at sub-1 K temperatures. We find a good agreement between the theory and the experiment.

PACS numbers: 63.20.Kr, 44.90.+c

Keywords: electron-phonon interaction, energy relaxation, disordered semiconductors

Since the low temperature hot electron experiments by Roukes et al. \cite{1}, the energy transport between electrons and phonons has continued to be a topical subject. Recently, there has been significant experimental and theoretical interest in the electron-phonon (e-ph) energy relaxation in metals and semiconductors at low temperatures \cite{2, 3, 4, 5, 6, 7, 8}. The understanding of thermal e-ph coupling is important for several low temperature devices such as microbolometers, calorimeters and on chip refrigerators \cite{4, 5}. This coupling plays also an important role in correct interpretation of low temperature experiments \cite{4} and the e-ph energy relaxation rate gives direct information about phonon mediated electron dephasing \cite{10}.

Interaction between electrons and phonons is strongly affected by the disorder of the electron system and, therefore, the problem is commonly divided into two special cases: pure and impure (or diffusive) limit of e-ph interaction. The cross-over between these two regions is defined as $q l = 1$, where $q$ is the phonon wavevector and $l$ the electron mean free path. If the whole phonon system is to be considered then the phonon wavevector can be conveniently replaced by the thermal phonon wave vector $q_T = k_B T / h v$, where $T$ is the temperature of the lattice and $v$ the sound velocity. Recent theory for single-valley semiconductors \cite{5} predicts that the e-ph energy relaxation is strongly enhanced when the system enters from the pure limit ($ql > 1$) to the diffusive limit ($ql < 1$). The behavior is the opposite in comparison to metals where it is well known, since the pioneering work by A. B. Pippard \cite{11}, that the disorder of the electron system tends to suppress the e-ph energy relaxation (see also Ref. \cite{2}). In semiconductors, due to small electron density, the e-ph interaction can be described by deformation potential coupling constants, which do not depend on the electronic variables, while in metals the coupling strongly depends on the electron momentum \cite{12}. This fundamental difference eventually leads to disorder enhancement of the relaxation in the diffusive limit in single-valley semiconductors \cite{5}.

In many-valley semiconductors the situation is further altered due to intervalley scattering, which is the topic of our work. Due to lack of screening the e-ph energy flow rate is strongly enhanced in many valley semiconductors in comparison to single valley ones at diffusive low temperature limit. We approach the e-ph energy transport problem by first considering the phonon energy attenuation rate due to electrons (or phonon-electron energy relaxation rate). This procedure is attractive, because it enables straightforward comparison between our work and previous literature, which has concentrated mainly on ultrasonic attenuation \cite{13, 14, 15, 16, 17}. We derive expression for the total e-ph energy flow rate (by using the phonon energy attenuation rate) and perform low temperature electron heating experiments to heavily doped n-type silicon samples. We find excellent agreement between the theoretical and the experimental e-ph

\[ T = \frac{\hbar v}{k_B}, \]

\[ q_l = 1, \]

\[ q_l > 1, \]

\[ q_l < 1. \]

\[ \tau_1, \]

\[ \tau_2. \]

FIG. 1: Schematic illustration of the constant energy ellipsoids of Si conduction band valleys. The valleys are located close to X-point in the first Brillouin zone. Elastic scattering rates $1/\tau_1$ and $1/\tau_2$ couple the different classes of the valleys.
temperature responses.

As discussed above the electron-phonon coupling in semiconductors can be described through deformation potential coupling constants, which do not depend on the electron variables (in a single valley). The strain induced conduction band energy shifts \( \delta \nu_l \) (\( l = 1, 2, \ldots, L \), \( L \) is the number of valleys) can be written conveniently in matrix notation as \( \delta \nu = D \epsilon \), where \( \{ \delta \epsilon \}_l = \delta \nu_l \) and \( D \) is the deformation potential \( L \times 6 \) matrix (containing the deformation potential coupling constants). \( \epsilon = [ \epsilon_{xx} \, \epsilon_{yy} \, \epsilon_{zz} \, \epsilon_{xy} \, \epsilon_{xz} \, \epsilon_{yz} ]^T \) is the strain component vector and \( \epsilon_{\alpha \beta} = \frac{1}{2} (\partial \nu_\alpha / \partial \alpha + \partial \nu_\beta / \partial \beta) \) are the symmetric strain components of displacement \( u \). For example, for the six Si conduction band minima (see Fig. 4) we have \( \delta \nu_l = \Xi_d (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + \Xi_u \vec{\epsilon}_l \) [18], where \( \Xi_d \) (\( \Xi_u \)) is the dilatational (uniaxial) deformation potential constant.

Here we deal with long wavelength limit where the phonon field can be identified with a classical acoustic wave \( \nu = \nu u \exp [-i (q \cdot r - \omega t)] \) with polarization \( \epsilon \) (|\( \epsilon \)| = 1). The strain now reduces to \( \epsilon_{\alpha \beta} = \frac{1}{2} (\partial \nu_\beta / \partial \alpha + \partial \nu_\alpha / \partial \beta) \) (\( \vec{\epsilon} = \frac{1}{2} \hat{q} u \)). This can be expressed in matrix form as \( \epsilon = -iqDSu \) and we find equation

\[
\delta \nu = -iqDSu, \tag{1}
\]

which describes how the displacement makes the band edges oscillate in a many valley system. In the diffusive long wavelength limit the phonon momentum itself cannot transfer the electrons from one minima to another, because this process would require large momentum \( q \sim 1/a \) (\( a \) is the lattice constant). Then the electron nonequilibrium, generated by the acoustic field, relaxes towards local equilibrium by two processes: diffusion and elastic intervalley impurity scattering. When the strain lifts the valley degeneracy elastic intervalley scattering provides a path for the electron system to relax towards local equilibrium. This path is favorable if the time scale related to diffusion over length \( \sim q^{-1} \) is sufficiently large, i.e., when \( q^2 D < 1/\tau_{iv} \), where \( 1/\tau_{iv} \) is the total elastic intervalley transition rate (\( D \) is the diffusion coefficient).

In this limit the linearized many-valley relaxation-time Boltzmann equation [19] reduces to a simple rate equation, which couples the change in the electron density \( \delta n_l \) of valley \( l \) to that of valley \( m \) via intervalley scattering rate \( \tau_{lm}^{-1} \):

\[
\frac{\partial \delta n_l}{\partial t} = \sum_m \frac{\tau_{lm}^{-1}}{\tau_{im}^{-1}} [\delta n_l - \delta n_m - 2\nu_l (\epsilon_F) (\delta \nu_l - \delta \nu_m)] . \tag{2}
\]

Here \( \nu_l (\epsilon_F) \) is the single spin and valley density of states at Fermi level \( \epsilon_F \gg k_B T \). We assume that strain equivalent valleys are coupled with rate \( \tau_{lm}^{-1} = \tau_1^{-1} \) and that the valleys whose degeneracy can be lifted with strain are coupled with rate \( \tau_{lm}^{-1} = \tau_2^{-1} \). In the case of Si the coaxial valleys are always equivalent whereas the degeneracy of the perpendicular valleys can be lifted (see Fig. 1). Now the solution of Eq. (2) is \( \delta \nu = 2\nu_1 (\epsilon_F) (1 + i\omega \tau_{iv})^{-1} M \delta \nu \), where \( \tau_{iv} = \tau_2 / L \) and \( \{ M \}_{l,m} = \delta_{l,m} - L^{-1} \). The phonon-electron relaxation rate \( 1/\tau_q \) is related to the dissipated heat \( Q \) of the acoustic field through standard relation

\[
1/\tau_q = Q/J = \omega \Im [\delta \nu] \cdot \Re [\delta \nu] / J, \tag{6}
\]

where \( J \) is the acoustic energy flux density and \( \langle \cdot \rangle \) stands for time average. Using this relation and Eq. (1) we find

\[
(\tau_{q})^{-1} = \frac{2\nu_1 (\epsilon_F) \omega_{q\lambda}^2 \tau_{iv}}{\rho \omega_{q\lambda}^2 / 1 + \omega_{q\lambda}^2 \tau_{iv}^2}, \tag{3}
\]

where we have used linear dispersion relations \( \omega_{q\lambda} = \omega_{\lambda} q \) (\( \lambda \) is the mode index). The factor \( \Phi_{\lambda} = e^\beta S^\lambda D^T M \Phi \) and it obviously depends only on the polarization \( \nu \), and on the deformation potential coupling constants. In the case of Si we have \( \Phi_{\lambda} = 2\Xi_\lambda^2 \{ \sum (\vec{q}_i \nu_i)^2 / 4(\vec{q} \cdot \nu)^2 \} \) and \( 1/\tau_{iv} = 6/\tau_2 \). Note that Eq. (3) does not depend on screening, because there are no total electron density fluctuations, i.e., \( \sum \delta n_l = 0 \).

We can describe a degenerate electron system by an equilibrium distribution at temperature \( T_\Sigma \). This holds even in the presence of net heat flow between electrons and phonons. The heat flow only creates a nonequilibrium between the electrons and phonons, which relaxes towards equilibrium at rate \( 1/\tau_{q} \) per single phonon mode. By following Perrin and Budd [20] this non-equilibrium can be expressed using the relaxation time approximation of the phonon-electron collision integral

\[
\left( \frac{\partial N(\omega_{q\lambda})}{\partial t} \right)_{ph-e} = -\frac{N(\omega_{q\lambda})}{\tau_{q\lambda}} - N_{T_e}(\omega_{q\lambda}) - N_{T_p}(\omega_{q\lambda}) \tag{4}
\]

where \( N(\omega_{q\lambda}) \) and \( N_{T_e}(\omega_{q\lambda}) \) = \( 1 - \exp(\hbar \omega_{q\lambda}/k_B T) \) are the nonequilibrium and equilibrium phonon distribution functions, respectively. The total stationary heat flow \( P \) through the coupled electron-phonon system is the energy average of the collision integral:

\[
P = \sum_{\lambda} \int dq \frac{\omega_{q\lambda}}{(2\pi)^3} h \omega_{q\lambda} \left( \frac{\partial N(\omega_{q\lambda})}{\partial t} \right)_{ph-e} \tag{5}
\]

where the summation is performed over the acoustic eigenmodes of the crystal. The only experimentally meaningful situation is such that the phonon system is coupled to some thermalizing bath, which is at temperature \( T_0 \). If the coupling is strong or \( P \) is small we can approximate \( N(\omega_{q\lambda}) \approx N_{T_{ph}}(\omega_{q\lambda}) \), where \( T_{ph} \) is the (possibly local) phonon temperature, and Eq. (5) reduces to the familiar form:

\[
P = F(T_e) - F(T_{ph}), \tag{6}
\]

where \( F(T) \) is the energy flow rate control function. Using Eqs. (3)-(6) and assuming that \( (k_B T / \hbar \tau_{iv})^2 \) is clearly below unity the energy flow rate control function
can be expressed in a closed form

\[ F(T) = \frac{\nu_{\text{f}}(\varepsilon_{\text{F}})B_5}{\pi^2 \rho_0 h^3} \sum_{\lambda} \left( \frac{\Phi_{\lambda}}{v_{\lambda}} \right) \tau_{\text{iv}} (k_B T)^6 \]

\[ = \frac{2\nu_{\text{f}}(\varepsilon_{\text{F}}) \varepsilon_2 B_5}{45\pi^2 \rho_0 h^3 v_F^2} \left[ \frac{17}{8} + \left( \frac{v_F}{v_L} \right)^5 \right] \tau_2 (k_B T)^6, \] (7)

where the first equality is valid for arbitrary many-valley system. The constant \( B_5 = \int_0^\infty dx x^3 / | 1 - \exp(x) | = 120 \pi^3 / 945 \) and \( \langle \cdot \rangle_{\Omega} \) stands for average over a solid angle. The second equality applies for silicon and there we have further assumed that the phonon eigenmodes are isotropic and that they are described by the longitudinal and transversal sound velocities \( v_L \) and \( v_T \).

Eq. (7) is valid when \((k_B T / h \tau_{\text{iv}})^2 \ll 1\) and \( q_T^2 D < 1 / \tau_{\text{iv}} \). At low temperatures the dominating condition is the latter and can be written also as \( q_T l \sqrt{\tau_{\text{iv}} / \tau} < 1 \), where \( \tau \) is the momentum relaxation time. Condition \( q_T l \sqrt{\tau_{\text{iv}} / \tau} = 1 \) defines the crossover temperature below which elastic intervalley scattering induced electron-phonon relaxation dominates over diffusion. If \( \tau_{\text{iv}} \) is not orders of magnitude larger than \( \tau \) this differs very little from the impure-pure threshold \( q_T l = 1 \).

Eq. (7) suggests that intervalley scattering induced electron-phonon energy relaxation rate \( \tau_{\text{iv}}^{-1} \propto \tau_{\text{iv}} T_e^4 \), which can be seen from approximate rate equation \( dP / dT_e = C_e \tau_{\text{iv}}^{-1} \), where \( C_e = \gamma T_e \) is the electron heat capacity. As the phonon mediated dephasing rate \( 1 / \tau_{\text{iv}} \) we find an important relation \( 1 / \tau_{\text{iv}} \propto \tau_{\text{iv}} T_e^4 \).

As already pointed above screening plays no role in \( 1 / \tau_{\text{ql}} \), and as a result intervalley scattering induced electron-phonon energy flow rate in Eq. (7) does not include any screening parameters, like for example screening wave vector \( \kappa \). Note, however, that there exists also single-valley contribution to the energy relaxation which is due to number density fluctuations in a single valley, but this contribution is strongly screened in doped semiconductors. By using the single valley result calculated by Sergeev et al. and Eq. (7) we find that the ratio between many-valley and single valley energy flow rate scales roughly as \( \sim 1500 (k\kappa)^2 (\tau_{\text{iv}} / \tau) (\kappa / T)^2 \), where \( [\kappa] = \text{nm}^{-1} \) and \( [T] = \text{K} \). Thus the many-valley effect is expected to fully dominate in the diffusive limit at high electron densities and low temperatures. We have tested Eq. (7) experimentally in the case of n+ Si:

The n+ Si samples were fabricated on unibond silicon-on-insulator substrates. Properties of the samples are listed in Table I and a detailed description about the sample fabrication can be found in [21]. The sample geometry and the experiment is depicted in Fig. 2(a). In the experiments the samples were mounted on a sample holder of a dilution refrigerator. The electron and phonon temperatures were simultaneously measured by utilizing the superconductor-semiconductor-superconductor (S-Sm-S) thermometry, while the electron gas in the Si film was heated with a DC power density \( P = \rho_{\text{e}} J^2 \) created by electric current density \( J \). Note that as the electronic coupling to the n+ Si film is made via superconducting Al the heat flow in the experiment follows accurately a path electrons–phonons–substrate/sample holder (phonons) and, therefore, the experimental \( P \) is equal to the left-hand-side of Eq. 4. Heating of the electron gas can cause a substantial increase in the temperature of the phonon thermometer, as reported recently for a similar n+ Si sample as discussed here. To assure that the nonequilibrium phonon distribution (of the phonons that interact with the electrons in the Si layer) can be reasonably described with an equilibrium distribution function we consider heating power range where \((T_{\text{ph}} - T_0) / T_0\) is clearly below unity.

![FIG. 2](image-url)

**FIG. 2**: (a) Schematic illustration of the sample geometry and the measurement setup. The ~9500 µm long n+ Si film is heated with a DC current density \( J \). \( T_e \) and \( T_{\text{ph}} \) are measured using current biased S-Sm-S (Al-Si-Al) contacts (only the biasing circuit for \( T_e \) is depicted). \( T_{\text{ph}} \) thermometer is electrically isolated from the main Si film by a ~1 µm gap. (b) The power density \( P = \rho_{\text{e}} J^2 \) vs. \( T_e^6 / T_{\text{ph}}^6 \) for samples with different carrier concentrations at bath temperature of 265 mK.

| Sample | \( N (10^{25} \text{m}^{-3}) \) | \( \rho_{\text{e}} (10^{-5} \Omega \cdot \text{m}) \) | \( l (\text{nm}) \) | \( d (\text{nm}) \) |
|--------|-------------------------------|-----------------|-----------------|-----------------|
| A      | 3.5                           | 1.04            | 5.06            | 70              |
| F      | 6.7                           | 0.63            | 5.42            | 58              |
| G      | 12.0                          | 0.51            | 4.54            | 58              |
| H      | 16.0                          | 0.44            | 4.34            | 58              |

TABLE I: The characteristics of the samples: \( N \) - carrier concentration, \( \rho_{\text{e}} \) - 1.5 K resistivity, \( l \) - electron mean free path, \( d \) - n+ Si film thickness. All samples have 400 nm thick buried oxide layer.
the condition that probes heat transport between electrons and one coherent acoustic mode coincides with our experiment that probes heat transport between electrons and phonon gas obeying quantum statistics. At high $N$ one would expect slowly decreasing or a roughly constant $\tau_2$, while our results show a weak increase as a function of $N$. This unexpected result could be explained by noting that our samples are in the limit of strong disorder ($k_F l \approx 3.6$ on average from Table I). Whereas, Eq. (4) is essentially based on a semiclassical free electron gas model, at least finally when the approximation $\nu_1(\varepsilon_F) = \nu_1^{\mathrm{el}}(\varepsilon_F)$ is made. Correction terms arising from interaction and quantum interference effects can be included to our model in the spirit of Ref. [10]. As similar terms appear in the conductivity the magnitude of these quantum corrections can be estimated from low field magnetoresistance and temperature dependency of resistivity. At the moment such data for thin film $n^+$ Si is not available.

Finally, we point out that the intervalley scattering induced electron-phonon energy relaxation can be observed also in several other material systems than $n^+$ Si. Canonical examples would be $n^+$ Ge and two-dimensional electron gas in (111) Si inversion layer. As the $\Gamma$-point in the valence band of elemental semiconductors is divided into heavy hole, light hole and split-off bands the effect should be particularly strong in various hole systems. However, due to complicated nature of the valence band maximum and effectively zero distance of the different bands in $k$-space the theory, which is valid for conduction band electrons, should be modified.

In summary, we have studied the effect of elastic intervalley transitions on the electron-phonon energy relaxation rate in many-valley semiconductors in the diffusive limit. We derived a general expression for the electron-phonon energy flow rate [Eq. (4)] and discussed the special case of $n^+$ silicon. Low temperature experiments on heavily doped Si samples were performed and good agreement between the theory and the experiment was found.

We want to acknowledge the skillful contribution of M. Markkanen in the sample fabrication. This work has been partially funded by the Academy of Finland (project numbers 46804, 205470, 205467 and 53903). PK also acknowledges financial support of Ulla Tuominen and Emil Aaltonen Foundations.

![FIG. 3: Slopes $S$ of the linear fits in Fig. 2(b) and intervalley scattering time $\tau_2$ [determined from $S$ and Eq. (2)] as a function of electron density $N$. The dashed curve is a polynomial fit that serves as a guide for the eye. The inset shows tabulated values of $S$ and $\tau_2$ (in the units of the axes).]
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