Inelastic interaction of electrons with lattice waves in many-valley-model semiconductors at low temperature

N. Chakrabarti and D. P. Bhattacharya
Department of Physics, Jadavpur University, Calcutta, 700032, India
(Received 26 March 1996; revised manuscript received 9 July 1996)

The rate of loss of energy of nonequilibrium electrons due to inelastic interactions with intravalley acoustic phonons in a high-purity many-valley model semiconductor has been calculated here under the conditions of low lattice temperature when the approximations of the well-known traditional theory are not valid. The rate now depends upon the average energy and the lattice temperature in a significantly different manner compared to what follows from traditional approximations. The nature of any such dependence is also different from that for the simple valley model unlike what the traditional theory predicts. Numerical results for Si and Ge show that the loss rates exceed the traditional values at lower energies for lower lattice temperatures. [S0163-1829(97)05115-1]

Through interaction with any lattice imperfection in a semiconductor the nonequilibrium carriers on an average lose energy with a rate characteristic of the type of imperfection.

For the phenomena of avalanche breakdown due to band-to-band transition in Ge and Si it has been rather arbitrarily assumed that just below the threshold for ionization the energy loss through emission of optical phonons exceeds that to acoustic phonons over a low range of the heating field. For higher fields, however, the loss to acoustic-mode lattice vibrations seems to dominate for electron energies of the order of the band gap or more.[1,2]

There exists a range of low lattice temperature ($T_L \leqslant 20$ K) when the free electrons in a high-purity covalent semiconductor interact dominantly only with intravalley deformation acoustic phonons and the electrons may become hot attaining a field-dependent effective temperature T_e, which exceeds T_L, for a field of only a few V/cm.[2–6] When the free carriers are sufficiently heated up, the optical phonon scattering may also control the electron transport even at low temperatures.[10]

At low lattice temperature, the phonon system may also significantly deviate from thermal equilibrium if the carrier concentration is enough to exceed some field-dependent critical value n_c. Under these conditions the average energy loss of a carrier may be calculated by solving the coupled system of the Boltzmann-type equation, treating electrons and phonons on equal footing.[2,7,8] But under the conditions when the electrons in high-purity materials are dominantly scattered only by acoustic phonons at low lattice temperatures around 5 K, since the carrier concentration is usually much lower than n_c at any field,[2–5] the phonons are essentially maintained in thermal equilibrium even when electrons are heated up in relatively weak fields. Under such conditions a traditional theory yields an average rate of energy loss to the acoustic modes for a nondegenerate ensemble of hot electrons, $\langle d\mathcal{E}/dt\rangle_{\rm ac} \sim T_e^{3/2}(1-T_L/T_e)$, be it a simple model or a many-valley semiconductor.

The traditional theory neglects the phonon energy $\varepsilon_{\rm ph}$ compared to the carrier energy $\varepsilon_{\mathbf{k}}$ and approximates the equilibrium phonon distribution by simple equipartition law. But the ratio $\varepsilon_{\rm ph}/\varepsilon_{\mathbf{k}} \sim 2v_s/v_{\rm th}$, $v_{\rm th}$ being the average thermal velocity of the electron that is in thermodynamic equilibrium with the lattice and v_s the average acoustic velocity in the material. At higher lattice temperatures ($T_L \geqslant 20$ K) this ratio is small indeed. But on lowering the lattice temperature the ratio increases and eventually $\varepsilon_{\rm ph}$ becomes comparable to $\varepsilon_{\mathbf{k}}$. The thermal energy now being small, the equipartition approximation for the phonon distribution is hardly valid. Hence, at the low lattice temperatures the neglect of the energy of the acoustic phonons and the equipartition approximation for their equilibrium distribution would result in a wrong balance of energy for the electron-phonon system.[4]

The calculations of the scattering rates and of some transport coefficients when made at low temperatures taking into account the finite energy of the acoustic phonons and their true equilibrium distribution, yield results[4,9,10] that are significantly different from what follows from traditional theory. The energy-loss rate in a model semiconductor similarly obtained elsewhere[11] also shows interesting features at low temperatures. The purpose of this paper is to derive an expression for the average rate of energy loss of an ensemble of nonequilibrium electrons to the acoustic modes in a many-valley band structure under the condition of low lattice temperature and when the phonon system remains in equilibrium giving due regard to the finite phonon energy and also to their true equilibrium distribution, and following the assumptions which have been used earlier.[4,12] The results thus obtained for Ge and Si will be compared with the traditional values for the identical interaction and with the loss rate for interaction with optical modes. It remains to be seen if one gets here also the same characteristics of loss rate as predicted by the traditional theory, irrespective of the band model under the prevalent condition of low lattice temperature.

We consider electronic transitions between states having wave vectors $\mathbf{k}$ and $\mathbf{k}'$ $(=\mathbf{k}+\mathbf{q})$ with attendant emission and absorption of a phonon of wave vector $\mathbf{q}$ in a volume V of a many-valley model semiconductor with ellipsoidal constant-energy surfaces. The interaction is allowed with transverse (t) as well as longitudinal (l) modes. When the valleys are centered on $\langle 100\rangle$ or $\langle 111\rangle$ axes in a Brillouin zone, symme-

try makes it possible to express all the intravalley deformation potential constants E_α in terms of two independent ones, viz., E_d and E_u for dilatation and uniaxial shear, respectively, leading to the matrix element between the initial state $\mathbf{k}_i$ and final state $\mathbf{k}_f$ as[2]

$$|\langle \mathbf{k}_f, N_{\mathbf{q}\alpha} \pm 1 | H'_{\rm ac} | \mathbf{k}_i, N_{\mathbf{q}\alpha} \rangle|^2 = \frac{E_\alpha^2 \hbar q}{2V\rho u_\alpha} \begin{bmatrix} N_{\mathbf{q}\alpha}+1 \\ N_{\mathbf{q}\alpha} \end{bmatrix}. \quad (1)$$

Here α indicates the polarization of phonons. $E_l = E_d + E_u \cos^2\theta$ and $E_t = E_u \sin\theta\cos\theta$, θ being the angle between $\mathbf{q}$ and the symmetry axis, $\hbar = h/2\pi$, h being Planck's constant, ρ is the density of the material and u_α is the acoustic velocity. $N_{\mathbf{q}\alpha}$ is the number of phonons of any $\mathbf{q}$ and α. The upper or lower signs (and $N_{\mathbf{q}\alpha}+1$ or $N_{\mathbf{q}\alpha}$) stand for the processes of emission and absorption, respectively.

In the presence of a strong electric field the average rate of energy loss of a carrier in a valley at an effective temperature T_e is[2]

$$\left\langle \frac{d\mathcal{E}}{dt} \right\rangle_{\rm ac} = -\frac{1}{n_1 V} \sum_{\mathbf{q},\alpha} \hbar u_\alpha q \left(\frac{\partial N_{\mathbf{q}\alpha}}{\partial t} \right), \quad (2)$$

where n_1 is the carrier concentration in a single valley, $(\partial N_{\mathbf{q}\alpha}/\partial t)$ is the rate of increase in the phonon number of any type and may be written from the perturbation theory as

$$\begin{aligned} \left(\frac{\partial N_{\mathbf{q}\alpha}}{\partial t} \right) = \frac{2\pi}{\hbar} \sum_{\mathbf{k}} & [|\langle \mathbf{k}, N_{\mathbf{q}\alpha}+1 | H'_{\rm ac} | \mathbf{k}', N_{\mathbf{q}\alpha} \rangle|^2 \\ & \times \delta(\varepsilon_{\mathbf{k},N_{\mathbf{q}\alpha}+1} - \varepsilon_{\mathbf{k}',N_{\mathbf{q}\alpha}}) f_0(\mathbf{k}') \\ & - |\langle \mathbf{k}', N_{\mathbf{q}\alpha}-1 | H'_{\rm ac} | \mathbf{k}, N_{\mathbf{q}\alpha} \rangle|^2 \\ & \times \delta(\varepsilon_{\mathbf{k}',N_{\mathbf{q}\alpha}-1} - \varepsilon_{\mathbf{k},N_{\mathbf{q}\alpha}}) f_0(\mathbf{k})], \end{aligned} \quad (3)$$

where $f_0(\mathbf{k})$ is the distribution function for the nonequilibrium electrons.

Substituting $k_\beta = k_\beta^* (m_\beta/m_0)^{1/2}$ for $\beta = x,y,z$ where x, y, and z are the principal axes, with z being the longitudinal axis, one can transfer to the starred system making $\varepsilon_{\mathbf{k}} = \hbar^2 k^{*2}/2m_0$ and $q = q^* \overline{\eta} (m_d/m_0)^{1/2}$ where m_0 is the free-electron mass. For ellipsoids of revolution, as in n-type Ge and Si if the longitudinal axis is taken to be the axis of symmetry, one can get $\overline{\eta}$, the mass anisotropy factor as $[(m_l+m_t)/2m_d]^{1/2}$ and m_d, the density of states effective mass as $(m_t^2 m_l)^{1/3}$; m_l being the effective mass along the major axis and m_t that in the transverse direction.

With $\mathbf{q}^*$ direction taken as the z axis the integration over θ^* and ϕ^* can be easily carried out. For the integration over k^* the limits as decided by the energy and momentum balance equations taking finite energy of the acoustic phonons into account come out to be $[q^*/2 - u_\alpha (m_d m_0)^{1/2} \overline{\eta}/\hbar]$ and ∞. If $f_0(\mathbf{k}^{*\prime})$ is expanded in a Taylor's series around $\mathbf{k}^*$, and $f_0(\mathbf{k}^*)$ is taken to be the Maxwell-Boltzmann distribution at an effective electron temperature T_e and the average energy $\langle \mathcal{E} \rangle = 3k_B T_e/2$, one can obtain considering the electrons of both spins,

$$\begin{aligned} \left(\frac{\partial N_{\mathbf{q}\alpha}}{\partial t} \right) = \mathcal{R}_{\rm ac} & \left[1 + (N_{\mathbf{q}\alpha}+1) \sum_{j=1}^{\infty} \frac{(-x_\alpha/T_n)^j}{j!} \right] \\ & \times \exp[-a_\alpha (x_\alpha - b_\alpha)^2], \end{aligned} \quad (4)$$

where

$$\mathcal{R}_{\rm ac} = \frac{E_\alpha^2 (m_t^2 m_l m_0)^{1/2}}{2\pi\hbar^4 \rho u_\alpha} k_B T_L \frac{n_1}{N_{c_1}(T_e)} T_n \overline{\eta} (m_d/m_0)^{1/2},$$

k_B is the Boltzmann constant, $N_{c_1}(T_e)$ is the effective density of states for a single valley given by $2(2\pi m_t^{2/3} m_l^{1/3} k_B T_e)^{3/2}/8\pi^3\hbar^3$, $x_\alpha = \hbar u_\alpha q/k_B T_L$, $T_n = T_e/T_L$, $b_\alpha = 2\overline{\eta}^2 u_\alpha^2 m_d/k_B T_L$, $a_\alpha = k_B T_L/8 m_d u_\alpha^2 \overline{\eta}^2 T_n$, and $N_{\mathbf{q}\alpha}$ is given by the Bose-Einstein distribution. By setting $m_l = m_t = m^*$, the scalar effective mass of the free carriers and $E_d = E_1$, $E_u = 0$ in Eq. (4), one can get the rate for a simple model semiconductor at the low-lattice temperatures.

At higher lattice temperatures ($T_L > 20$ K) when the phonon energy is negligibly small compared to the carrier energy, $x_\alpha \ll 1$; $b_\alpha \ll 1$ and the phonon ensemble obeys the equipartition law. Expression (4) now reduces to

$$\left(\frac{\partial N_{\mathbf{q}\alpha}}{\partial t} \right) = \mathcal{R}_{\rm ac} \left[1 - \frac{1}{T_n} \right] \exp[-a_\alpha, x_\alpha^2]. \quad (5)$$

Thus, when the phonon energy is taken into account, the number of phonons increases distinctly at a different rate in comparison to what occurs in the traditional approximation of negligible phonon energy. The number of phonons now increases at a slower rate, and the rate depends upon the phonon wave vector and T_n in a rather complex manner, decreasing with the former at a faster rate with the lowering of T_n. The effect of finite energy of the phonons is felt more and more the higher the value of the acoustic velocity for any polarization α and the lower the lattice temperature. It is also to be noted that at any lattice temperature the effect is more pronounced the lower the value of T_n.

The integration over vector $\mathbf{q}$ in Eq. (2) can be likewise carried out after assigning a true expression for the equilibrium phonon distribution that is valid at the low-lattice temperature. It may be taken as[12]

$$N_{\mathbf{q}\alpha}(x_\alpha) = \begin{cases} \displaystyle\sum_{m=0}^{\infty} \frac{B_m}{m!} x_\alpha^{m-1}, & x_\alpha \leqslant \overline{x} \\ \exp(-x_\alpha), & x_\alpha > \overline{x}, \end{cases} \quad (6)$$

here B_m are Bernoulli's numbers. For integration over the magnitude of the phonon wave vector q, the upper limit may be assumed to be infinity since $(\partial N_{\mathbf{q}\alpha}/\partial t)$ given by Eq. (4) falls off rapidly for large q. Thus one can obtain

$$\begin{aligned} \left\langle \frac{d\mathcal{E}}{dt} \right\rangle_{\rm ac} = -\mathcal{B}_{\rm ac} \Bigg[\mathcal{D}_{\alpha{\rm ac}} \Bigg\{ & \sum_{m=0}^{\infty} \frac{B_m}{m!} (\mathcal{A}_{e\alpha} - \mathcal{A}_{a\alpha}) \\ & + \exp[b_\alpha (T_n+1)] S_{\alpha 1} + S_{\alpha 2} \\ & - \exp[b_\alpha (T_n-1)] S_{\alpha 3} \Bigg\} \Bigg], \end{aligned} \quad (7)$$

where

$$\mathcal{B}_{\rm ac} = (m_t^2 m_l/2)^{1/2} (2\pi^{3/2} \rho \hbar^4 m_d \overline{\eta}^2)^{-1} (k_B T_L)^4/(k_B T_e)^{1/2},$$

$$\mathcal{D}_{l{\rm ac}} = u_l^{-4} [E_d^2 + 2E_d E_u m_l/(3\overline{\eta}^2 m_d) + E_u^2 m_l^2/(5\overline{\eta}^4 m_d^2)],$$

$$\mathcal{D}_{t{\rm ac}} = 2u_t^{-4} E_u^2 m_l m_t/(15\overline{\eta}^4 m_d^2),$$

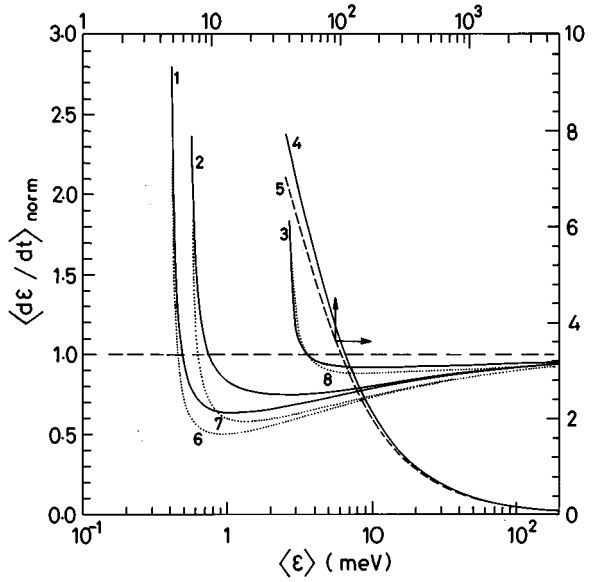

FIG. 1. Normalized rates of energy loss of nonequilibrium electrons in the many-valley model due to interaction with intravalley acoustic and optical phonons. Curves 1–5 are for Ge. 1, 2, and 3 are for acoustic interactions at 3, 4, and 20 K, respectively, and when the rates are normalized to their traditional values, and 4 and 5 are for optical interaction at 4 K and when the rates are normalized, respectively, to what follows from the theory developed here, and the traditional values due to acoustic interactions. Curves 6, 7, and 8 are for Si corresponding to the acoustic interactions at the temperatures of 3, 4, and 20 K, respectively.

$$\mathcal{A}_{e\alpha}=\sum_{r=0}^{m+2} {}^{m+2}C_r(-b_\alpha)^{m+2-r}(2a_\alpha^{(r+1)/2})^{-1}\times\left[\Gamma\left\{\frac{r+1}{2},a_\alpha b_\alpha^2\right\}-\Gamma\left\{\frac{r+1}{2},a_\alpha(\overline{x}+b_\alpha)^2\right\}\right],$$

$$\mathcal{A}_{a\alpha}=\sum_{r=0}^{m+2} {}^{m+2}C_r(b_\alpha)^{m+2-r}(2a_\alpha^{(r+1)/2})^{-1}\times\left[\Gamma\left\{\frac{r+1}{2},a_\alpha b_\alpha^2\right\}-\Gamma\left\{\frac{r+1}{2},a_\alpha(\overline{x}-b_\alpha)^2\right\}\right],$$

$$\mathcal{S}_{\alpha 1}=\sum_{r=0}^{3} {}^{3}C_r(-d/2a_\alpha)^{3-r}(2a_\alpha^{(r+1)/2})^{-1}\times\left[\Gamma\left\{\frac{r+1}{2},a_\alpha(\overline{x}+d/2a_\alpha)^2\right\}\right],$$

$$\mathcal{S}_{\alpha 2}=\sum_{r=0}^{3} {}^{3}C_r(-b_\alpha)^{3-r}(2a_\alpha^{(r+1)/2})^{-1}\left[\Gamma\left\{\frac{r+1}{2},a_\alpha b_\alpha^2\right\}\right],$$

$$\mathcal{S}_{\alpha 3}=\sum_{r=0}^{3} {}^{3}C_r(-e/2a_\alpha)^{3-r}(2a_\alpha^{(r+1)/2})^{-1}\times\left[\Gamma\left\{\frac{r+1}{2},a_\alpha(\overline{x}+e/2a_\alpha)^2\right\}\right],$$

${}^mC_n$'s are binomial coefficients, $\Gamma\{\alpha,\beta\}$ is an incomplete gamma function,[13] $d=(2T_n+1)/2T_n$, $e=(2T_n-1)/2T_n$.

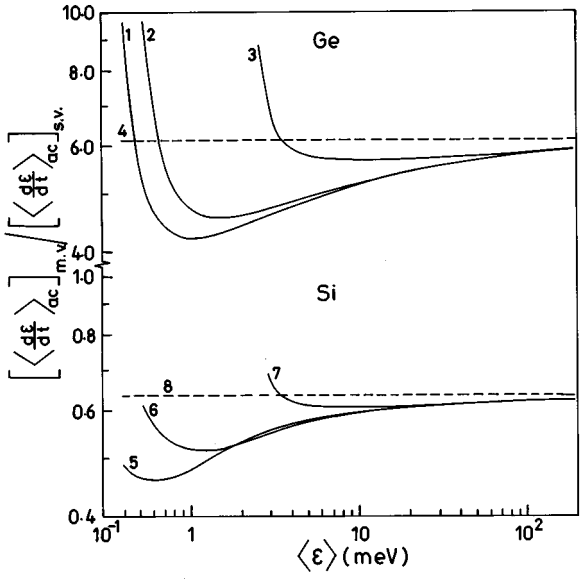

FIG. 2. Energy-loss rates of nonequilibrium electrons to acoustic-mode lattice vibrations in the many-valley (m.v.) model normalized to the corresponding values for the simple-valley (s.v.) model. Curves 1, 2, and 3 for Ge are obtained from the theory developed here at 3, 4, and 20 K, respectively, and curve 4 can be obtained from the traditional approximations. Curves 5, 6, and 7 for Si follow from the theory developed here at 3, 4, and 20 K, respectively, and curve 8 can be obtained from the traditional approximations.

It may be noted that under the condition where the lattice temperature is high so that both x_α and b_α are small and the phonons obey equipartition law, expression (7) reduces to its traditional form,

$$\left\langle\frac{d\mathcal{E}}{dt}\right\rangle_{ac}=-\mathcal{R}_{1ac}(E_0')^2(1-1/T_n),\tag{8}$$

where

$$\mathcal{R}_{1ac}=8\sqrt{2}(m_t^2m_l)^{1/2}m_d\overline{\eta^2}(k_BT_e)^{3/2}/(\pi^{3/2}\rho\hbar^4),$$

$$(E_0')^2=E_d^2+2E_dE_um_l/(3\overline{\eta^2}m_d)+(3+2m_t/m_l)E_u^2m_l^2/(15\overline{\eta^4}m_d^2).$$

Equating both m_t and m_l to the scalar effective mass m^* and putting $E_u=0$ and $E_d=E_1$, one can recover the loss rates for the simple model semiconductor from Eqs. (7) and (8) under the conditions of low temperature,[11] and in the light of traditional approximations,[2] respectively. The loss rates to optical mode in Ge have been estimated from Eq. (2) for energies exceeding the optical phonon energy.[2] The results are shown in Fig. 1 for comparison.

Thus the energy-loss rate calculated here depends upon the average energy in a more complex manner compared to what is given by traditional theory. If the average carrier energy is high, there is only a little dependence of the rate of energy loss on the lattice temperature, be it the loss to the acoustic modes obtained from the traditional approximations for any model of the valley, simple or many, or the loss to optical modes. However, for the acoustic interaction the

lattice-temperature dependence of the loss rate calculated here is seen to be relatively more involved.

The above formulations may be used for samples of Si and Ge having the well-known parameter values,[14] and $\overline{x}$ may be taken to be 3.5.

Figure 1 reveals how the condition of low lattice temperature brings significant changes in the dependence of the loss rate upon the average energy. Compared to the traditional results, our theory at any lattice temperature leads to higher values of the loss rate in the lower-energy regime and lower values in the higher-energy regime. For any material, both rates would assume equal value at some energy, and this critical energy increases with the lattice temperature. The discrepancy of the loss rates relative to the traditional value is greater the lower the lattice temperature since the phonon energy becomes more and more significant there. Our theory leads again to the same results as that given by traditional theory for higher values of the average energy with a rate which is greater, the lower the lattice temperature. It may also be noted that in Ge the loss rate exceeds that due to optical modes for higher values of the average energy compared to what is given by traditional theory.

Figure 2 shows that the theory developed here predicts characteristically different dependence of the loss rates upon the average energy for the many-valley model compared to the same for the simple-valley model, unlike the identical dependence given by traditional theory. The qualitative difference is ascribed to the finite energy of the acoustic phonons, which makes the interaction inelastic, and the equipartition approximation for the phonon distribution invalid at low temperatures.

One of the authors (N.C.) is thankful to the University Grants Commission, New Delhi, India for support.

[1] W. Shockley, *Proceedings of the International Conference on Semiconductor Physics, Prague, 1960* (Czechoslovakian Academy of Sciences, Prague, 1961).

[2] E. M. Conwell, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1967), Suppl. 9.

[3] Z. S. Kachlishvili, Fiz. Tekh. Poluprovodn. **2**, 580 (1968) [Sov. Phys. Semicond. **2**, 478 (1968)].

[4] C. Canali, C. Jacoboni, F. Nava, G. Ottaviani, and A. Alberigi-Quaranta, Phys. Rev. B **12**, 2265 (1975).

[5] S. H. Koenig, R. D. Brown, and W. Schillinger, Phys. Rev. **128**, 1668 (1962).

[6] V. V. Mitin, Appl. Phys. A **39**, 123 (1986).

[7] V. V. Paranjape, Proc. Phys. Soc. London **80**, 971 (1962).

[8] V. D. Dorn, Z. Naturforsch. **12a**, 739 (1957).

[9] C. Jacoboni, F. Nava, C. Canali, and G. Ottaviani, Phys. Rev. B **24**, 1014 (1981).

[10] A. K. Ghorai and D. P. Bhattacharya, Phys. Rev. B **47**, 13 858 (1992).

[11] N. Chakrabarti and D. P. Bhattacharya, Phys. Rev. B **53**, 6885 (1996).

[12] C. Jacoboni and L. Reggiani, Rev. Mod. Phys. **55**, 645 (1983).

[13] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965).

[14] L. Reggiani, *Hot Electron Transport in Semiconductors* (Springer-Verlag, Berlin, 1985).