Inelastic interaction of nonequilibrium electrons with acoustic phonons at low lattice temperatures

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The rate of loss of energy of the nonequilibrium electrons to the acoustic mode lattice vibrations is obtained here under conditions when the lattice temperature is low, so that the approximations of the well-known traditional theory are not valid. Evaluating the loss rates in Si and Ge we find that there have been significant changes in the rates which exceed the traditional values at lower energies, the lower the lattice temperature.

In the studies of the avalanche multiplication due to band-to-band transitions in some semiconducting materials such as Ge and Si it has been a rather arbitrary custom to assume that just below the threshold for ionization, the dominant energy-loss process for the free carriers is through emissions of optical phonons. The rate of energy loss to the optical mode lattice vibrations has been taken to exceed that to the acoustic mode over a low range of the heating electric field. For higher fields, however, loss to acoustic modes seems to dominate for electron energies of the order of the band gap and larger.[1–5]

It is well known that there is a range of low lattice temperatures ($T_L \leqslant 20$ K) when the free carriers in a high-purity covalent semiconductor interact dominantly with intravalley acoustic phonons. At such low temperatures the electrons become hot in relatively weak fields, and under favorable circumstances they may even lead to the onset of the reversible, and as such, nondestructive impurity breakdown due to impact ionization of the donor levels at a field of only a few volts per centimeter. The electron transport under these conditions is limited by the acoustic phonon scattering of the nonequilibrium carriers.[4,6–13] The optical phonon scattering in Ge is also known to limit the transport under high-field conditions when the carriers deviate significantly from the state of thermodynamic equilibrium even at low lattice temperatures.[14]

In the light of the traditional theory the rate of loss of energy of the hot electrons to the deformation acoustic mode lattice vibrations has already been obtained.[4] However, the traditional theory is based on a number of simplifying approximations that are hardly valid at the low lattice temperatures of the order of a few tens of degrees or less. First, the theory neglects the acoustic phonon energy $\varepsilon_{\rm ph}$ in relation to the carrier energy $\varepsilon_{\bar{k}}$. But the ratio $\varepsilon_{\rm ph}/\varepsilon_{\bar{k}}$ is of the order of $2u_l/v_{\rm th}$. $v_{\rm th}$ is the average thermal velocity of an electron and u_l is the velocity of longitudinal acoustic mode in the material.[4] At higher lattice temperatures when $T_L > 20$ K this ratio being very small, the phonon energy is indeed only a negligible fraction of the electron energy. On lowering the temperature this ratio increases and the phonon energy tends to be more and more comparable with the electron energy. In fact it is this small amount of energy exchanged in the collision between the free carriers and the phonons that ensures stationarity of the electron-phonon system in the presence of any electric field under the condition when no other dissipative mechanism except the emission of acoustic phonons is effective.[7] Second, when $T_L > 20$ K since the average thermal energy of the free carriers tends to be much greater than the phonon energy, the energy distribution of the phonon is approximated in the traditional theory by the simple equipartition law. Obviously at the low lattice temperatures, the equipartition approximation for the phonon distribution is not valid. Hence a wrong balance of energy of the electron-phonon system may result unless the true phonon population and the finite energy of the acoustic phonons are taken into account with sufficient precision at the low lattice temperatures.

The calculation of the acoustic scattering rate of the free electrons made without using the traditional approximations shows that except for an intermediate range of the carrier energy there have been significant changes in both the qualitative and quantitative aspects of the energy and temperature dependence of the scattering rates at low lattice temperatures in comparison to what follows from the traditional theory. The theoretical calculation of the transport characteristics of the materials when made using the new scattering rates under the condition of low lattice temperature leads to encouraging features.[7,15,16] Hence it would be interesting to study the effect of finite energy carried by the acoustic phonons on the energy loss of the nonequilibrium electrons to the acoustic modes at low temperatures since the possibility of obtaining materials of desired purity is already within the scope of the present stage of semiconductor technology. The purpose of this paper is to calculate the average rate of energy loss of the nonequilibrium electrons to acoustic mode lattice vibrations under the condition of low lattice temperature when the phonon energy can neither be neglected in comparison with the carrier energy nor the phonon distribution be represented by the equipartition law. The theory is then used to obtain the energy-loss rate in Ge and Si. The results are compared with (i) that obtained from the traditional approximations for the identical interactions of the free carriers and (ii) that obtained for the interaction with optical mode lattice vibrations so as to assess the effect of finite energy of acoustic phonons on the energy loss for different values of the lattice temperature.

We shall consider a volume V of a model isotropic semiconductor with a single, parabolic, spherically symmetric conduction band. Let there be any electronic state with wave vector k and transitions between this state and another having wave vector k' $(=k+\bar{q})$ involving either emission or

absorption of a phonon of wave vector $\bar{q}$, resulting in an increase in $N_{\bar{q}}$, the number of phonons. The rate of increase in the number of phonons may be written using the perturbation theory as[4]

$$\left(\frac{\partial N_{\bar{q}}}{\partial t}\right)=\frac{2\pi}{\hbar}\sum_{k}\left[|\langle \bar{k},N_{\bar{q}}+1|H'_{\rm ac}|\bar{k}',N_{\bar{q}}\rangle|^2\delta(\varepsilon_{\bar{k}},N_{\bar{q}}+1-\varepsilon_{\bar{k}'},N_{\bar{q}})f_0(\bar{k}')-|\langle \bar{k},N_{\bar{q}}-1|H'_{\rm ac}|\bar{k},N_{\bar{q}}\rangle|^2\delta(\varepsilon_{\bar{k}'},N_{\bar{q}}-1-\varepsilon_{\bar{k}},N_{\bar{q}})f_0(\bar{k})\right], \tag{1}$$

where the square of the matrix element between the initial state k_i and final state k_f is given by

$$|\langle \bar{k}_f,N_{\bar{q}}\pm 1|H'_{\rm ac}|\bar{k}_i,N_{\bar{q}}\rangle|^2=\frac{E_1^2\hbar q}{2V\rho u_l}\begin{bmatrix}N_{\bar{q}}+1\\ N_{\bar{q}}\end{bmatrix}. \tag{2}$$

Here $\hbar=h/2\pi$, h being Planck's constant, $f_0(\bar{k})$ is the distribution function for the nonequilibrium electrons, E_1 is the deformation potential constant, and ρ is the density of the material. The upper or lower sign (and $N_{\bar{q}}+1$ or $N_{\bar{q}}$) stands for the processes of emission and absorption, respectively.

The summation over k may be converted to an integration over spherical coordinates k, θ, and ϕ with the $\bar{q}$ direction taken as the z axis. Considering the electrons of both spins the integration over the polar and azimuthal angles yields

$$\left(\frac{\partial N_{\bar{q}}}{\partial t}\right)=\frac{E_1^2 m^*}{2\pi\rho\hbar^2 u_l}\int_k[(N_{\bar{q}}+1)f_0(\bar{k}')-N_{\bar{q}}f_0(\bar{k})]k\,dk. \tag{3}$$

Under the conditions of low temperature since the phonon energy cannot be neglected, the limits for the integration over k, as ascertained from the energy and momentum balance equations may be taken to be $(q/2-m^*u_l/\hbar)$ and ∞. If $f_0(\bar{k}+\bar{q})$ is now expanded in a Taylor's series around k and $f_0(k)$ be a Maxwellian distribution at an effective electron temperature T_e and the average energy $\langle\varepsilon\rangle=3k_BT_e/2$, one can obtain

$$\left(\frac{\partial N_{\bar{q}}}{\partial t}\right)=\frac{u_l n_0 T_n}{2l_{\rm ac}N_c(T_e)}\left[1+(N_{\bar{q}}+1)\sum_{j=1}^{\infty}\frac{(-x/T_n)^j}{j!}\right]\times\exp[-a(x-b)^2], \tag{4}$$

where n_0 is the free carrier concentration, $l_{\rm ac}$ the mean free path for deformation potential scattering by acoustic phonons obeying the equipartition law. $N_c(T_e)$, the effective density of states, is given by $2(2\pi m^*k_BT_e)^{3/2}/8\pi^3\hbar^3$, k_B is Boltzmann's constant, and m^* is the effective mass of free carriers, $x=\hbar u_l q/k_BT_L$, $b=2m^*u_l^2/k_BT_L$, $T_n=T_e/T_L$, and $a=k_BT_L/8m^*u_l^2T_n$. Under the condition of high lattice temperature when the phonon energy can indeed be neglected and the equipartition law holds good, from (4) one can readily recover the traditional expression[4] for the rate of increase of the phonon number.

Thus under the low-temperature condition when the phonon energy is taken into account in the energy balance equation with sufficient precision the phonon number increases at a slower rate compared to what is predicted from the traditional theory. $(\partial N_{\bar{q}}/\partial t)$ now depends upon q and T_n in a rather complex manner, decreasing with q at a faster rate with the lowering of T_n. The effect of the significant phonon energy can be felt more and more with lower lattice temperature and higher acoustic velocity in the material. When numerical calculations are done considering the samples of Si and Ge with the material parameters given in Table I, one can obtain Figs. 1 and 2.

The figures show how significantly the finite value of the phonon energy changes the rate of increase of the phonon number at any T_n for different values of the lattice temperature in comparison to what follows from the traditional theory. It is also apparent that the finite phonon energy brings in only little changes in the phonon population if T_L is higher than 20 K. This is obviously moreso in Ge than in Si because it is the significance of the phonon energy relative to the thermal energy of the carriers that actually brings in the changes. All these observations make it interesting to see how the same effect influences the subsequent calculations of the energy loss of the nonequilibrium carriers under the conditions of low lattice temperatures.

The average rate of energy loss of a carrier to the acoustic mode lattice vibrations is given by

$$\left\langle\frac{d\varepsilon}{dt}\right\rangle_{\rm ac}=-\frac{1}{n_0V}\sum_{\bar{q}}\hbar u_l q\left(\frac{\partial N_{\bar{q}}}{\partial t}\right). \tag{5}$$

Now in order to carry out the integration in $\bar{q}$ space, expressions for $N_{\bar{q}}$ and the limits for the magnitude of q must be ascertained under the conditions of low temperature of inter-

TABLE I. Material parameters of Si and Ge (Ref. 17). m_0 is the free electron mass.

Physical parameters	Si	Ge
Acoustic deformation Potential constant E_1 (eV)	9.0	20.29
Longitudinal acoustic Velocity u_l ($\times10^5$ cm s^{-1})	9.037	5.4
Effective mass m^*	$0.32m_0$	$0.12m_0$
Density ρ (g cm^{-3})	2.329	5.32
Debye temperature θ_D (K)	730	430
Optical deformation Potential constant D ($\times10^8$ eV cm^{-1})		5.5

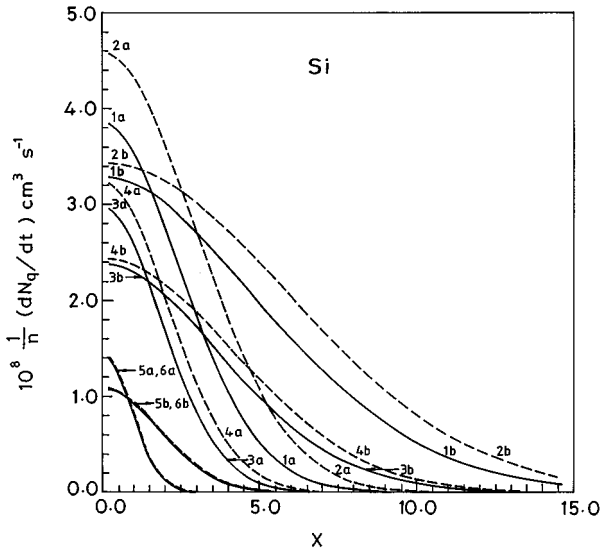

FIG. 1. Rate of increase of phonon number in Si due to interaction of nonequilibrium electrons with the intravalley acoustic phonons. Curves 1 and 2, 3 and 4, 5 and 6 are for lattice temperatures of 2, 4, and 20 K, respectively, of which the solid curves 1, 3, and 5 are obtained from the theory developed here and, the dashed ones 2, 4, and 6 are obtained from the traditional theory. The curves marked *a* are for $T_n=2.5$ whereas those marked *b* are for $T_n=10$.

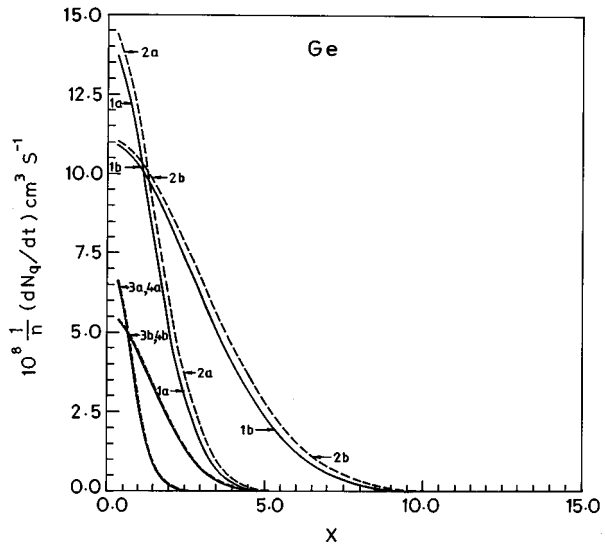

FIG. 2. Rate of increase of phonon number in Ge due to interaction of nonequilibrium electrons with the intravalley acoustic phonons. Curves 1 and 2, 3, and 4 are for lattice temperatures of 1 and 4 K, respectively, of which the solid curves 1 and 3 are obtained from the theory developed here and, the dashed ones 2 and 4 are obtained from traditional theory. The curves marked *a* are for $T_n=2.5$ whereas those marked *b* are for $T_n=10$.

est here. A good approximation of the true $N_{\bar{q}}$ in the low-temperature region is given by the truncated Laurent's expansion of the form[7]

$$N_{\bar{q}}(x)=\begin{cases}\dfrac{1}{x}-\dfrac{1}{2}+\dfrac{1}{12}x-\dfrac{1}{720}x^3 & \text{for } x<\bar{x}\\ \exp(-x) & \text{for } x\geqslant\bar{x},\end{cases} \tag{6}$$

where $\bar{x}=3.5$. Since $(\partial N_{\bar{q}}/\partial t)$ given by (3) falls off rapidly for large q the upper limit may be taken to be $\propto$. Hence one obtains

$$\left\langle\frac{d\varepsilon}{dt}\right\rangle_{\rm ac}=-\mathscr{A}_{\rm ac}\left[D_{\rm ac}+\frac{1}{2}\sum_{j=1}^{\infty}(-1)^j\frac{G_j}{j!(T_n)^j}\right], \tag{7}$$

where $\mathscr{A}_{\rm ac}=(k_BT_L)^4u_lT_n/4\pi^2(\hbar u_l)^3N_c(T_e)l_{\rm ac}$,

$$D_{\rm ac}=\frac{1}{2a^2}\Gamma(2,ab^2)+\frac{3b}{2a^{3/2}}\Gamma(3/2,ab^2)+\frac{3b^2}{2a}\Gamma(1,ab^2)+\frac{b^3}{2a^{1/2}}\Gamma(1/2,ab^2),$$

$$G_j=\sum_{r=0}^{j+2}g_2(j)\Gamma_{12}+\sum_{r=0}^{j+3}g_3(j)[(1/2)\Gamma_{12}+\Gamma_2]+(1/12)\sum_{r=0}^{j+4}g_4(j)\Gamma_{12}-(1/720)\sum_{r=0}^{j+6}g_6(j)\Gamma_{12}+\exp[-(ab^2-d^2/4a)]\sum_{r=0}^{j+3}h(j)\Gamma_3,$$

$$g_m(j)=\binom{j+m}{r}a^{-(r+1)/2}b^{j+m-r},\quad \text{where } m \text{ is integer},$$

$$h(j)=\binom{j+3}{r}a^{[(r-1)/2]-j-3}(d/2)^{j+3-r},$$

$$\binom{P}{n}=\frac{P(P-1)\cdots(P-n+1)}{1.2\cdots n},\quad \binom{P}{0}=1,$$

$$\Gamma_1=\Gamma\left[\frac{(r+1)}{2},ab^2\right],$$

$$\Gamma_2=\Gamma\left[\frac{r+1}{2},a(\bar{x}-b)^2\right],$$

$$\Gamma_3=\Gamma\left[\frac{r+1}{2},a(\bar{x}-d/2a)^2\right],$$

$\Gamma_{12}=\Gamma_1-\Gamma_2$, $\Gamma(\alpha,\beta)$ is incomplete Γ function,[18] and $d=(1/2T_n-1)$.

It is easy to see that under the condition when the lattice temperature is high so that both x and b are small and the phonons carrying negligibly small energy obey equipartition law, the expression (7) reduces to its traditional form obtained elsewhere.[4]

The average rates of energy loss of the nonequilibrium electrons in Si and Ge to the acoustic mode lattice vibration for any value of the average energy are calculated from (7) at different lattice temperatures. The same rates are obtained from the traditional results[4] for a comparison. Again in order to compare these results and the results for the rate of energy loss to optical modes $\langle d\varepsilon/dt\rangle_{\rm op}$ in Ge the latter has been calculated from the expression that may also be obtained from (1) for energies exceeding the optical phonon energy. We repeat here the expression for a ready reference:[4]

$$\left\langle\frac{d\varepsilon}{dt}\right\rangle_{\rm op}=-\frac{(m^*)^{3/2}D^2(2k_BT_e)^{1/2}}{\pi^{3/2}\hbar^2\rho}B(x_0,x_e), \tag{8}$$

where

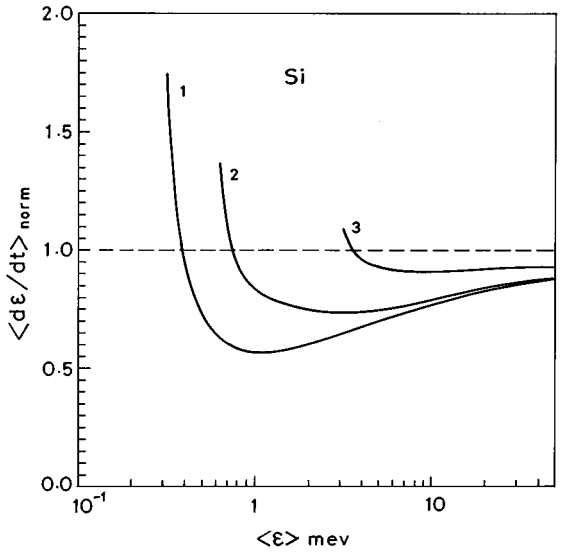

FIG. 3. Rates of energy loss of nonequilibrium electrons, normalized to their traditional values, in Si due to interaction with intravalley acoustic mode lattice vibrations. Curves 1, 2, and 3 are for lattice temperatures of 2, 4, and 20 K, respectively.

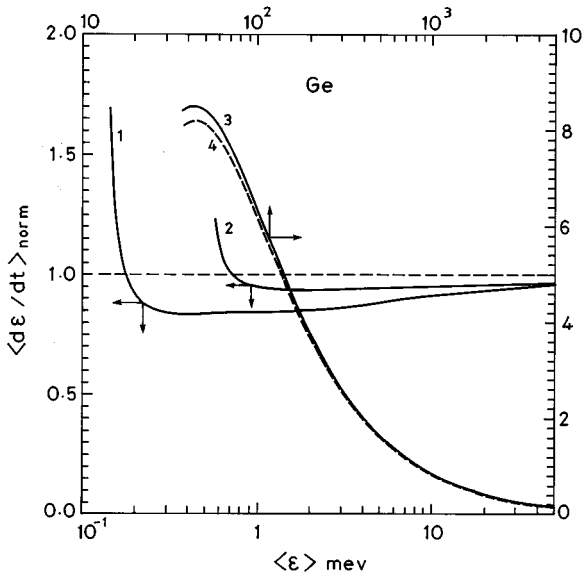

FIG. 4. Normalized rates of energy loss of nonequilibrium electrons in Ge due to interaction with intravalley acoustic and optical mode lattice vibrations. Curves 1 and 2 are for acoustic interaction at 1 and 4 K, respectively, and when the rates are normalized to their traditional values. Curves 3 and 4 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 interaction.

$$B(x_0,x_e)=\frac{\exp(x_0-x_e)-1}{\exp(x_0)-1}\,\frac{x_e}{2}\exp\left(\frac{x_e}{2}\right)K_1\left(\frac{x_e}{2}\right);$$

$x_e=\hbar\omega_0/k_BT_e$, $x_0=\hbar\omega_0/k_BT_L$. K_1 is Bessel function of the second kind. ω_0 is the optical phonon frequency, D is the interaction constant for nonpolar optical modes.

It may be noted here that the traditional result for $\langle d\varepsilon/dt\rangle_{ac}$ as well as the result for $\langle d\varepsilon/dt\rangle_{op}$ do not much depend upon the lattice temperature if $T_e\gg T_L$. However, for acoustic interaction the change in energy-loss rate relative to the traditional value indeed depends upon the lattice temperature, making it lower for the higher temperatures. The results of the calculation of the normalized loss rates in Si and Ge are plotted in Figs. 3 and 4, respectively. It may be seen how the finite phonon energy of the acoustic phonons brings in distinct changes in the energy-loss rates of the nonequilibrium electrons at low lattice temperatures. For lower values of $\langle\varepsilon\rangle$ the absolute rates are now greater than what can be predicted from the traditional theory. The significant discrepancy of our results from those of the traditional theory increases with the decrease of the lattice temperature. Moreover, it is again the significant value of the relative energy of the acoustic phonons that makes the corresponding loss rate exceed the traditional values at lower energies the lower the lattice temperature, and in Ge it exceeds that due to optical modes for higher values of the energy compared to what follows from the traditional theory.

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[1] P. A. Wolff, Phys. Rev. **95**, 1415 (1954).
[2] W. Shockley, *Proceedings of the International Conference on Semiconductor Physics, Prague, 1960* (Czechoslovakian Academy of Sciences, Prague, 1961).
[3] G. A. Baraff, Phys. Rev. **133**, A26 (1964).
[4] E. M. Conwell, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1967), Suppl. 9.
[5] T. N. Morgan, Bull. Am. Phys. Soc. **2**, 265 (1959).
[6] Z. S. Kachlishvili, Fiz Tekh. Poluprovodn. **2**, 580 (1968) [Sov. Phys. Semicond. **2**, 478 (1968)].
[7] C. Canali, C. Jacoboni, F. Nava, G. Ottaviani, and A. Alberigi Quaranta, Phys. Rev. B **12**, 2265 (1975).
[8] S. H. Koenig, R. D. Brown, and W. Schillinger, Phys. Rev. **128**, 1668 (1962).
[9] J. Yamashita, J. Phys. Soc. Jpn. **16**, 720 (1961).
[10] A. Zylbersztejn, Phys. Rev. **127**, 744 (1962).
[11] V. F. Banaya, L. I. Veselova, E. M. Gershenzon, and V. A. Chuenkov, Fiz. Tekh. Poluprovodn. **7**, 1972 (1973) [Sov. Phys. Semicond. **7**, 1315 (1974)].
[12] F. A. Khan and D. P. Bhattacharya, J. Phys. C **17**, 3463 (1984).
[13] T. K. Pramanik and D. P. Bhattacharya, Phys. Status Solidi B **177**, 425 (1993).
[14] V. V. Mitin, Appl. Phys. A **39**, 123 (1986).
[15] S. S. Paul and D. P. Bhattacharya, Phys. Rev. B **39**, 13 521 (1989).
[16] A. K. Ghorai and D. P. Bhattacharya, Phys. Rev. B **47**, 13 858 (1992).
[17] L. Reggiani, *Hot Electron Transport in Semiconductors* (Springer-Verlag, Berlin, 1985).
[18] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965).