Letters to the Editor

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Inelasticity of acoustic scattering in Monte Carlo transport calculation for nonparabolic semiconductor

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Inclusion of the inelasticity of the deformation potential acoustic scattering in hot electron transport calculations is important inasmuch as the acoustic energy loss increases with increasing electric field and may contribute significantly to the total energy loss in situations where acoustic scattering predominates, (Conwell 1967) Formulas for incorporating the inelasticity of the acoustic scattering in the Monte Carlo study of hot carrier problems have been recently reported for parabolic and spherical energy bands, (Sheng & Westgate 1973) In narrow-gap semiconductors, however, the energy wavevector relation for the carriers is nonparabolic and one ought to consider this nonparabolicity in a realistic treatment of the transport coefficients In this note we shall describe how to incorporate the inelasticity of the acoustic scattering in the Monte Carlo calculation of hot electron transport in nonparabolic semiconductors

The electron energy wavevector ($E-\boldsymbol{k}$) relation for nonparabolic bands is written as (Conwell & Vassel 1968)

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(E) = E(1+\alpha E) \qquad \ldots (1)$$

where $\hbar$ is the Drac constant, m^* is the band-edge effective mass, and α is given by

$$\alpha = \frac{1}{E_g}\left(1-\frac{m^*}{m_0}\right)^2 \qquad \ldots (2)$$

m_0 is the free electron mass, and E_g is the direct gap energy.

In the treatment of acoustic scattering, as usual, we have not distinguished between longitudinal and transverse waves, and have assumed a spherical symmetry. The rate of transition from wavevector $\boldsymbol{k}$ to $\boldsymbol{k}'$ due to this scattering is then expressed as (Conwell 1967)

$$S_a{}^{\pm}(\boldsymbol{k}, \boldsymbol{k}') = \frac{2\pi}{\hbar} B_a(\boldsymbol{k}, \boldsymbol{k}')(N_a + \tfrac{1}{2} \mp \tfrac{1}{2})\delta[E(\boldsymbol{k}') - E(\boldsymbol{k}) \mp \hbar u q] \qquad \ldots (3)$$

the upper and the lower signs referring to the processes of absorption and emission respectively. Here

$$B_a(\boldsymbol{k}, \boldsymbol{k}') = \frac{E_1^2 \hbar q}{2V\rho u} G(\boldsymbol{k}, \boldsymbol{k}') \qquad \ldots (4)$$

E_1 is the acoustic deformation potential constant. $\boldsymbol{q}$ is the phonon wavevector, V is the crystal volume, ρ is the mass density, u is the acoustic velocity and N_a is the acoustic phonon occupation number. $G(\boldsymbol{k}, \boldsymbol{k}')$ is the overlap integral representing the admixture of p-type valence band wave functions, and can be written as (Kane 1957)

$$G(\boldsymbol{k}, \boldsymbol{k}') = (a_k a_{k'} + c_k c_{k'} \cos\beta')^2 \qquad \ldots (5)$$

where

$$a_k = \left[\frac{1 + \alpha E(\boldsymbol{k})}{1 + 2\alpha E(\boldsymbol{k})} \right]^{\frac{1}{2}} \qquad \ldots (6)$$

$$c_k = \left[\frac{\alpha E(\boldsymbol{k})}{1 + 2\alpha E(\boldsymbol{k})} \right]^{\frac{1}{2}} \qquad \ldots (7)$$

and β' is the angle between $\boldsymbol{k}$ and $\boldsymbol{k}'$

It may be mentioned that eqs (1), (5), (6) and (7) have been obtained on the assumption that the spin-orbit splitting of the valence band, Δ is negligibly small. However, Fawcett *et al* (1970) have shown that they are still a good approximation when Δ is large

Substituting eq (4) into eq (3) and integrating over all $\boldsymbol{k}'$ we have for the total scattering rate from the state $\boldsymbol{k}$:

$$\lambda_a^{\pm}(k) = \frac{E_1^2}{8\pi^2\rho u} \int_{q=q_{min}}^{q_{max}} \int_{\beta=0}^{\pi} \int_{\phi=0}^{2\pi} q^3 G(\boldsymbol{k}, \boldsymbol{k}')(N_a + \tfrac{1}{2} \mp \tfrac{1}{2}) \delta[E(\boldsymbol{k}') - E(\boldsymbol{k}) \mp \hbar u q] \times \sin\beta \, d\beta \, d\phi \, dq \qquad \ldots (8)$$

where (q, β, ϕ) are the spherical coordinates of $\boldsymbol{q}$ with the $\boldsymbol{k}$-direction chosen as the polar axis. Evaluating the angular integrations in eq (8) gives.

$$\lambda_a^{\pm}(k) = \frac{E_1^2 m^*}{4\pi\rho u\hbar^2 k} \int_{q_{min}}^{q_{max}} q^2 [G(\boldsymbol{k}, \boldsymbol{k}')]_{\beta=\beta_0} (N_a + \tfrac{1}{2} \mp \tfrac{1}{2})(1 + 2\alpha E \pm 2\alpha\hbar u q) dq \qquad \ldots (9)$$

β_0 represents the value of β for which the argument of the δ-function in eq. (8) is zero, and is given by

$$\cos\beta_0 = \mp \frac{q}{2k} + \frac{m^* u}{\hbar k} (1 + 2\alpha E \pm \alpha \hbar u q) \qquad \ldots (10)$$

To obtain $[G(\boldsymbol{k}, \boldsymbol{k}')]_{\beta=\beta_0}$ we note that $\alpha E < 1$, and $m^* u/\hbar k \ll 1$. Furthermore, we can neglect $\alpha \hbar u q$ with respect to αE without any serious error, (Costato & Reggiani 1972). We may then write from eqs. (5), (6), (7) and (10), to a good approximation

$$[G(\boldsymbol{k}, \boldsymbol{k}')]_{\beta=\beta_0} = \left(1 - \frac{q^2}{2k^2} \cdot \frac{\alpha E}{1+2\alpha E}\right)^2. \quad \ldots (11)$$

Eq. (9) then reduces to

$$\lambda_a^{\pm}(k) = \frac{E_1^2 m^*}{4\pi\rho u^2 \hbar k} \int_{q_{mi_n}}^{q_{ma_x}} q^2 \left(1 - \frac{q^2}{2k^2} \cdot \frac{\alpha E}{1+2\alpha E}\right)^2 (N_a + \tfrac{1}{2} \mp \tfrac{1}{2})(1 + 2\alpha E \pm 2\alpha \hbar u q) dq \quad \ldots (12)$$

The limits of integration q_{mi_n} and q_{ma_x} are obtained from the condition $|\cos\beta| \leqslant 1$ with the requirement that the argument of the δ-function vanishes. The result is

$$q_{mi_n} = 0 \quad \ldots (13)$$

$$q_{ma_x} = \frac{2k \pm \frac{2m^* u}{\hbar}(1+2\alpha E)}{1 - 2\alpha m^* u^2} \simeq 2k \pm \frac{2m^* u}{\hbar}(1+2\alpha E) \quad \ldots (14)$$

since $2\alpha m^* u^2 \ll 1$. We shall now substitute eqs (13) and (14) into eq (12), make the equipartition approximation for N_a

$$N_a + \tfrac{1}{2} = \frac{k_B T_L}{\hbar u q} \quad \ldots (15)$$

k_B and T_L being the Boltzmann constant and the lattice temperature respectively, and retain only the terms up to the first order in $m^* u/\hbar k$. The approximations are valid for most materials above about 20°K. We then obtain from eq (12)

$$\lambda_a^{\pm}(k) = \frac{m^{*3/2} E_1^2 k_B T_L \gamma^{\frac{1}{2}}(E)}{\sqrt{2}\pi\rho\hbar^4 u^2} \left[\frac{(1+\alpha E)^2 + (1/3)\alpha^2 E^2}{1+2\alpha E} \pm \frac{\sqrt{2m^* u}}{\gamma^{\frac{1}{2}}(E)} \left\{1 - 2\xi_a(E)\gamma(E)\left(\frac{1}{k_B T_L} - \frac{4\alpha}{1+2\alpha E}\right)\right\}\right] \quad \ldots (16)$$

where,

$$\xi_a(E) = \frac{35 + 56\alpha E + 32\alpha^2 E^2}{105(1+2\alpha E)}. \quad \ldots (17)$$

From eqs. (12) and (15) we obtain the phonon wavevector probability distribution

$$P_a^{\pm}(q) = A\left[q^2\left(1 - \frac{q^2}{2k^2} \cdot \frac{\alpha E}{1+2\alpha E}\right)^2 \left(\frac{k_B T_L}{\hbar u q} \mp \tfrac{1}{2}\right)(1 + 2\alpha E \pm 2\alpha \hbar u q)\right] \quad \ldots (18)$$

where A is a normalizing coefficient. To choose q for a given value of k, use

is made of eq. (18). If r is a uniformly distributed random number between 0 and 1, we have

$$r = \int_{q_{min}}^{q} P_a^{\pm}(q)dq \Big/ \int_{q_{min}}^{q_{max}} P_a^{\pm}(q)dq \qquad (19)$$

which may be solved for q. For weak nonparabolicity, fairly high lattice temperatures and not very high electric fields, eq. (19) yields approximately

$$q \approx q_{max}\sqrt{r}. \qquad \ldots (20)$$

The absorption and emission events are determined with the aid of eq. (16) by the usual procedure. (Fawcett *et al* 1970) q is determined from eq. (19) and β_0 is calculated from eq. (10). If another uniformly distributed random number is generated between 0 and 2π to fix the azimuthal angle ϕ, the final electron state after scattering is completely specified.

It may be noted that the sum of λ_a^+ and λ_a^- given by eq. (16) yields the expression for the total acoustic scattering rate in the elastic approximation, (Fawcett *et al* 1970). Furthermore, by setting $\alpha = 0$ in eqs. (10), (16) and (18) one readily obtains the expressions for a parabolic band structure.

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Partial structure factors for liquid alloys

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Recent studies (Gopala Rao & Murthy 1974, 1975a, 1975b) proved the usefulness of square well potential in the theoretical investigations of conducting fluids like liquid metals. In this note we propose to extend the same to binary liquid alloys, taking Na—K alloy as an example, for calculating the partial structure factors, S_{ij}, under the mean spherical model (MSM) approximation (Gopala Rao & Murthy, 1974)