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Theory of non-radiative capture of carriers by multiphonon processes for deep centres in semiconductors

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Abstract. A quantum-mechanical calculation of the non-radiative transition rate by multiphonon processes is performed by employing a more direct mathematical approach than those used by previous workers. Based on the trap potential model proposed by Lucovsky and the optical deformation form of electron-phonon interaction, the analytical expression for the carrier capture cross section is brought to a transparent form for easy comparison with experiments after some transcriptions. The effect due to the charge state of the deep centre is also discussed. Both the absolute magnitude and the temperature-dependent behaviour of the capture cross section predicted in our calculations are well supported by the experimental results of various deep centres in semiconductors. In particular, good fits are obtained for the temperature dependence of the experimental electron capture cross sections reported by Henry and Lang for B and A centres in GaAs. The accuracy of the Huang–Rhys factor and the phonon energy obtained for the B centre is corroborated by the good fittings obtained for the photoionization cross section data reported by Wang *et al.* The results of our theory are also shown to be useful in identifying more accurately the charge state of a deep centre.

1. Introduction

Quantum-mechanical calculations of non-radiative multiphonon (NMP) transition rate in solids have been performed by many previous workers [1–4]. However, their results, being complicated, need to be simplified by assuming some specific temperature range before they can be used to fit the experimental data. Thus the comparison between theory and experiment is unavoidably limited. An example is the fit to the electron capture cross section of the B centre in GaAs [5]. Some progress towards the solution of the problem has been made recently by Goguenheim and Lannoo [6], who obtained a compact expression for the capture cross section valid for the whole temperature range. However, the estimation of the absolute magnitude of the capture cross sections in deep centres for semiconductors remains to be worked out. Such calculations would require detailed models of the electronic states and the electron–phonon interaction. Nonetheless, the use of these models would also contribute towards physical understanding of carrier capture mechanism in semiconductors.

In this paper an analytical calculation of the carrier capture cross section of deep centres in semiconductors is presented. Section 2 outlines a quantum-mechanical calculation of NMP transition rate in solids, which is based on a more direct mathematical approach than those of the previous workers. In section 3 a set of trap-related parameters for semiconductors is calculated based on a simple potential proposed by Lucovsky [7]. The form of electron-phonon interaction used in the calculation is that of optical deformation, which is believed to be dominant [8]. The relations of the trap-related parameters so obtained are used in section 4 to simplify the expression for the capture cross section to a more transparent form

for comparison with experiments. The theoretical estimates of the absolute magnitudes and the temperature-dependent behaviour of the capture cross sections for typical neutral centres are found to be well supported by the experimental results reported in [9]. In section 5 detailed fits of our theory to Henry and Lang's experimental data [9] for the B and A centres in GaAs are performed. The values of the Huang–Rhys factor S and average phonon energy $\hbar\omega$, extracted from our fit to the data for the B centre, are quite different from those obtained by Goguenheim and Lannoo [6]. In order to corroborate the accuracy of the values of S and $\hbar\omega$ that we obtained, they are used to obtain the photoionization cross-section curves $\sigma_B^{\text{ph}}(h\nu)$ of the B centre reported by Wang *et al* [10]. The good fits to all the curves at various temperatures indicate that our values of S and $\hbar\omega$ are able to explain the observed thermal broadening effect of $\sigma_B^{\text{ph}}(h\nu)$.

2. Calculation of non-radiative multiphonon transition rate in solids

The NMP transitions of electrons in solids are believed to be due to the breakdown of the adiabatic approximation since the Born–Oppenheimer wavefunction $\Psi_{in}(r, Q)$ chosen for the stationary state of a system cannot be strictly stationary. The breakdown of the adiabatic approximation leads to a perturbation Hamiltonian \mathcal{H}_{NA} that mediates the transition of electrons from one state to another. The operator is defined by [11]

$$\mathcal{H}_{\text{NA}}\Psi_{in}(r, Q) = -\frac{\hbar}{2} \sum_s \left(X_{in}(Q) \frac{\partial^2}{\partial Q_s^2} \Phi_i(r, Q) + 2 \frac{\partial}{\partial Q_s} X_{in}(Q) \frac{\partial}{\partial Q_s} \Phi_i(r, Q) \right) \quad (1)$$

where $\Phi_i(r, Q)$ and $X_{in}(Q)$ are respectively the electronic and the lattice vibrational parts of the Born–Oppenheimer wavefunction $\Psi_{in}(r, Q)$, and they satisfy the following eigenvalue equations:

$$\begin{aligned} [\mathcal{H}_e + \mathcal{H}_{\text{el}}]\Phi_i(r, Q) &= U_i(Q)\Phi_i(r, Q) \\ [\mathcal{H}_l + U_i(Q)]X_{in}(Q) &= E_i X_{in}(Q). \end{aligned} \quad (2)$$

In the equations above, \mathcal{H}_e , \mathcal{H}_l and \mathcal{H}_{el} are the electronic, the lattice vibrational and the electron–phonon coupling parts of the total Hamiltonian. Here r is the position vector of the electron and Q is the configuration coordinate, which denotes symbolically all the lattice coordinates Q_s .

The radiationless transition rate W_{ab} from state a to b due to the breakdown of the adiabatic approximation is given by the Fermi–golden rule:

$$W_{ab} = \frac{2\pi}{\hbar} \text{Ave}_n \sum_{n'} |\langle \Psi_{bn'} | \mathcal{H}_{\text{NA}} | \Psi_{an} \rangle|^2 \delta(E_b - E_a) \quad (3)$$

where Ave_n denotes a thermal average over all the states of the lattice vibrations in the initial state a .

Linear electron–lattice interaction is usually assumed, and may be expressed by

$$\mathcal{H}_{\text{el}} = \sum_s G_s(r)(Q_s - Q_s^a) \quad (4)$$

where Q_s^a is the equilibrium position of the lattice vibrations in the initial state a . In solving equation (2), the term \mathcal{H}_{el} is treated as a perturbation. The equilibrium position of the lattice vibrations may then be expressed as

$$Q_s^i = -\langle \Phi_i^0 | \mathcal{G}_s(r) | \Phi_i^0 \rangle / \hbar \omega_s$$

where $|\Phi_i^0\rangle$ is the zeroth-order electronic wavefunction, which satisfies $\mathcal{H}_e |\Phi_i^0\rangle = U_i^0 |\Phi_i^0\rangle$, and ω_s is the angular frequency of the lattice vibration for the s th mode. With the assumption of linear electron-phonon interaction, the lattice vibrations are still harmonic oscillators and their angular frequencies remain unchanged. The lattice vibrational part of the wavefunction may then be expressed as

$$|X_{in}(Q)\rangle \prod_s |n_s(Q_s - Q_s^i)\rangle$$

where n_s is the quantum number of the lattice vibrations. The difference in the total energy between the two states a and b is then given by

$$E_b - E_a = -E_T + \sum_s (n'_s - n_s) \hbar \omega_s \tag{5}$$

where E_T is the electronic energy separation between the states a and b . The shift Λ of the equilibrium position of the lattice vibrations during the transition from state a to b is defined by

$$\Lambda_s = Q_s^b - Q_s^a.$$

The Huang-Rhys factor S , which will be used later, is then defined as

$$S = \frac{1}{2} \sum_s \Lambda_s^2.$$

Within the so-called non-Condon approximation in solving equation (2), the transition matrix element in equation (3) can be reduced to the form [12]:

$$\langle \Psi_{bn'} | \mathcal{H}_{NA} | \Psi_{an} \rangle = \sum_s \langle \Phi_b^0 | \mathcal{G}_s(r) | \Phi_a^0 \rangle \langle X_{bn'} | Q_s - Q_s^a | X_{an} \rangle. \tag{6}$$

With the equation above and the notation $V_s = \langle \Phi_b^0 | \mathcal{G}_s(r) | \Phi_a^0 \rangle$, the transition rate W_{ab} is then expressed as

$$W_{ab} = \frac{2\pi}{\hbar} \text{Ave}_n \sum_{n'} \left| \sum_s V_s \langle X_{bn'} | Q_s - Q_s^a | X_{an} \rangle \right|^2 \delta(E_b - E_a). \tag{7}$$

Before performing the detailed calculation of the vibration overlaps in equation (7), it is necessary to assume that all modes of lattice vibrations have the same frequency ω . This assumption is needed in order to obtain simple applicable results. The detailed calculation is given in the appendix, where we reproduce by using a more direct mathematical approach the same results as obtained by Gustche [4] and by Goguenheim and Lannoo [6]. A more compact form of W_{ab} can be obtained if we make use of a relation for modified Bessel functions as was done in [6]. This compact form would permit us to gain deeper insight into the behaviour of W_{ab} with respect to its parameters. The relation used is

$$I_{m-1}(\zeta) - I_{m+1}(\zeta) = (2m/\zeta) I_m(\zeta). \tag{8}$$

The compact form of W_{ab} so obtained from equation (A5) is

$$W_{ab} = \frac{2\pi}{\hbar} \left[\frac{|V\Lambda|^2}{4} \left(1 - \frac{E_T}{S\hbar\omega} \right)^2 G(E_T) + \frac{|V|^2}{2} \left(1 - \frac{|V\Lambda|^2}{2S|V|^2} \right) [\bar{n}G(E_T + \hbar\omega) + (\bar{n} + 1)G(E_T - \hbar\omega)] \right]. \tag{9}$$

The auxiliary function $G(E_T)$ and the notations $|V\Lambda|^2$ and $|V|^2$ are defined in the appendix.

3. Evaluation of the trap parameters for semiconductors

The behaviour of NMP transition rate with respect to temperature is governed by the three parameters S , $|V|^2$ and $|V\Lambda|^2$. These matrix elements depend on the form of electron-phonon coupling (which is assumed to be linear in the lattice displacement) and also on the electronic wavefunctions of both the initial and final states. For thermal capture of carriers in semiconductors, the free state f and the bound state b are taken as the initial and final states, respectively. For convenience of discussion, we will assume that the free carriers are electrons, although our theory applies equally well to holes.

To build up the bound-state wavefunction, we use the trap potential model proposed by Lucovsky [7], which has been used successfully in the calculation of photoionization in deep centres. The bound-state wavefunction $\Psi_b^0(r)$ for the model may be expressed as

$$\Phi_b^0(r) = A \exp(-r/a)/r \quad (r > R_0) \quad (10)$$

where $a = \hbar/(2m^* E_T)^{1/2}$, $A = 1/(2m^* a)^{1/2}$, R_0 is the radius of the effective potential of the trap, and m^* is the electron effective mass.

As a deep bound state is very localized relative to a free state, the free-state wavefunction used in performing the integrals on the matrix elements is limited to the region where $r \rightarrow 0$. To take into account the scattering effect on the free-state wavefunction, it is assumed that, beyond the short-range attractive potential, there is a long-range Coulomb potential with charge Z . Under such a model, the free-state wavefunction for $r \rightarrow 0$ is given by

$$\Phi_f^0 = (1/V_c^{1/2})C_0^{1/2}(\epsilon) \quad (11)$$

where V_c is the volume of the whole crystal and $C_0(\epsilon)$ is the Sommerfeld factor [13].

For the electron-phonon coupling, we consider the form based on the optical deformation potential:

$$\mathcal{G}_s(r) = D_0 \exp(iq_s \cdot r) \quad (12)$$

where q_s is the phonon wavevector and D_0 is a q_s -independent constant.

The matrix elements S , $|V|^2$ and $|V\Lambda|^2$ are then evaluated by ignoring the weaker short-wavelength contributions, i.e. $q_s a \gg 1$. Moreover, the following important relations of the matrix elements are obtained:

$$\begin{aligned} |V|^2 &= [16\pi a^3 C_0(\epsilon)/V_c] S(\hbar\omega)^2 \\ |V\Lambda|^2 &= [32\pi a^3 C_0(\epsilon)/V_c] S^2(\hbar\omega)^2. \end{aligned} \quad (13)$$

From these relations, it can be seen that the second term of equation (9) for NMP transition rate, which has the factor

$$(1 - |V\Lambda|^2/2S|V|^2)$$

is zero. This important result leads to a very much simplified expression for W_{fb} , which is

$$W_{fb} = [16\pi^2 a^3 C_0(\epsilon)/\hbar V_c](E_T - S\hbar\omega)^2 G(E_T). \quad (14)$$

In contrast, Goguenheim and Lannoo [6] obtained their W_{fb} in terms of $G(E_T)$ by reducing the term $\bar{n}G(E_T + \hbar\omega) + (\bar{n} + 1)G(E_T - \hbar\omega)$ of equation (9) approximately to $G(E_T)$ through a certain relation of the modified Bessel functions. Therefore, even after the reduction, their equation for W_{fb} is still more complex for interpretation than ours.

4. Capture cross sections

The transition of capturing processes considered above refers to that from the bottom of the conduction band to the trap level. However, owing to the distribution of free electrons in the conduction band, it is required to take an average of the capture coefficient $C_p(T)$, which is

$$\bar{C}_p(T) = \int_{\text{CB}} V_c W_{fb} f(\epsilon) \rho(\epsilon) d\epsilon \quad (15)$$

where ϵ is the thermal energy of a free electron, $f(\epsilon)$ is the normalized distribution of the free electrons in the conduction band and $\rho(\epsilon)$ is the density of states of the conduction band. It can be seen easily that the main contribution in the integration of equation (15) comes from a range $\epsilon < \epsilon_{\text{max}}$, where ϵ_{max} is the upper limit of ϵ in which $C_0(\epsilon)f(\epsilon)\rho(\epsilon)$ still has a significant value for the integration. Typically ϵ_{max} is of the order of kT .

In order to perform the integration of equation (15), we need to simplify the function $G(E_T + \epsilon, T)$ in $C_p(E_T + \epsilon, T)$. With the following relation [6] for the modified Bessel function I_m , which is valid for $(m^2 + \zeta^2)^{1/2} \gg 1$ (a condition satisfied by all deep centres),

$$I_{m-1}(\zeta) + I_{m+1}(\zeta) \simeq 2[(m^2 + \zeta^2)^{1/2}/\zeta]I_m(\zeta)$$

and equation (8), we obtain the approximate relation for integers $\Delta m \ll m$:

$$I_{m+\Delta m}(\zeta) \simeq [(m^2 + \zeta^2)^{1/2} - m]/\zeta)^{\Delta m} I_m(\zeta).$$

With this result and noting that $\epsilon_{\text{max}} \ll E_T$ (for deep centres), the integration of equation (15) would lead to

$$\bar{C}_p(T) \simeq (16\pi^2 a^3 / \hbar)(E_T - S\hbar\omega)^2 G(E_T, T) F(T) \quad (16)$$

where

$$F(T) = \int_0^{\epsilon_{\text{max}}} \left(\frac{(P^2 + \zeta^2)^{1/2} - P}{2\bar{n}S} \right)^{\epsilon/\hbar\omega} C_0(\epsilon) f(\epsilon) \rho(\epsilon) d\epsilon \quad (16a)$$

is a charge-state-dependent function with argument T and $P = E_T/\hbar\omega$. It is evident from equation (16) that the capture coefficient of a deep centre by NMP transition processes is modified by the factor $F(T)$ due to the charge state of the deep centre and the averaging of the free-electron distribution. Moreover, we have obtained an expression for $\bar{C}_p(T)$ in which the charge-state-dependent component $F(T)$ is separated from the NMP-dependent component $(E_T - S\hbar\omega)^2 G(E_T, T)$. Given the charge state of a deep centre, the exact values of $F(T)$ given by equation (16a) can be computed numerically. Such calculations have been performed for various types of deep centres. The results of the charge-state-dependent behaviour are too involved to be discussed in detail in the present paper and will be presented in another publication. Nonetheless an important result of our findings is that, when the temperature-dependent behaviour of $\bar{C}_p(T)$ is dominated by the NMP process, i.e. the $G(E_T, T)$ term, the charge-state-dependent function $F(T)$ can be approximated as a constant. Hence one can accurately reproduce the exact results of equation (16) by adopting the following expression:

$$\bar{C}_p(T) = F_Z (16\pi^2 a^3 / \hbar)(E_T - S\hbar\omega)^2 G(E_T, T). \quad (17)$$

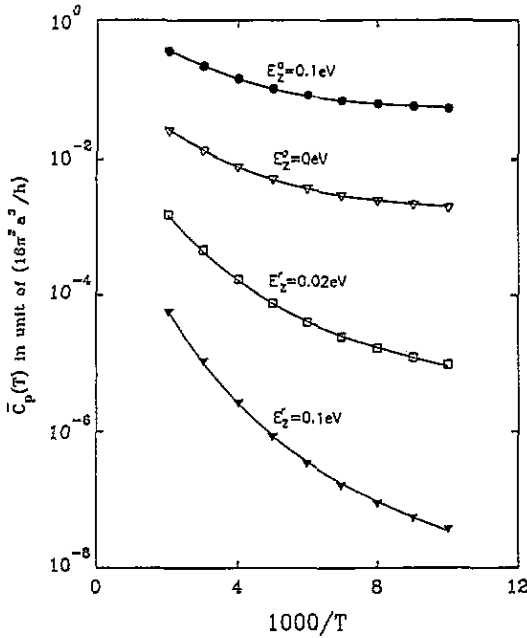


Figure 1. The symbols shown in the figure are the values of $\bar{C}_p(T)$ calculated numerically by using equation (16) with $E_T = 0.4$ eV, $\hbar\omega = 0.025$ eV and $S = 6$; E_Z^a is the Bohr energy for an attractive centre, E_Z^0 for a neutral centre and E_Z^r for a repulsive centre. The $\bar{C}_p(T)$ given by the approximate expression of equation (17) are shown as full curves.

Here $\hbar\omega$ is the effective average phonon energy, which has taken into account the effects of the charge state of a deep centre and the free-electron distribution, and F_Z is a charge-state-dependent constant. The ability of equation (17) to reproduce the exact results of $\bar{C}_p(T)$ is well demonstrated in figure 1, where we compare the $\bar{C}_p(T)$ computed by numerical integration of equation (16) with that given by equation (17) for typical centres.

In principle, F_Z is indicative of the magnitude of the function $F(T)$, which can be computed by numerical integration. For a neutral centre, F_Z is about the order of unity. For an attractive centre, F_Z will be larger than that for a neutral centre. For a repulsive centre, F_Z is a number generally very much less than one. Therefore, an examination of the value of F_Z obtained by the fit of equation (17) to experimental data would immediately reveal the nature of the charge state of a deep centre.

The carrier capture cross section $\sigma(T)$ can be easily found by dividing $\bar{C}_p(T)$ by the thermal velocity of the carriers:

$$\sigma(T) = \sigma_0 \frac{(S\hbar\omega)^2}{(E_T kT)^{1/2}} \left(1 - \frac{E_T}{S\hbar\omega}\right)^2 G(E_T, T) \quad (18)$$

where $\sigma_0 = (2\pi^{5/2}\hbar^2/m^*E_T)F_Z$ is a prefactor that depends on the charge state of the trap centre via F_Z . Equation (18) shows that the temperature dependence of the NMP capture cross section is governed by the auxiliary function $G(E_T, T)$. The function $G(E_T, T)$, as defined, is a polynomial, which can be approximated by an analytic form of the modified Bessel function $I_m(\zeta)$ [14] valid for $(m^2 + \zeta^2)^{1/2} \gg 1$ (a condition satisfied by all deep centres):

$$G(E_T, T) \simeq \frac{1}{\hbar\omega(2\pi)^{1/2}} (P^2 + \zeta^2)^{-1/4} \left(\frac{\zeta}{P + (P^2 + \zeta^2)^{1/2}} \right)^P \times \exp \left((P^2 + \zeta^2)^{1/2} - (2\tilde{n} + 1)S + \frac{P\hbar\omega}{2kT} \right). \quad (19)$$

Such an analytical function of $G(E_T)$ is particularly convenient if a rapid fit of theory to experiment is called for. We would like to remark here that the expression of the auxiliary function $G(E_T)$ in equation (19) is different from those in equation (29) of [6] and equation (12) of [15] unless we let $\zeta = 1$ in the term $\{\zeta/[P + (P^2 + \zeta^2)^{1/2}]\}^P$ of equation (19).

The temperature-dependent behaviour of the capture cross section and its absolute magnitude for various coupling strengths (Huang–Rhys factor) S is illustrated in figure 2 for a typical neutral centre of $E_T = 0.4$ eV and $\hbar\omega = 0.025$ eV. It is easily seen in figure 2 that the temperature dependence of the capture cross section under the NMP mechanism becomes weaker as the temperature is lowered. From the curves drawn in figure 2 and the asymptotic form of equation (18) it can be seen that the extrapolation of the values of the capture cross section σ_∞ as $T \rightarrow \infty$ are confined to a range of 10^{-13} – 10^{-15} cm², which is consistent with Henry and Lang's data [9]. Furthermore, the temperature-dependent behaviours shown in figure 2 are also well supported by the experimental data of [9].

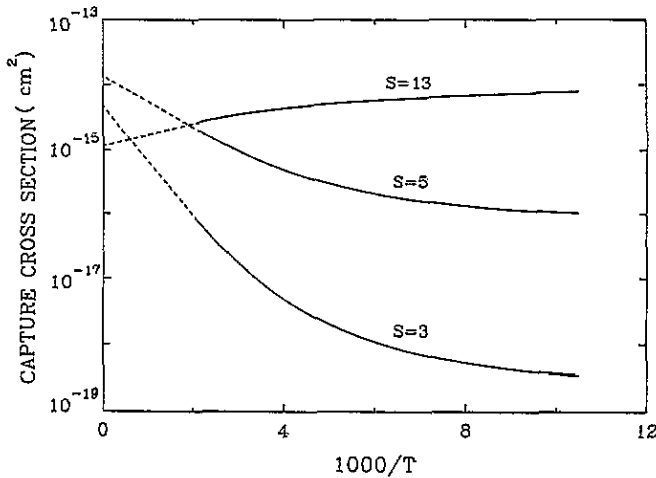


Figure 2. Theoretical curves of the capture cross section versus inverse absolute temperature for neutral centres: $E_T = 0.4$ eV, $\hbar\omega = 0.025$ eV and with $S = 3, 5$ and 13 respectively. The effective mass m^* is taken as $0.067m_0$ for the centres. The broken lines are the extrapolations of the curves at $T \rightarrow \infty$ as done by Henry and Lang [9].

5. Discussion and comparison with experiment

The expression for the capture cross section given in equation (18) can readily be used to fit the experimental data. Fittings have been carried out on the experimental temperature-dependent electron capture cross sections of the native deep centres A and B in GaAs reported by Henry and Lang [9]. The thermal ionization energy E_T used in the fit for each centre is the value reported in experiments such as Hall measurement or capacitive spectroscopy techniques. The free parameters used in the fittings are the Huang–Rhys factor S , the average phonon energy $\hbar\omega$ and σ_0 . Results of the best fit are shown in figure 3. It is found that the temperature-dependent behaviours of the fittings are very sensitive to

the two parameters S and $\hbar\omega$. The values of the parameters used in performing the fits are listed in table 1, which reflect a stronger electron-phonon coupling in the A centre than in the B centre. The average phonon energies $\hbar\omega$ obtained for the two centres coincide with the longitudinal optic (LO) mode phonon energy [18] of GaAs. The theoretically calculated values of the parameter σ_0 assuming neutral centres are also listed in table 1 for comparison with those obtained from the fits. The fairly good agreement between the theoretical and the best-fit values of σ_0 for the B centre implies that the centre is nearly neutral, whereas the larger difference in the values for the A centre indicates that the centre is slightly repulsive. Results on the B centre also demonstrate that a small capture cross section does not necessarily imply that the trap potential is repulsive, a conclusion often drawn by experimentalists.

Table 1. The parameters used in best fittings for A and B centres in GaAs

	A	B
Energy level relative to valence band edge E_v (eV) [9]	$E_v + 0.4$	$E_v + 0.71$
Binding energy at 300 K E_T (eV) [9]	1.03	0.72
Huang-Rhys factor, S	14.34	3.87 (0.56 [6])
Phonon energy, $\hbar\omega$ (meV)	30	30 (34 [6])
Frank-Condon shift, $S\hbar\omega$ (eV)	0.43	0.116 (0.019 [6])
Charge-dependent factor, σ_0 (cm ²)	8.7×10^{-15}	11.7×10^{-13}
Theoretical estimate of σ_0 (cm ²) (assuming neutral centre) ^a	3.9×10^{-13}	5.5×10^{-13}

^a Effective mass m^* taken as $0.067m_0$ for GaAs [8]

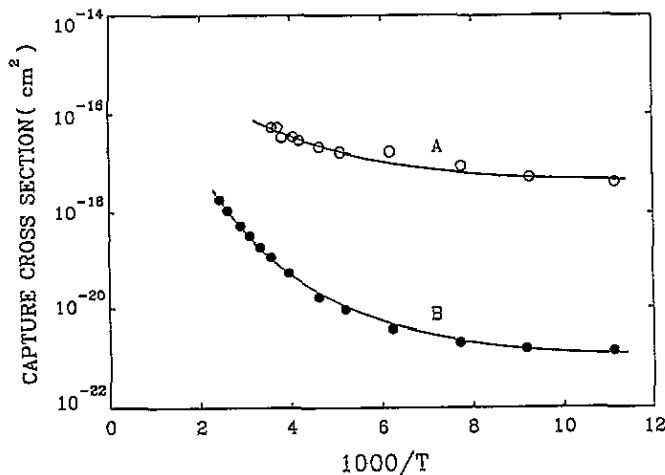


Figure 3. The theoretical best fits of the experimental capture cross sections [9] of the B centre (●) and the A centre (○) in GaAs by using equation (18). The best-fit parameters employed are listed in table 1.

The fit to the electron capture cross section of the B centre has also been performed by Goguenheim and Lannoo [6] using their theory. The parameters S and $\hbar\omega$ of their

best fit are also given in table 1. Their values are quite different from ours. In order to confirm the accuracy of our values for S and $\hbar\omega$, we use them to obtain the experimental electron photoionization cross sections of the B centre, which have been carefully measured at various temperatures by Wang *et al* [10]. The expression for the photoionization cross section with phonon coupling used in our fittings is as follows [16]:

$$\sigma_B^{\text{ph}}(h\nu) = \sum_{p'=-\infty}^{p'_{\text{max}}} \sigma_0^{\text{ph}}(h\nu, E_T + E_{p'})G(E_{p'}) \quad (20)$$

where $\sigma_0^{\text{ph}}(h\nu, E_T + E_{p'})$ is the photoionization cross section with ionization energy equal to $E_T + E_{p'}$ in the absence of phonon coupling, $G(E_{p'})$ is just the expression given by equation (A4) and $E_{p'} = p'\hbar\omega$ is the phonon energy emitted for positive p' or absorbed for negative p' by the electron during a transition process. There is a maximum value for $E_{p'}$, which is required by the condition that the kinetic energy of the electron excited to the conduction band must be positive. For the photoionization cross section $\sigma_0^{\text{ph}}(h\nu, E)$, we use the result calculated by Lucovsky [7]:

$$\sigma_0^{\text{ph}}(h\nu, E) = K_0 E^{1/2} (h\nu - E)^{3/2} / (h\nu)^3 \quad (21)$$

where K_0 is a constant. The only free parameter used in our fittings is the thermal ionization energy E_T . Using our values of S and $\hbar\omega$ for the B centre listed in table 1, the values of E_T obtained in the best fits range monotonically from 0.823 to 0.780 eV for the curves from 79 to 247 K. As shown in figure 4, the fits to all the experimental curves are very good. On the other hand, by using the values of S and $\hbar\omega$ reported by Goguenheim and Lannoo [6], the resultant theoretical curves, such as the one shown in figure 4 for 79 K, cannot account for the thermal broadening effect observed in the experiment [10].

6. Conclusion

Using the relations of the trap-related parameters based on a trap model and optical deformation form of electron-phonon coupling potential, the carrier capture cross section is brought into a simple and transparent form for easy comparison with experiment. Very good fits to the electron capture cross section for A and B centres in GaAs are obtained, from which we can extract the Huang-Rhys factor S , the average phonon energy $\hbar\omega$ and the charge-state factor σ_0 . The accuracy of the two parameters S and $\hbar\omega$ for the B centre has been corroborated by the good fits of the experimental data of the temperature-dependent photoionization cross section. This consistency supports the theory developed in this paper. Hence we believe that we have a reliable method for extracting more accurate values of deep trap parameters, such as Huang-Rhys factor S , average phonon energy $\hbar\omega$ and thermal ionization energy E_T . Accurate values of these parameters are definitely useful in identifying traps and in understanding the mechanism of the carrier capture and emission processes. The values of $\hbar\omega$ obtained for B and A centres in GaAs are both 30 meV, which coincides with that of the LO mode. This seems to imply the major involvement of optical phonons during multiphonon capturing processes.

We have also described the charge-state effect on the carrier capture cross section. In particular, the charge-state factor σ_0 introduced has been shown to be useful in identifying the charge state of a trap centre.

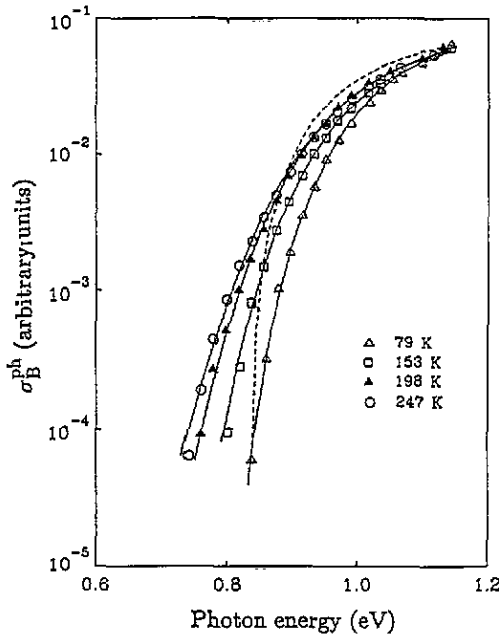


Figure 4. Theoretical best fits of experimental photoionization cross sections $\sigma_B^{ph}(h\nu)$ for $T = 79, 153, 198$ and 247 K by using equations (20) and (21) and with our values of S and $\hbar\omega$ in table 1. The broken curve is for $T = 79$ K, using the value of S and $\hbar\omega$ reported in [6].

Acknowledgment

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Appendix

In the evaluation of the transition matrix elements needed for the expression of W_{ab} only the lattice vibration modes will be considered. Contributions from the local modes, if any, do not affect our result because of the physically similar action of the local modes to that of the lattice modes, as mentioned by Ridley [3]. N lattice modes are assumed and the vector components V_s and Λ_s , which will be summed over all modes, contain a factor $1/N^{1/2}$. For simplicity, we choose the origin of lattice configuration coordinates to be at the equilibrium position Q^a of lattice vibrations in the initial state a . The arguments of $Q - Q^a$ and $Q - Q^b$ will then be replaced by Q and $Q - \Lambda$ respectively. Expanding the squared matrix elements of equation (7) in the text as

$$\left| \sum_s V_s \langle X_{bn'} | Q_s | X_{an} \rangle \right|^2 = \sum |V_s \langle n'_s | Q_s | n_s \rangle|^2 \prod_{i \neq s} |\langle n'_i | n_i \rangle|^2 + \sum_s \sum_{s' \neq s} (V_s \langle n'_s | Q_s | n_s \rangle \langle n'_s | n_s \rangle)^* (V_{s'} \langle n'_{s'} | Q_{s'} | n_{s'} \rangle \langle n'_{s'} | n_{s'} \rangle) \prod_{i \neq s, s'} |\langle n'_i | n_i \rangle|^2 \tag{A1}$$

where the notations

$$|n_s\rangle = |n_s(Q_s)\rangle \quad |n'_s\rangle = |n'_s(Q_s - \Lambda_s)\rangle$$

have been used for brevity, we may rewrite equation (7) as follows:

$$W_{ab} = \frac{2\pi}{\hbar} \left[\sum_s \sum_{n'_s} |V_s \langle n'_s | Q_s | \bar{n}_s \rangle|^2 G(E_T - n'_s \hbar \omega) + \sum_s \sum_{s' \neq s} \left(\sum_{n'_s} V_s \langle n'_s | Q_s | \bar{n}_s \rangle \langle n'_s | \bar{n}_s \rangle \right)^* \right. \\ \left. \times \left(\sum_{n'_s} V_{s'} \langle n'_s | Q_{s'} | \bar{n}_{s'} \rangle \langle n'_s | \bar{n}_{s'} \rangle \right) G(E_T - (\bar{n}'_s + n'_s) \hbar \omega) \right]. \quad (\text{A2})$$

Here \bar{n}_s is the thermal average over the phonon occupation number and has same value for all modes:

$$\bar{n}_s = \bar{n} = 1/(e^{\hbar\omega/kT} - 1). \quad (\text{A3})$$

$G(E)$ is defined by

$$G(E) = \text{Ave}_n \sum_{n'} \prod_i | \langle n'_i | n_i \rangle |^2 \delta \left(\sum_s (n'_s - n_s) \hbar \omega - E \right)$$

which has been evaluated by Huang and Rhys [11] and shown to be

$$G(E) = \frac{1}{\hbar\omega} \exp \left(-(2\bar{n} + 1)S + \frac{E}{2kT} \right) \sum_m I_m(\zeta) \delta(m\hbar\omega - E) \quad (\text{A4})$$

where $\zeta = 2S[\bar{n}(\bar{n} + 1)]^{1/2}$ and $I_m(\zeta)$ is a modified Bessel function. We notice that the overlap integration $\langle n'_s | \bar{n}_s \rangle$ of the oscillator wavefunctions leads to a factor $(1/N^{1/2})^{n'_s - \bar{n}_s}$. Hence a change in the vibrational quantum number $n'_s - \bar{n}_s$ by more than 1 can be ignored in the sum over n'_s in the calculation of W_{ab} . Using the following calculated expressions

$$\langle n'_s | Q_s | \bar{n}_s \rangle = [(\bar{n}_s + 1)/2]^{1/2} \langle n'_s | \bar{n}_s + 1 \rangle + (\bar{n}_s/2)^{1/2} \langle n'_s | \bar{n}_s - 1 \rangle$$

$$\langle n'_s = \bar{n}_s + 1 | \bar{n}_s \rangle = (\bar{n}_s/2)^{1/2} \Lambda_s$$

$$\langle n'_s = \bar{n}_s | \bar{n}_s \rangle = e^{-(\bar{n}_s - 1)} \Lambda_s^2 / 2$$

$$\langle n'_s = \bar{n}_s - 1 | \bar{n}_s \rangle = -[(\bar{n}_s + 1)/2]^{1/2} \Lambda_s$$

and the notations

$$|V\Lambda|^2 = \left| \sum_s V_s \Lambda_s \right|^2 \quad |V|^2 = \sum_s |V_s|^2$$

we obtain finally the result for W_{ab} as

$$W_{ab} = (2\pi/\hbar) \sum_{j=-2}^2 B_j G(E_T - j\hbar\omega) \quad (\text{A5})$$

where

$$B_{-2} = \frac{1}{4}|V\Lambda|^2\bar{n}^2$$

$$B_{-1} = \frac{1}{2}|V\Lambda|^2\bar{n} + \frac{1}{2}|V|^2\bar{n}$$

$$B_0 = -\frac{1}{4}|V\Lambda|^2(2\bar{n}^2 + 2\bar{n} - 1)$$

$$B_1 = -\frac{1}{2}|V\Lambda|^2(\bar{n} + 1) + \frac{1}{2}|V|^2(\bar{n} + 1)$$

$$B_2 = -\frac{1}{4}|V\Lambda|^2(\bar{n} + 1)^2.$$

These results are exactly the ones obtained by Gustche [4] and by Goguenheim and Lannoo [6]. It can be easily proven that the expression for W_{ab} above satisfies the detailed balance equation.

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