One-Phonon Transition Rate in Impurity Conduction

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The one-phonon transition rate for carrier transfer from an occupied impurity center to the empty one was calculated on the basis of the formalism given by Gummel and Lax. The deformation potential is used as the perturbation and the dependence of the equilibrium position of the lattice atoms on the state of the carrier is taken into account. This dependence influences seriously the one-phonon transition rate. The general formula for the transition rate was investigated in detail in two regions of temperature. Numerical data are given for n- and p-type Si and Ge in the approximation of the simple parabolic band. The usefulness of the Gummel and Lax treatment is discussed.

IN a previous paper[1] (to be referred in the following as I) we investigated the two-phonon transition rates in the low-concentration impurity conduction in semiconductors. The tunneling of carriers from the ground state of an occupied shallow impurity center to the ground state of an empty one was treated in the general formalism developed by Gummel and Lax.[2] In this formalism the deformation potential is used as the perturbation and the dependence of the equilibrium position of the lattice atoms on the state of the carrier is taken into account. In the present note we are concerned with the influence of this dependence on the one-phonon transition rate for carrier transfer. As in paper I, only longitudinal acoustic phonons are taken into account.

According to Gummel and Lax the total rate of the one-phonon transition from the carrier state a to the state b is[2]

$$W_{ba}{}^{1\,\mathrm{tot}}=W_{ba}{}^{1}(1-2A+B)\exp(-\alpha), \tag{1}$$

where

$$A=[\gamma^* g(-\Delta E_{ba}/\hbar)+\gamma g^*(-\Delta E_{ba}/\hbar)]/2h(-\Delta E_{ba}/\hbar), \tag{2}$$

$$B=|\gamma|^2 f(-\Delta E_{ba}/\hbar)/h(-\Delta E_{ba}/\hbar), \tag{3}$$

$$W_{ba}{}^{1}=2\pi\hbar^{-2}h(-\Delta E_{ba}/\hbar). \tag{4}$$

$W_{ba}{}^{1}$ is the one-phonon transition rate if we neglect the dependence of the equilibrium position of the lattice atoms on the state of the carrier. As can be seen from the following, it is just the transition rate treated by Miller and Abrahams in their work on the impurity conduction at low concentrations.[3] $\Delta E_{ba}=E_b(0)-E_a(0)$ is the energy difference between the carrier states b and a in the nondeformed crystal lattice if we neglect the difference of the lattice relaxation energies in the two carrier states. This can be done when we deal with the ground states of two impurity centers of the same kind. ΔE_{ba} is then simply the difference of the electrostatic energy of the carrier in the two centers, the electrostatic potential being given by the ionized majority and minority centers and the external field. By definition,

$$\alpha=\int_{-\infty}^{+\infty} f(\omega)d\omega, \tag{5}$$

$$\gamma=\int_{-\infty}^{+\infty} g(\omega)d\omega. \tag{6}$$

The functions $f(\omega)$, $g(\omega)$, and $h(\omega)$ are the distribution functions for phonons.

TOTAL ONE-PHONON TRANSITION RATE

We shall use now the formulas derived in paper I. From (I.8)–(I.11), (I.14)–(I.18), and (I.26)–(I.28) we obtain, neglecting again the oscillating function $\cos(\tau\boldsymbol{\Omega}\cdot\mathbf{R})$ as was done in (I.31), (I.32), and in reference 3,

$$f(\omega)=(E_1{}^2|\omega|/4\pi^2\hbar v^5 d)\exp(\hbar\omega/2kT)\times[\sinh(\hbar|\omega|/2kT)]^{-1}U(|\omega|/v), \tag{7}$$

$$g(\omega)=-C(\hbar E_1{}^2|\omega|^3/4\pi^2 v^5 d\Delta E_{ba})\exp(\hbar\omega/2kT)\times[\sinh(\hbar|\omega|/2kT)]^{-1}U(|\omega|/v), \tag{8}$$

$$h(\omega)=|C|^2(\hbar^3 E_1{}^2|\omega|^5/4\pi^2 v^5 d\Delta E_{ba}{}^2)\exp(\hbar\omega/2kT)\times[\sinh(\hbar|\omega|/2kT)]^{-1}U(|\omega|/v). \tag{9}$$

E_1 is the deformation potential constant, v the velocity of sound, and d the density of the crystal. C is independent of ω,[1,3] and $U(\tau)$ is by definition

$$U(\tau)=(4\pi)^{-1}\int\left|\int u^*(\mathbf{r})\exp(i\tau\boldsymbol{\Omega}\cdot\mathbf{r})u(\mathbf{r})d\mathbf{r}\right|^2 d\boldsymbol{\Omega}. \tag{10}$$

Here $u(\mathbf{r})$ is the wave function of the ground state of the impurity center in nondeformed crystal lattice. The second integration is over all directions of a unit vector $\boldsymbol{\Omega}$.

From the formulas (2), (3), (5)–(9), and using as integration variable $x=\hbar\omega/|\Delta E_{ba}|$, we obtain

$$\alpha=(E_1{}^2\Delta E_{ba}{}^2/4\pi^2\hbar^3 v^5 d)\int_{-\infty}^{+\infty} U(|\Delta E_{ba}||x|/\hbar v)|x|\times\exp(|\Delta E_{ba}|x/2kT)\times[\sinh(|\Delta E_{ba}||x|/2kT)]^{-1}dx, \tag{11}$$

[1] J. Mycielski, Phys. Rev. **125**, 46 (1962).
[2] H. Gummel and M. Lax, Ann. Phys. **2**, 28 (1957).
[3] A. Miller and E. Abrahams, Phys. Rev. **120**, 745 (1960).

$$A=(E_1^2\Delta E_{ba}^2/4\pi^2\hbar^3v^5d)\int_{-\infty}^{+\infty}U(|\Delta E_{ba}||x|/\hbar v)|x|^3\times\exp(|\Delta E_{ba}|x/2kT)\times[\sinh(|\Delta E_{ba}||x|/2kT)]^{-1}dx, \quad (12)$$

$$B=A^2. \quad (13)$$

In our case we can therefore write the formula (1) in the form

$$W_{ba}{}^{1\,\mathrm{tot}}=W_{ba}{}^1(1-A)^2\exp(-\alpha). \quad (14)$$

LOW TEMPERATURES

We shall investigate the formulas (11) and (12) in two limiting cases: for low and "high" temperatures. First we treat the case $T\to 0$. Then

$$\lim_{T\to 0}\{\exp(|\Delta E_{ba}|x/2kT)[\sinh(|\Delta E_{ba}||x|/2kT)]^{-1}\}=\begin{cases}2 & \text{if } x>0,\\ 0 & \text{if } x<0.\end{cases} \quad (15)$$

In the vicinity of the point $x=0$

$$\exp(|\Delta E_{ba}|x/2kT)[\sinh(|\Delta E_{ba}||x|/2kT)]^{-1}\cong 2kT/|\Delta E_{ba}||x|. \quad (16)$$

In the formulas (11) and (12), $|x|$ appears in the first power at least, thus in the limit $T\to 0$ we can neglect the contributions to the integrals from the singularity (16) and use (15). We have then

$$\alpha_{T\to 0}=(E_1^2\Delta E_{ba}^2/2\pi^2\hbar^3v^5d)\times\int_0^\infty U(|\Delta E_{ba}|x/\hbar v)xdx, \quad (17)$$

$$A_{T\to 0}=(E_1^2\Delta E_{ba}^2/2\pi^2\hbar^3v^5d)\times\int_0^\infty U(|\Delta E_{ba}|x/\hbar v)x^3dx. \quad (18)$$

In the case of a simple spherical and parabolic band and shallow, hydrogen-like impurity states, we have from (10)

$$U(\tau)=(1+e^4\tau^2/16\epsilon^2E_I^2)^{-4}, \quad (19)$$

ϵ being the static dielectric constant and E_I the ionization energy of the impurity center. $U(\tau)$ depends rather weakly on the structure of the wave function of carrier at the impurity center; hence we can use (19) as a reasonable approximation in many real cases. The formulas (17) and (18) with (19) give

$$\alpha_{T\to 0}{}^H=4\epsilon^2E_1^2E_I^2/3\pi^2e^4\hbar v^3d, \quad (20)$$

$$A_{T\to 0}{}^H=32\hbar\epsilon^4E_1^2E_I^4/3\pi^2e^8vd\Delta E_{ba}^2. \quad (21)$$

We want now to discuss the temperature T' below which we can use (20) and (21). Owing to the rather weak dependence of $U(\tau)$ on the structure of the wave function, T' gives also the range of validity of formulas (17) and (18). The contribution from the singularity (16) is relatively greater in the expression (11). This singularity is given by (16) approximately in the interval $(-kT/|\Delta E_{ba}|, kT/|\Delta E_{ba}|)$ and the relative contribution in (11) is about [we use (19)]

$$(2kT/|\Delta E_{ba}|)\int_{-kT/|\Delta E_{ba}|}^{kT/|\Delta E_{ba}|}U(|\Delta E_{ba}||x|/\hbar v)dx/2\int_0^\infty U(|\Delta E_{ba}|x/\hbar v)xdx<3e^4k^2T^2/4\hbar^2\epsilon^2v^2E_I^2. \quad (22)$$

This is small, hence formulas (20) and (21) are valid, if the temperature is below

$$T'=\hbar\epsilon vE_I/2e^2k. \quad (23)$$

"HIGH" TEMPERATURES

Now we shall treat the case $T\to\infty$. Then

$$\exp(|\Delta E_{ba}|x/2kT)[\sinh(|\Delta E_{ba}||x|/2kT)]^{-1}\cong 2kT/|\Delta E_{ba}||x|. \quad (24)$$

The formulas (11), (12), and (24) yield

$$\alpha_{T\to\infty}=(kE_1^2|\Delta E_{ba}|T/\pi^2\hbar^3v^5d)\times\int_0^\infty U(|\Delta E_{ba}|x/\hbar v)dx, \quad (25)$$

$$A_{T\to\infty}=(kE_1^2|\Delta E_{ba}|T/\pi^2\hbar^3v^5d)\times\int_0^\infty U(|\Delta E_{ba}|x/\hbar v)x^2dx. \quad (26)$$

Using (19) in (25) and (26), we obtain

$$\alpha_{T\to\infty}{}^H=5k\epsilon E_1^2E_IT/8\pi e^2\hbar^2v^4d, \quad (27)$$

$$A_{T\to\infty}{}^H=2k\epsilon^3E_1^2E_I^3T/\pi e^6v^2d\Delta E_{ba}^2. \quad (28)$$

We want now to estimate the temperature T'' above which the formulas (27) and (28) hold. T'' gives also approximately the range of validity of (25) and (26). Let us denote by x'' the position of the maximum most remote from $x=0$ among the maxima of the functions in (11) and (12). It is the point $x''>0$ in which the function in (12) has the maximum. The approximation (24) can be used if it is valid at $x=\pm x''$. Therefore we write the condition $|\Delta E_{ba}|x''/2kT<1/2\sqrt{3}$. Using (19) and computing x'', we arrive at

$$T''=4\hbar\epsilon vE_I/e^2k=8T'. \quad (29)$$

DISCUSSION OF RESULTS

In Table I we summarize the values obtained from the formulas (23), (29), (20), (21), and (14) for the

TABLE I. Influence of the dependence of the equilibrium position of the lattice atoms on the state of the carrier on the one-phonon transition rate of carrier in n- and p-type Si and Ge.

Material	ϵ_3 (10^{-3} ev)	T_I (°K)	T' (°K)	T'' (°K)	$\alpha_{T<T'^H}$	$A_{T<T'^H}$	$W_{ba^{1\,\mathrm{tot}}}/W_{ba^1}$ ($T<T'$)	$E_{LR}{}^H$ (10^{-3} ev)
n-Si	4.8	15	10	80	0.56	0.59	0.10	1.1
p-Si	5.0	20	12	90	0.27	0.34	0.33	0.63
n-Ge	0.99	3	2	17	0.08	0.08	0.78	0.033
p-Ge	0.323	4	2	18	0.05	0.55	0.19	0.021

samples of n- and p-type silicon and germanium used in Table I in paper I. As was done there, we take for $|\Delta E_{ba}|$ the observed activation energy of conductivity, ϵ_3. The temperature T_I about which the impurity conduction sets up, i.e., becomes greater than the band conductivity, is also given. All experimental data and references are the same as in Table I in paper I.

As one sees, the approximation for $T<T'$ covers a great part of the impurity conduction range. On the other hand, $T''\gg T_I$ for our samples and therefore we do not give the numerical values of the expressions (27) and (28).

A fair agreement of the theoretical values of conductivity, obtained from the transition rate $W_{ba}{}^1$, with the experimental data was gotten by Miller and Abrahams for n-type germanium.[3] From Table I we see that in the n-Ge sample, $W_{ba}{}^{1\,\mathrm{tot}}$ is close to $W_{ba}{}^1$. For other samples, however, the effect of the dependence of the equilibrium position of the lattice atoms on the state of the carrier is of great importance and must be taken into account in calculation of the conductivity. As one sees from (21) and (28), this effect rises with decreasing impurity concentration (i.e., decreasing $|\Delta E_{ba}|$).

In the Gummel and Lax formalism used here, only the terms independent and linear in elastic wave amplitudes are taken into account in the wave functions of the carrier. The necessary condition to justify this simple, clear-cut approximation is that the relaxation energy E_{LR} of the lattice deformed by interaction with the localized carrier be small compared with the energy difference between two states, in our case about ϵ_3. From the formula (3.17) and the footnote 7 in the Gummel and Lax paper,[2] we obtain

$$E_{LR}=(E_1{}^2/4\pi^2v^2d)\int_0^\infty U(\tau)\tau^2d\tau. \tag{30}$$

If we use $U(\tau)$ in the form (19), we have

$$E_{LR}{}^H=\epsilon^3E_1{}^2E_I{}^3/2\pi e^6v^2d. \tag{31}$$

This formula is given in the paper of Toyozawa.[4]

The numerical values of expression (31) are given in the last column of Table I. The condition $E_{LR}{}^H\ll\epsilon_3$ is fulfilled with the exception of n-Si.

Independently of the value E_{LR}, however, the linear formalism of Gummel and Lax can give a reasonable results only if the change of the one-phonon transition rate because of the dependence of the equilibrium position of the lattice atoms on the state of the carrier is not too great. In other words, α and A must be rather small compared with unity. Because of that, as one sees from Table I, the usefulness of our formulas for the samples of n-Si and p-Ge is doubtful. Generally it will be doubtful whenever the sample has very low impurity concentration (i.e., very small ϵ_3) or strong carrier-phonon interaction.

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[4] Y. Toyozawa, Progr. Theoret. Phys. (Kyoto) **23**, 378 (1960).