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Phonon Scattering by Neutral Donors in n-Type Silicon

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The scattering of phonons by neutral n-type impurities in silicon is studied. Following Keyes, who determined the phonon relaxation time for scattering by neutral impurities in n-type germanium, the relaxation time for the silicon band structure is developed. This scattering comes about due to the large effect of strain on the hydrogen-like donor ground-state energy level. The change in energy of the ground state due to the strain caused by phonons is calculated and the resulting phonon scattering relaxation rate is derived.

KEY WORDS: donors; impurities; phonons; scattering; silicon.

1. INTRODUCTION

Neutral donor scattering was first seen by Goff and Pearlmann [1] in germanium at low temperatures, and a theory was given by Keyes [2]. This theory applies to lightly doped samples in which the impurity wave functions are localized. This theory accounts for the large amount of phonon scattering in lightly doped germanium at low temperatures. It also accounts for the piezothermal conductivity effect in germanium [3]. Keyes' theory applies to Ge and in the present paper the scattering of phonons by neutral n-type impurities in lightly doped silicon is studied and the phonon relaxation time is derived.

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2. DONOR GROUND-STATE WAVE FUNCTIONS AND ENERGIES

The ground-state wave functions of shallow impurity states in silicon are, in the effective mass theory [4–7], given by

$$\psi(\vec{r}) = \sum_{j=1}^{N} \alpha_j F_j(\vec{r})\,\phi_j(\vec{r}) \tag{1}$$

where in this context N is the number of equivalent conduction band minima, the α_j are numerical coefficients, $\phi_j(\vec{r})$ is the Bloch function at the jth minimum, and the functions $F_j(\mathbf{r})$ are hydrogen-like envelope functions. The envelope functions $F_j(\mathbf{r})$ are solutions of the effective mass equation:

$$\left[E_j\left(\frac{1}{i}\nabla\right) - \frac{e^2}{\kappa r}\right] F_j(\mathbf{r}) = EF_j(\mathbf{r}) \tag{2}$$

where κ is the static dielectric constant of the host material, $E_j(\mathbf{k}-\mathbf{k}_j)$ is the energy of the conduction band near $\mathbf{k}=\mathbf{k}_j$, and E is the energy of the donor state relative to the conduction band minimum. In this theory the ground state of the impurity is N-fold degenerate, however, when corrections to the effective mass approximation are taken into account this degeneracy is reduced. The remaining degeneracy, and the values of the numerical constants α, may be determined solely from the symmetry of the Hamiltonian of the impurity state, T_d [8]. The N degenerate functions form the basis of a representation of the group T_d; this representation may be reduced into the irreducible representations of the group and the linear combinations of Eq. (1) belonging to each irreducible representation are the ground-state wave functions of the impurity [4]. The wave functions corresponding to any one particular irreducible representation are degenerate and this remaining degeneracy cannot be lifted by any tetrahedrally symmetric perturbation.

The conduction band minima in silicon consist of six equivalent minima along the $\langle 100 \rangle$ axes. In this analysis it is convenient to use as basis wave functions a modification of the "decoupled basis" introduced by Price [9] in his theory of thermoelectric effects in Ge and used by Keyes [2] in his study of low-temperature thermal conductivity in Ge. The basis set to be used in this study of the Si symmetry is

$$\begin{aligned}\Psi_x^+ &= \frac{1}{\sqrt{2}}(\psi_{[100]} + \psi_{[-100]}) \\ &= \frac{1}{\sqrt{2}}(F_{[100]}\phi_{[100]} + F_{[-100]}\phi_{[-100]})\end{aligned}$$

$$\Psi_x^- = \frac{1}{\sqrt{2}}(\psi_{[100]} - \psi_{-[100]})$$

$$= \frac{1}{\sqrt{2}}(F_{[100]}\phi_{[100]} - F_{[\quad 100]}\phi_{[-100]})$$

etc. In the effective mass approximation there would be no off-diagonal terms in the Hamiltonian matrix in this bases, and there would be six degenerate ground states. However, in the vicinity of an impurity this degeneracy is split through the intervalley interaction due to the impurity potential. Price [9] introduced a phenomenological perturbation with off-diagonal matrix elements in this basis due to the intervalley interaction; this "chemical shift" lifts the degeneracy. In this representation the matrix of the Hamiltonian is

$$H_0 + H_1 = \begin{pmatrix} E_0 & -\Delta & -\Delta & 0 & 0 & 0 \\ -\Delta & E_0 & -\Delta & 0 & 0 & 0 \\ -\Delta & -\Delta & E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_0 + \beta & 0 & 0 \\ 0 & 0 & 0 & 0 & E_0 + \beta & 0 \\ 0 & 0 & 0 & 0 & 0 & E_0 + \beta \end{pmatrix} \tag{3}$$

Here H_1 is the phenomenological perturbation introduced by Price which is responsible for the off-diagonal matrix elements Δ and β, and Δ and β are due to the overlap attributed to the intervalley interaction. The off-diagonal elements of the impurity Hamiltonian connecting the Ψ_j $(j = x, y, z)$, and those connecting any Ψ_j^- with any Ψ_j^+, are zero by virtue of the symmetry of the conduction band minima and the chosen form for the basis set of $\Psi_j^{(+,\ )}$. The best demonstration of the adequacy of the phenomenological Hamiltonian in germanium is provided by the piezothermal conductivity experiments of Fritzsche [10, 11] and Keyes and Sladek [3].

The eigenvalues of this Hamiltonian matrix are a singlet of energy $E_0 - 2\Delta$, a doublet of energy $E_0 + \Delta$, and a triplet of energy $E_0 + \beta$. It is known that Δ is positive [12] and thus that the singlet is the state of lowest energy and also that the doublet and triplet states have nearly the same energy, with the doublet lying slightly higher than the triplet [12]. For phosphorous donors in si $3\Delta \approx 13$ meV, and $\beta - \Delta \approx 1.3$ meV [12]. The eigenvectors associated with these energy levels are

$$
\begin{aligned}
\Psi_{\mathrm{S}} &= \frac{1}{\sqrt{3}}\left(\Psi_x^+ + \Psi_y^+ + \Psi_z^+\right) \\
\Psi_{\mathrm{D1}} &= \frac{1}{\sqrt{2}}\left(\Psi_x^+ - \Psi_y^+\right) \\
\Psi_{\mathrm{D2}} &= \frac{1}{\sqrt{6}}\left(\Psi_x^+ + \Psi_y^+ - 2\Psi_z^+\right) \\
\Psi_{\mathrm{T1}} &= \Psi_x^- \\
\Psi_{\mathrm{T2}} &= \Psi_y^- \\
\Psi_{\mathrm{T3}} &= \Psi_z^-
\end{aligned}
\tag{4}
$$

where the subscripts S, D, and T refer to the singlet, doublet, and triplet states, respectively. In this new basis the Hamiltonian matrix $H_0 + H_1$ is diagonal.

In the presence of a strain the band edge energies will change [9, 13] and thus the energies of the ground states will change. The change in energy of the functions $\Psi_j^{(+,-)}$ in this analysis is given by [13]

$$
u_j^{(+,-)} = \int \mathbf{\Xi} \cdot \vec{\eta}(\mathbf{r})\, |\Psi_j^{(+,-)}|^2\, dV \tag{5}
$$

where $\mathbf{\Xi}$ is the deformation potential tensor and $\vec{\eta}(\mathbf{r})$ is the strain tensor. The strain of interest here is the strain due to phonons and the perturbation due to the phonons is small compared to the intervalley interaction. It is also noted that $u_x^+ = u_x^- = u_x$, etc., because the strain energy comes from the distortion of each band edge minimum and thus there are no cross terms between, for example, $F_{[100]}\psi_{[100]}$ and $F_{[\bar{1}00]}\psi_{[\bar{1}00]}$. Thus the change in energy of the singlet state to second order in the strain is

$$
\delta E_{\text{singlet}} = \frac{1}{3}\left(u_x + u_y + u_z\right) - \frac{1}{27\Delta}\left[3\left(u_x^2 + u_y^2 + u_z^2\right) - \left(u_x + u_y + u_x\right)^2\right] \tag{6}
$$

3. EVALUATION OF STRAIN ENERGY

The change in energy given in Eq. (6) has terms which are second order in the strain, and the theory of Klemens [14, 15] shows that these terms will lead to a scattering of phonons.

To evaluate this change in energy of the ground state it is necessary to calculate the u_j given in Eq. (5). The deformation potential is given by [13]

$$
\mathbf{\Xi}^i = \Xi_{\mathrm{d}}\mathbf{1} + \Xi_{\mathrm{u}}\mathbf{a}^i\mathbf{a}^i \tag{7}
$$

where $\mathbf{a}^i$ is the unit vector along the axis of revolution of valley i, $\Xi_{\rm d}$ is the dilatation deformation potential, $\Xi_{\rm u}$ is the shear deformation potential, and $\mathbf{1}$ is the identity matrix. Thus, $\Xi^{[100]} = \Xi^{[-100]}$, $\Xi^{[010]} = \Xi^{[0-10]}$, and $\Xi^{[001]} = \Xi^{[00-1]}$. The displacement vector may be expanded in terms of phonon raising and lowering operators as

$$\mathbf{d}(\mathbf{r}) = \frac{1}{\sqrt{G}} \sum_{\mathbf{q},j} \vec{\varepsilon}_j a_{\mathbf{q},j} e^{i\mathbf{q}\cdot\mathbf{r}} \tag{8}$$

where the $j = \pm 1$, ± 2, ± 3, $a_{\mathbf{q},j}$ are the phonon raising and lowering operators, $a_j(-\mathbf{q}) = a_j^\dagger(\mathbf{q})$, $\vec{\varepsilon}_j$ is the polarization vector, and G is the number of unit cells in the lattice. The raising and lowering operators obey the commutation relation $[a_{\mathbf{q},j}, a^\dagger_{\mathbf{q},j}] = -\hbar/M\omega(\mathbf{q})$, where M is the mass of a unit cell, and $\omega(\mathbf{q})$ is the frequency of the phonon with wave vector $\mathbf{q}$. The ground-state envelope functions $F(\mathbf{r})$ are of the form

$$F(\mathbf{r}) = \frac{1}{(\pi a^3)^{1/2}} \exp\left[-\frac{r}{a_0}\right] \tag{9}$$

where $a_0 = \hbar^2\kappa/m_{\rm eff}e^2$ is the Bohr radius of the orbital in the effective mass approximation, κ is the static dielectric constant, $m_{\rm eff}$ is the effective electronic mass, and e is the electronic charge. Using Eqs. (8) and (9) the change in the ground-state energy which is second order in the strain is, from Eq. (6),

$$\begin{aligned} \delta E(\mathcal{O}\varepsilon^2) = {} & -\frac{1}{27\Delta}\frac{\Xi_{\rm u}^2}{G} \sum_{\mathbf{q},j} \sum_{\mathbf{q}',j'} [2(\chi_1\chi_1' + \chi_2\chi_2' + \chi_3\chi_3') \\ & - \chi_1(\chi_2' + \chi_3') - \chi_2(\chi_1' + \chi_3') - \chi_3(\chi_1' + \chi_2')] \\ & \times a_{\mathbf{q},j} a_{\mathbf{q}',j'} \left(1 + \frac{a_0^2 q^2}{4}\right)^{-2} \left(1 + \frac{a_0^2 q'^2}{4}\right)^{-2} \end{aligned} \tag{10}$$

where $\chi_i = \varepsilon_i q_i$.

4. CALCULATION OF PHONON RELAXATION TIME

The expression in Eq. (10) is second order in the phonon operator. Klemens has shown [14, 15] that if the perturbation Hamiltonian is of the form

$$H' = \sum_{\mathbf{q},\mathbf{q}'} c_2(\mathbf{q}, \mathbf{q}') a_{\mathbf{q}} a^\dagger_{\mathbf{q}} \tag{11}$$

then the relaxation time of the mode **q** is given by

$$\frac{1}{\tau} = \frac{V}{(2\pi)^3} 2\pi \frac{1}{M^2\omega^2} \sum_{j'} \oint dS'_{j'} \frac{1}{v'_g} |c_2(\mathbf{q}, \mathbf{q}')|^2 \tag{12}$$

where for the receiving mode j' represents the polarization, $\omega' = \omega$, v'_g is the group velocity of the phonon, V is the crystal volume, and the surface integral is over surfaces of constant ω. From Eq. (10),

$$\begin{aligned} c_2(\mathbf{q}, \mathbf{q}')^2 = {} & \left(\frac{1}{27\Delta}\right)^2 \frac{\Xi_u^4}{G^2} \\ & \times [A\chi_1'^2 + B\chi_2'^2 + C\chi_3'^2 + D\chi_1'\chi_2' + E\chi_1'\chi_3' + F\chi_2'\chi_3'] \\ & \times \left(1 + \frac{a_0^2 q^2}{4}\right)^{-4} \left(1 + \frac{a_0^2 q'^2}{4}\right)^{-4} \end{aligned} \tag{13}$$

where

$$\begin{aligned} A &= 4\chi_1^2 + \chi_2^2 + \chi_3^2 + 2\chi_2\chi_3 - 4\chi_1\chi_2 - 4\chi_1\chi_3 \\ B &= 4\chi_2^2 + \chi_1^2 + \chi_3^2 + 2\chi_1\chi_3 - 4\chi_1\chi_2 - 4\chi_2\chi_3 \\ C &= 4\chi_3^2 + \chi_1^2 + \chi_2^2 + 2\chi_1\chi_2 - 4\chi_1\chi_3 - 4\chi_2\chi_3 \\ D &= -4\chi_1^2 - 4\chi_2^2 + 2\chi_3^2 + 10\chi_1\chi_2 - 2\chi_1\chi_3 - 2\chi_2\chi_3 \\ E &= -4\chi_1^2 - 4\chi_3^2 + 2\chi_2^2 + 10\chi_1\chi_3 - 2\chi_1\chi_2 - 2\chi_2\chi_3 \\ F &= -4\chi_2^2 - 4\chi_3^2 + 2\chi_1^2 + 10\chi_2\chi_3 - 2\chi_1\chi_2 - 2\chi_1\chi_3 \end{aligned}$$

Note that these parameters do not contain any primed variables. By substituting Eq. (13) into Eq. (12), the phonon relaxation time can be found.

The integral in Eq. (12) becomes

$$\begin{aligned} \oint dS'_{j'} \frac{1}{v_{j'}} |c_2(\mathbf{q}, \mathbf{q}')|^2 = {} & \frac{1}{v_j} \left(\frac{1}{27G}\right)^2 \left(\frac{\Xi^2}{\Delta}\right)^2 \left(1 + \frac{a_0^2 q^2}{4}\right)^{-8} q^6 \\ & \times (\mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV} + \mathrm{V} + \mathrm{VI}) \end{aligned} \tag{14}$$

where

$$\begin{aligned} \mathrm{I} &= \frac{A}{q^2} \oint \frac{\varepsilon_1^2 q_1^2}{q^2} \sin\theta \, d\theta \, d\varphi, & \mathrm{II} &= \frac{B}{q^2} \oint \frac{\varepsilon_2^2 q_2^2}{q^2} \sin\theta \, d\theta \, d\varphi \\ \mathrm{III} &= \frac{C}{q^2} \oint \frac{\varepsilon_3^2 q_3^2}{q^2} \sin\theta \, d\theta \, d\varphi, & \mathrm{IV} &= \frac{D}{q^2} \oint \frac{\varepsilon_1\varepsilon_2 q_1 q_2}{q^2} \sin\theta \, d\theta \, d\varphi \\ \mathrm{V} &= \frac{E}{q^2} \oint \frac{\varepsilon_1\varepsilon_3 q_1 q_2}{q^2} \sin\theta \, d\theta \, d\varphi, & \mathrm{VI} &= \frac{F}{q^2} \oint \frac{\varepsilon_2\varepsilon_3 q_1 q_2}{q^2} \sin\theta \, d\theta \, d\varphi \end{aligned} \tag{15}$$

Table I. Components of the Wave Vector and the Longitudinal and Transverse Components of the Polarization Vector

Wave vector, **q**	Polarization vector, $\bar{\varepsilon}$		
	Longitudinal	Transverse 1	Transverse 2
$q_1 = q \sin\theta \cos\varphi$	$\varepsilon_1 = \sin\theta\cos\varphi$	$\varepsilon'_1 = \sin\varphi$	$\varepsilon''_1 = \cos\theta\cos\varphi$
$q_2 = q \sin\theta \sin\varphi$	$\varepsilon_2 = \sin\theta\sin\varphi$	$\varepsilon'_2 = -\cos\varphi$	$\varepsilon''_2 = \cos\theta\sin\varphi$
$q_3 = q \cos\varphi$	$\varepsilon_3 = \cos\theta$	$\varepsilon'_3 = 0$	$\varepsilon''_3 = -\sin\theta$

Note that the integration variables are no longer primed for convenience of notation. The components of the polarization vector and the wave vector are functions of θ and φ; the components in terms of the integration variables are given in Table I. Table II gives the values of the integrals in Eqs. (15). It should be noted that the polarizations of the transverse branches are arbitrary and that any mutually orthogonal set would give the same results; this set was chosen for convenience. Using these values the relaxation time given in Eq. (12) is found to be

$$\frac{1}{\tau} = N_{\text{nd}} \frac{2}{5}\left(\frac{1}{27}\right)^2 \left(\frac{\Xi_{\text{u}}^2}{\Delta}\right)^2 \frac{a^6}{\pi M^2}\left(\frac{2}{v_{\text{L}}^7}+\frac{3}{v_{\text{T}}^7}\right)\left(1+\frac{a_0^2 q^2}{4}\right)^{8} \omega^4 \times \left[\frac{1}{q^2}(\chi_1^2+\chi_2^2+\chi_3^2-\chi_1\chi_2-\chi_1\chi_3-\chi_2\chi_3)\right] \qquad (16)$$

Table II. The Values of the Integrals Given in Eqs. (15) for the Components Given in Table I

Integral	L	T1	T2
I	$\frac{A}{q^2}\frac{4}{5}\pi$	$\frac{A}{q^2}\frac{1}{3}\pi$	$\frac{A}{q^2}\frac{3}{15}\pi$
II	$\frac{B}{q^2}\frac{4}{5}\pi$	$\frac{B}{q^2}\frac{1}{3}\pi$	$\frac{B}{q^2}\frac{3}{15}\pi$
III	$\frac{C}{q^2}\frac{4}{5}\pi$	0	$\frac{C}{q^2}\frac{8}{15}\pi$
IV	$\frac{D}{q^2}\frac{4}{15}\pi$	$-\frac{D}{q^2}\frac{1}{3}\pi$	$\frac{D}{q^2}\frac{1}{15}\pi$
V	$\frac{E}{q^2}\frac{4}{15}\pi$	0	$-\frac{E}{q^2}\frac{4}{15}\pi$
VI	$\frac{E}{q^2}\frac{4}{15}\pi$	0	$-\frac{E}{q^2}\frac{4}{15}\pi$

where N_{nd} is the density of neutral donors. The term in square brackets is a dimensionless factor, the value of which is dependent on the direction of the phonon wavevector and the polarization. In polycrystalline materials the random orientation of the grains will have the effect of averaging over all phonon directions. In this case averaging the terms in square brackets over all directions, it is found that this term has an average value of 2/5 for longitudinal phonons and 3/5 for transverse phonons. Substituting these factors into Eq. (16), the averaged relaxation time becomes

$$\frac{1}{\tau} = N_{\mathrm{nd}} \frac{2}{5} \left(\frac{1}{27}\right)^2 \left(\frac{\Xi_{\mathrm{u}}^2}{\Delta}\right)^2 \frac{a^6}{\pi M^2} \left(\frac{2}{v_{\mathrm{L}}^7} + \frac{3}{v_{\mathrm{T}}^7}\right) \left(1 + \frac{a_0^2 q^2}{4}\right)^{8} \omega^4 \tag{17}$$

The change in energy of the doublet state will also have terms second order in the strain energy, and as in the case of the singlet state this will give rise to phonon scattering. The relaxation time for scattering by this state has not been calculated in detail but it will be assumed that the change in energy, and hence the scattering rate, will be of the same order as that calculated for the singlet state. The triplet state does not have terms which are second order in the strain and thus will not give rise to phonon scattering.

5. DISCUSSION AND CONCLUSIONS

The form of the reciprocal relaxation time given in Eq. (17) for the scattering of phonons by the ground state of neutral n-type impurities in silicon has several features of interest. The reciprocal relaxation time goes as ω^4, which is the form for point defect scattering; however, unlike normal point defect scattering, which continuous to increase in strength for higher-frequency phonons, the factor $[1 + (a_0^2 q^2/4)]^{8}$ cuts this scattering mechanism off, and thus this scattering is appreciable only for low-frequency phonons.

The neutral donor scattering relaxation time was used by White et al. [16] to calculate the effect of neutral donors on the thermal conductivity of heavily doped Si–Ge alloys at high temperatures. It was found in that case that neutral donors would have little effect on the thermal conductivity above 300 K. This was attributed to several factors including the fact that this mechanism competes with phonon–electron scattering and mass defect-distortion scattering. Phonon–electron scattering, which scatters phonons only in the low-frequency range, is a function of the number of electrons in the conduction band; at lower temperatures fewer electrons will be present in the conduction band and scattering by this mechanism will be less strong. The maximum phonon frequency effected by phonon–electron scattering is given by [16], $\omega_c = (4\pi v/h)\sqrt{2mKT}$, where v is the phonon velocity, h is Planck's constant, m is the electron mass, K is Boltzmann's constant, and T is the absolute temperature. This cutoff frequency decreases with temperature and thus decreases the range over which phonon–electron scattering competes with neutral donor scattering. Mass defect-distortion scattering is very strong in these alloyed materials and also competes with neutral donor scattering. Table III gives the phonon–electron cutoff frequency, and the inverse relaxation times for mass defect-distortion scattering (τ_m^{-1}) and neutral donor scattering (τ_{nd}^{-1}) at the phonon–electron cutoff frequency for an 80% Si/20% Ge alloy. The mass defect scattering relaxation time was calculated as in Ref. 16. In this case a donor concentration of $N_d = 10^{26} m^{-3}$ was assumed and the neutral donor concentration, given by $N_d - n_0$, where n_0 is the free electron density, was calculated using the equation [17]

$$n_0 = \frac{2N_d N_c}{(N_c + 0.27N_d) + [(N_c - 0.27N_d)^2 + 8N_d N_c \exp(E_d/KT)]^{1/2}} \quad (18)$$

which assumes no compensation, where $N_c = 2[2\pi mKT/h^2]^{3/2}$ and E_d is the depth of the donors below the conduction band, taken as 0.04 eV in this case (approximately the depth of phosphorous donors in silicon). From Table III it is seen that at 300 K neutral donor scattering is not as strong as mass defect scattering at the cutoff frequency. At lower temperatures the neutral donor scattering becomes stronger than the mass defect scattering at the cutoff frequency. The maximum of the inverse neutral donor relaxation time is centered at a phonon frequency of $2.7 \times 10^{12}\ s^{-1}$, and it is seen that as the temperature decreases, the cutoff frequency becomes less than this value. Along with these results it is noted that at lower temperatures the high-frequency portion of the phonon spectrum is not significantly occupied, thus increasing the overall percentage of heat-carrying phonons

Table III. Calculated Values of the Phonon–Electron Cutoff Frequency, Mass Defect-Distortion Scattering Inverse Relaxation Time, and Neutral Donor Scattering Inverse Relaxation Time at ω_c for an 80% Si/20% Ge Alloy with a Donor Concentration of $10^{26} m^{-3}$

T(K)	ω_c (s^{-1})	τ_m^{-1} (s^{-1})	τ_{nd}^{-1} (s^{-1})
300	5.63×10^{12}	1.6×10^8	7.9×10^7
100	3.24×10^{12}	1.6×10^8	5.3×10^8
50	2.30×10^{12}	1.6×10^8	5.4×10^8

effected by neutral donor scattering. Thus neutral donor scattering will begin to have an effect on the thermal conductivity at these lower temperatures.

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