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EFFECT OF SUBBAND-INTERACTION ON RELAXATION TIME OF HOLE IN *p*-TYPE SILICON AND GERMANIUM

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ABSTRACT

Considering the warping and the non-parabolicity of equi-energy surfaces and also the existence of three types of holes, we calculated the relaxation times of holes due to lattice scattering including the non-polar optical phonon scattering, the impurity scattering with neutral center as well as with ionized center scattering.

The effect of interaction between three subbands in the valence band is recognized most significantly in the non-polar optical phonon scattering of silicon. For silicon whose split-off energy is considerably small, it is very important to consider the effect of the subband-interaction if we want to estimate accurate values of relaxation times due to lattice scattering and also ionized impurity center scattering.

In highly doped samples (over 10^{17} cm^{-3}), one should consider the effect of neutral center scattering with accurate screening distance.

1. Introduction

Although the valence band of Ge-family semiconductors is constructed of three complicated subbands, scattering of holes have usually been approximately treated neglecting the existence of split-off holes and even assuming the parabolic band form.

Silicon has, however, the small split-off energy (44 meV) so that the subband-interaction begins to occur in rather low energy states and consequently the effect of warping and non-parabolicity is larger, and also the probability of the existence of holes in split-off subbands is considerably higher. One should take into account the interaction between these subbands in the valence band, introducing both of their warping and non-parabolicity and consider also the contribution from three type holes (heavy, light and split-off holes) accurately.

In this paper, using the two typical band models (DKK and Kane model) which are obtained by the $k \cdot p$ perturbation theory including the spin-orbit interaction, we determine the band structure near the valence band edge and calculate the

density of states for three subbands holes. Then we consider the effect of interaction between three subbands in the valence band on the relaxation time by acoustic, non-polar optical phonon and ionized impurity scattering, respectively.

2. Theory

2-1. Band Structure and Density of States near the Valence Band Edge

The energy band structure near the valence band edge of Ge-family semiconductors have been obtained using the method of the $k \cdot p$ perturbation theory including the spin-orbit interaction [1] and [2]. Dresselhaus et al. obtained the energy eigenvalues for three subbands with the approximation that the interaction between heavy, light and split-off holes can be neglected because those terms affect the roots of the secular equation only to the order k^4/Δ . Kane solved the secular equation and Asche et al. [3] have rewritten the $E\text{-}\mathbf{k}$ dispersion relation in spherical coordinate. In this paper we used these two typical band model as DKK model proposed by Dresselhaus, Kip and Kittel and Kane model by Kane and Asche et al.

From the above two band models we have obtained the density of states. For DKK model, the following solution can be obtained [4];

$$g_i = \frac{1}{8\pi^3} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} I \sqrt{E} \quad \text{for heavy and light holes,} \quad (1)$$

and

$$g_i = \frac{1}{8\pi^3} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} S \sqrt{E - \Delta} \quad \text{for split-off hole,} \quad (2)$$

where g_i ($i=H, L$ and S) means the density of states for each subband holes, respectively. I ($=H$ and L) or S is the modified coefficient which represents the anisotropy of the equi-energy surfaces for DKK model and relates to the band parameters [4]. The density of states for Kane model are given as [4].

$$g_i = \frac{1}{8\pi^3} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} \int \left| \frac{\partial U_i}{\partial E} \right| U_i^{1/2} d\Omega, \quad (3)$$

where the integration should be carried out on the equi-energy surfaces.

The numerical calculation was performed as follows; each equi-energy surface was divided in 1152 elements and the integration was performed by Simpson's method. The integration was found to converge when the division more than 648 elements were used.

2-2. Relaxation Times

We consider the scattering by the lattice vibration including the effects of optical phonons and the scattering by the ionized impurity centers. In order to simplify the calculation of the transition matrix elements, we introduce the follow-

ing two major assumptions; (i) the scattering processes are perfectly elastic except the case of the non-polar optical phonon scattering, and (ii) all holes are scattered isotropically so that the relaxation times can be assumed to depend only on the energy of holes.

2-2-1. Overlap Integral and Anisotropy of Scattering

By using the Born approximation the scattering probability per unit time P_f^i for each of types of hole is given by,

$$P_f^i = \frac{2\pi}{\hbar} |I_{\mathbf{k}, \mathbf{k}'}|^2 G_{\mathbf{k}\mathbf{k}'} \delta(E_f - E_i) \quad , \quad (4)$$

with

$$G_{\mathbf{k}\mathbf{k}'} = \frac{1}{2} \sum_{s1, s2} \left| \int \mathbf{u}_{s1, \mathbf{k}}^* \mathbf{u}_{s2, \mathbf{k}'}(r) d\mathbf{r} \right|^2 \quad , \quad (5)$$

where the sum is taken over spin states. $I(\mathbf{k}' - \mathbf{k})$ is the $(\mathbf{k}' - \mathbf{k})$ -th Fourier coefficient of the perturbing Hamiltonian which determines the scattering process. The wave vectors of holes at the initial and final state are denoted as \mathbf{k} and \mathbf{k}' , respectively. One should account accurately for the overlap integral between periodic parts $\mathbf{u}_{s, \mathbf{k}}(r)$ of the wave functions in the matrix between the initial and final Bloch states, which gives the anisotropy of the scattering probability.

Wiley [5] has investigated the overlap integral with the use of Kane's Bloch function for III-V compounds. Costato et al. [6] have applied their results to IV-semiconductors. They showed that the \mathbf{k} -dependence of the overlap integral is negligible and also showed that the overlap integral is dependent only on the scattering angle θ .

According to Wiley [5], the overlap integrals for heavy and light hole have remarkably strong anisotropy [4] and are represented as follows,

$$G_{HH} = G_{LL} = \frac{1}{4} (1 + 3 \cos^2 \theta) \quad \text{for intra-subband transition} \quad , \quad (6)$$

and

$$G_{HL} = G_{LH} = \frac{3}{4} \sin^2 \theta \quad \text{for inter-subband transition} \quad . \quad (7)$$

Therefore the probability of holes scattered into the heavy hole subband is given by,

$$\frac{1}{\tau_{HH}} = \int G_{HH} F_H d\Omega' \quad , \quad (8)$$

and

$$\frac{1}{\tau_{LH}} = \int G_{LH} F_H d\Omega' \quad , \quad (9)$$

where $F_i (i=H \text{ and } L)$ is determined from the scattering matrix elements. In low

energy states where the split-off subband doesn't appear, the total probability of holes scattered into the heavy hole subband is

$$\frac{1}{\tau_H} = \frac{1}{\tau_{HH}} + \frac{1}{\tau_{LH}} = \int (G_{HH} + G_{LH}) F_H d\Omega' . \quad (10)$$

From eqs. (6) and (7), the relaxation time can be reduced as,

$$\frac{1}{\tau_H} = \int F_H d\Omega' . \quad (11)$$

This result agrees with that when one takes overlap integral being unity.

When the electron energy becomes larger than the split-off energy, one should consider the existence of the split-off hole subband. Since the magnitude of the wave vector of both heavy and light holes, which occupy the energy states greater than the split-off energy, is considerably larger, the probability of inter-subband transition as H - S or L - S is very small so that it can be neglected in comparison with that of S - S intra-subband transition. Moreover the equi-energy surface of the split-off hole subband is almost isotropic [4]. Considering these two points we take the overlap integral G_{ss} to be unity.

From the above consideration we see the difference of the overlap integral between the plane waves and those for the Bloch holes may affect hardly the mobility [7]. Therefore we introduce the approximation that the overlap integral is unity and the k -dependence of the overlap is neglected. According to Tiersten [7] and Costato et al. [6] the relaxation times are found to be very nearly isotropic. They also showed that the assumption that the scattering depends only on energy leads to an error less than 1% for each subbands holes. However they pointed out that fairly large errors would be introduced at the stage of integration over equi-energy surfaces, if the pure parabolic bands were taken instead of the non-parabolic and warped ones.

The major lattice scattering processes in Ge-family semiconductors are the acoustic phonon scattering and non-polar optical phonon scattering. Bir et al. [8] and Tiersten [7] have shown that the deformation potential approach is adequate to describe these scattering phenomena in these semiconductors.

2-2-2. Acoustic Phonon Scattering

By using the deformation potential approximation the relaxation times of holes scattered into i -th subband by acoustic phonons is given as,

$$\frac{1}{\tau_{AC}^i} = \frac{\pi}{\hbar} \frac{k_B T}{\rho u_i^2} E_{ef}^2 g_{i(E)} , \quad (12)$$

and the total relaxation time τ_{AC}^T is represented as,

$$\frac{1}{\tau_{AC}^T} = \sum_i \frac{1}{\tau_{AC}^i} , \quad (13)$$

where g_i means the density of states defined in sec. 2-1 and symbols k_B , ρ , u_i is the Boltzmann constant, the density of the material and the longitudinal sound

velocity, respectively. E_{eff} is the deformation potential constant in Lawaetz's notation [9].

2-2-3. Non-Polar Optical Phonon Scattering

The transition probability due to non-polar optical phonon scattering was found to be given by an equation analogous to that by acoustic phonon [8]. The optical phonons, however, have the large energy $\hbar w_0$ at long wave length so that the scattering due to these phonons is inelastic [10]. Neglecting the dispersion of optical phonons and using the optical phonon coupling constant ($D_t K$), the relaxation time by optical phonon scattering for three subbands is calculated to be;

$$\frac{1}{\tau_{op}^i} = \frac{\pi (D_t K)^2}{2 \rho w_0} [N_q g_{i(E+\hbar w_0)} + (N_q + 1) g_{i(E-\hbar w_0)}], \quad (14)$$

where N_q is the Bose-Einstein phonon distribution with optical phonon frequency w_0 .

The expression for the relaxation time is slightly complicated because the scattering by optical phonons is inelastic with creation and annihilation of phonons. Considering the energy conservation and also the existence of three type holes, the total relaxation time is formally given as,

$$\frac{1}{\tau_{OP}^i} = \sum_i \frac{1}{\tau_{OP}^i}, \quad (15)$$

where the summation is followed to Fig. 1.

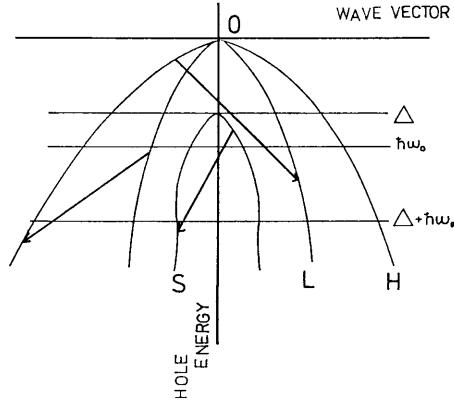


Fig. 1. Possible transitions of holes in the valence band due to non-polar optical phonon scattering for silicon type ($\Delta < \hbar w_0$). Although there are many other inter- and intra-subband transitions, we show only some typical transitions in order to avoid complications. Symbols Δ and w_0 are the split-off energy and the optical phonon frequency, respectively. H, L and S represent heavy, light and split-off hole subband, respectively.

2-2-4. Ionized Impurity Center Scattering

We assumed also that the scattering by ionized impurity centers is perfectly elastic and used the two approaches to describe the transition matrix element;

one of them is the CW formula proposed by Conwell and Weisskopf [11] and the other is the BH formula due to Brooks [12] and Herring [13]. The difference between above the two is the choice of the screening distance of the impurity potential.

The relaxation time due to these two scattering models is written as,

$$\frac{1}{\tau_{IM}^{ij}} = \frac{N_I}{\kappa^2} \left(\frac{\hbar^2}{2m_0} \right)^{1/2} \int G_{ij} H_i d\Omega', \quad (16)$$

where κ, N_I and G_{ij} is a dielectric constant of silicon or germanium, a net concentration of impurities and the above defined overlap integral respectively. H_i is determined from the scattering matrix element and defined as follow;

$$H_i = \frac{U'_i}{U_i^{3/2}} \frac{1 - \cos \theta}{[(1 - \cos \theta) + 1/(2\hbar^2 R^2)]^2}, \quad (17)$$

where R is the screening distance,

$$R^{BH} = (\kappa k_B T / e^2 N_I)^{1/2} \quad \text{for BH model}, \quad (18)$$

and

$$R^{CW} = N_I^{-1/3} / 2 \quad \text{for CW model}, \quad (19)$$

In Table 1, all parameters used in our calculation were summarized.

Table I. Parameters used in calculation in this paper. Symbols in this table have been defined in text. Atomic unit used here is $\hbar=1, m_0=1/2$ and $e^2=2$ system.

Parameter		Unit	Si	ref.	Ge	ref.
BAND parameter	A	ATOMIC UNIT	-4.42	9	-13.27	15
	B		-0.79		-8.63	
	C		4.78		12.4	
warping coef.	H	ATOMIC UNIT	4.92	4	2.59	4
	L		0.78		0.11	
	S		1.45		0.26	
ρ		g/cm^3	2.329		5.32	
u_l		cm/sec	9.04×10^5		5.4×10^5	16
T_{opt}		K	735		430	16
κ		ϵ_0	11.7		16.0	
Δ		meV	44.0	17	295	20
E_{eff}		eV	5.3	18	5.3	15
$D_t K$		eV/cm	6.6×10^5	19	9.1×10^5	15

3. Results and Discussion

3-1. Acoustic Phonon Scattering and its Anisotropy

The energy dependence of the relaxation time for heavy and light hole follows nearly the $E^{-0.5}$ law below 10 meV (silicon), respectively (Fig. 2). One, however, finds deviations from this dependence (even in the DKK model) near the split-off energy where the interaction between subbands occurs. Above 100 meV, the $E^{-0.5}$ dependence of the relaxation time is found to be recovered. The total relaxation time associated with intra- and inter-subband transition is mostly predominated by heavy holes. The DKK model seems to be adequate to describe only low energy states (below about 10 K for silicon and 100 K for germanium).

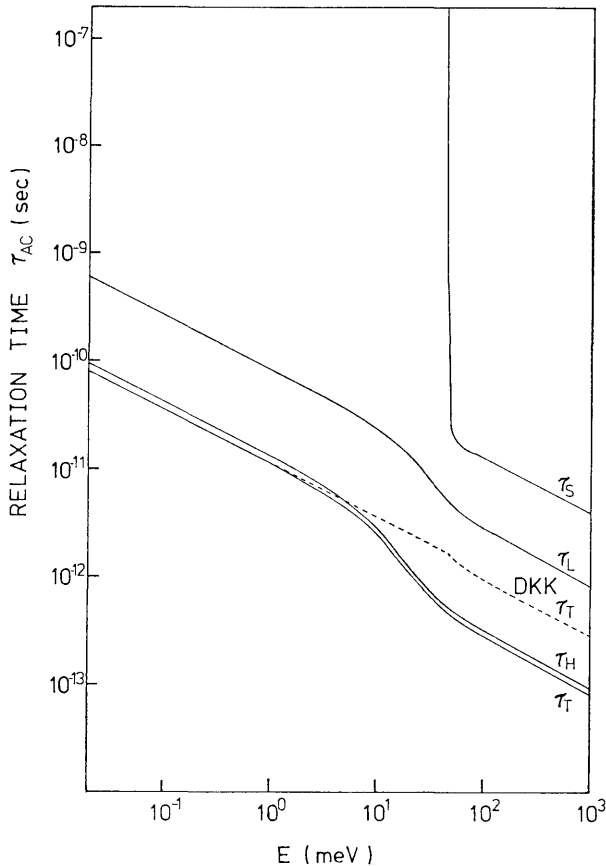


Fig. 2. Energy dependence of relaxation times due to acoustic phonon scattering. Symbols τ_H , τ_L , τ_S and τ_T are the relaxation times defined in text. The solid lines represent the relaxation times calculated from the Kane model and the dashed line represents the total relaxation time calculated from the DKK model.

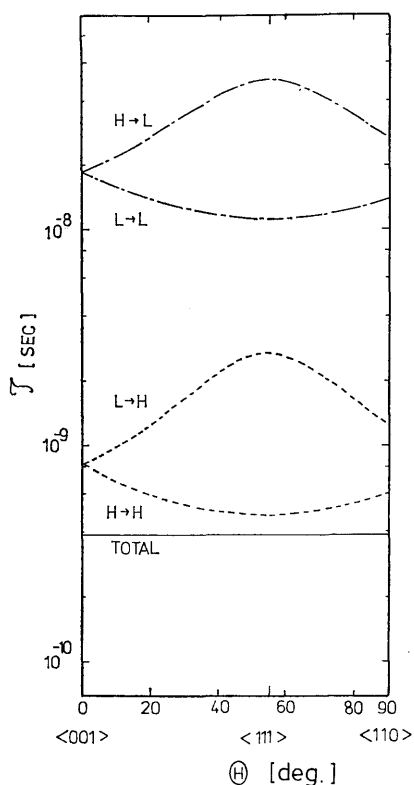


Fig. 3. Angular dependence of relaxation times due to acoustic phonon scattering for germanium. Symbol I-J means the transition from I-subband to J-subband. θ is the scattering angle.

In Fig. 3, we show the angular dependence of the relaxation times by the acoustic phonon scattering in which both heavy and light holes initially occupy in the (110) plane in the Brillouine zone. One finds that the anisotropy of the inter-subband transition is more remarkable than that of the intra-subband transition. Only on $\langle 100 \rangle$ direction, the relaxation time of holes scattered into the same final subband by the intra- and inter-subband transition ($H-H$ and $L-H$, or $L-L$ and $H-L$) has the same value. When the initial holes exist in $\langle 111 \rangle$ direction in the Brillouine zone, it is noted that the relaxation time due to the inter-subband transition has the maximum value while that due to the corresponding intra-subband transition has the minimum value. This means that the intra-subband transition occurs more frequently than the inter-subband transition. The total relaxation time doesn't show the variation so far as we neglect the k -dependence of the overlap integral.

3-2. Optical Phonon Scattering

By using both Fig. 1 and eq. (15), the resulting relaxation times by non-polar

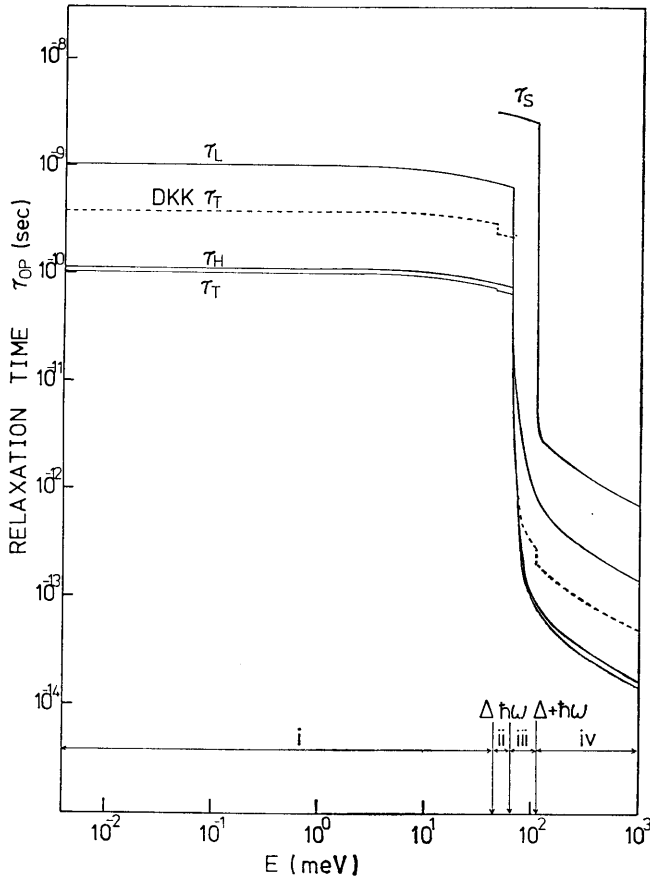


Fig. 4. Energy dependence of relaxation times due to non-polar optical phonon scattering for silicon at 100 K.

optical phonon scattering at 100 K for silicon are obtained and are shown in Fig. 4. The relaxation time is shown to be nearly independent on energy of holes below the split-off energy Δ , and the magnitude of those values are much larger than that by other scattering processes as long as the temperature is not too high. When the split-off hole band appears, the total relaxation time is affected; above $\Delta + \hbar\omega_0$ its value decreases very rapidly since the scattering processes with both creation and annihilation of phonons begin to occur in all three subbands.

The values of those relaxation times of silicon calculated from the DKK model are different from those calculated from the Kane model because the scattering process due to optical phonons is inelastic. Since the values of the relaxation times from the DKK model is about two times larger than that from the Kane model, one should consider the warping and non-parabolicity of equi-energy surfaces and also the effects of three subband holes in order to estimate the accurate value for relaxation times.

The effect of subband-interaction on the relaxation times appears differently

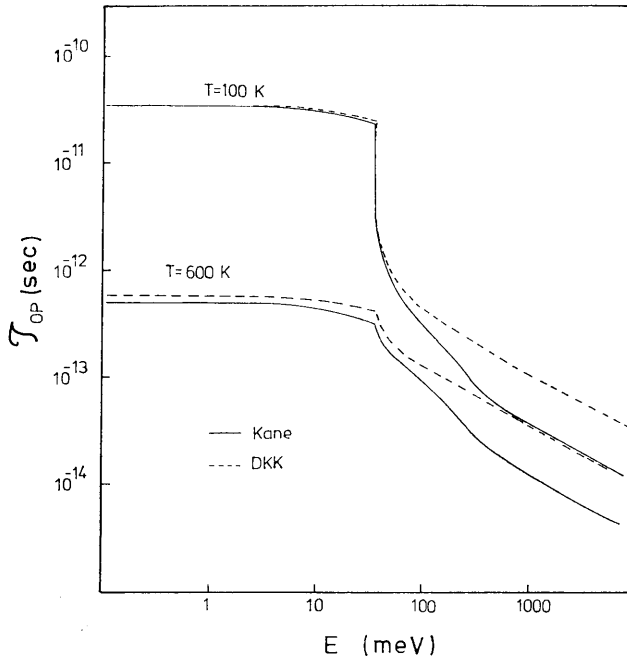


Fig. 5. Comparison of relaxation times for germanium due to non-polar optical phonon scattering calculated from Kane band model (solid line) with that calculated from DKK model (dashed line).

in silicon and germanium; for silicon one finds some difference in the relaxation times calculated from the above two band models (Kane and DKK model) even at very low temperature, while for germanium two relaxation times have certain good similarity (Fig. 5). The reason for this is considered to be the following two points. The first is that the split-off energy of germanium is so much larger that it causes decrease the anisotropy of equi-energy surfaces in lower energy states and the second is that the optical phonon energy of germanium is smaller than its split-off energy. From Figs. 2 and 4, one can estimate that the dominant scattering process would change from the acoustic phonon scattering below 100 K to the optical phonon scattering (for silicon).

3-3. Ionized Impurity Center Scattering

In Fig. 6 the resulting relaxation times calculated from CW and BH formula are shown for varying concentrations of the ionized impurities. The energy dependence of the relaxation time calculated from CW formula shows a strangely $E^{-1.5}$ power law in lower energy states, which is similar to that due to acoustic phonon scattering. In higher energy region the dependence for three subband holes, however, changes to $E^{1.5}$ law. The major hole which predominates the total relaxation time changes from heavy one to light one and further to split-off holes above 4. When the concentration of impurity centers becomes high, the value of the relaxation time decreases and that magnitude in lower energy states is less

than those due to acoustic or optical phonon scattering.

In the BH theory the dominant scattering process is, however, affected not by heavy holes but by light holes and changes to split-off holes when the split-off band appears. So long as the concentration of ionized impurity centers is low, the energy dependence of relaxation time shows the $E^{1.5}$ power law as is the case for the simple band model. Similarly to the CW formula, the magnitude of the relaxation time in low energy states is small enough to predominate the value of the total relaxation time associated with acoustic phonon, optical phonon and ionized impurity center scattering.

For the ionized impurity scattering, the difference of the values of two relaxation times calculated from the DKK model and from the Kane model is small

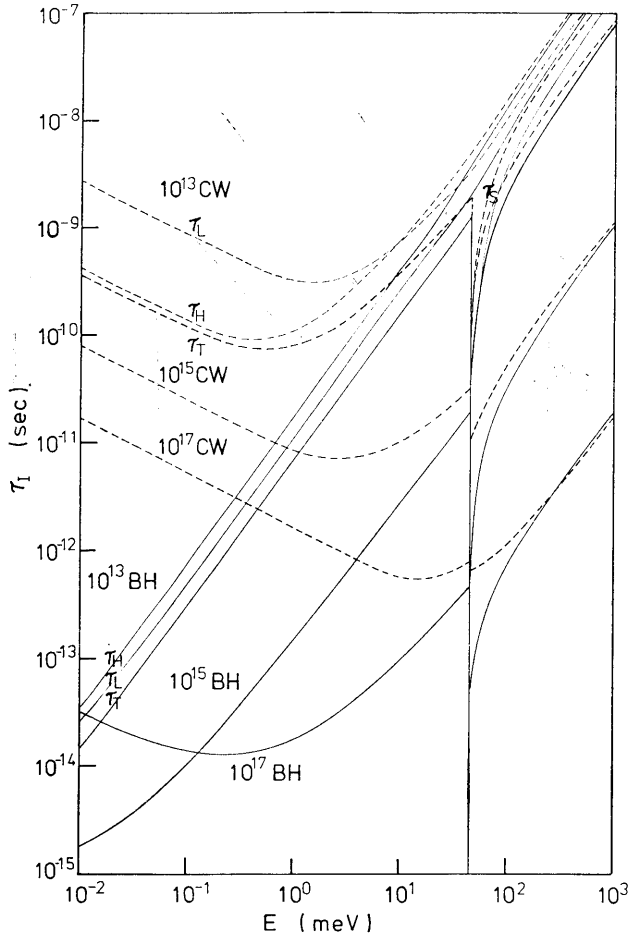


Fig. 6. Energy dependence of relaxation times due to ionized impurity scattering for silicon. We used two scattering models (CW and BH model) and the Kane model. Symbol 10^{13} CW means that the value is calculated by the CW model with 10^{13} cm^{-3} of ionized impurity concentration.

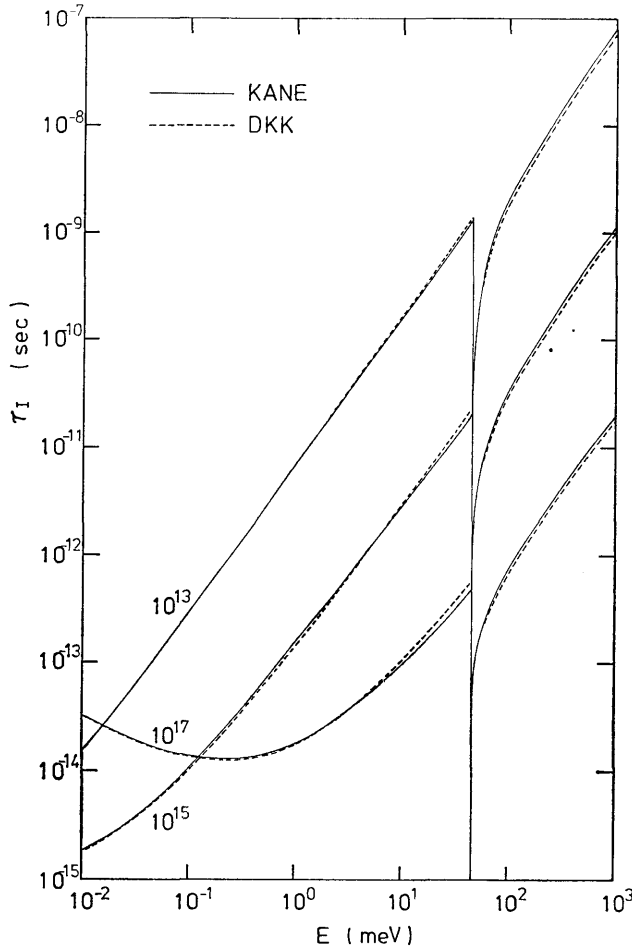


Fig. 7. Comparison of relaxation times due to ionized impurity scattering calculated from the Kane model with that from the DKK model. The BH theory is used for silicon.

(Fig. 7) so that the DKK model seems to adequately describe the ionized impurity center scattering if one assumes that the overlap integral is nearly unity and that the perturbing potential by ionized impurity centers is represented by the screened potential whose screening distance is taken as the average spacing $N_I^{-1/3}$ (CW) or Debye length (BH).

We have also considered the temperature dependence of the net concentration of ionized impurity centers assuming that the impurities have the localized acceptor level E_A in the band gap and the degree of the ionization of impurity takes the Maxwell-Boltzmann distribution for a simplicity. Then neutral impurities exist in the semiconductors and one should also consider the scattering by these neutral centers.

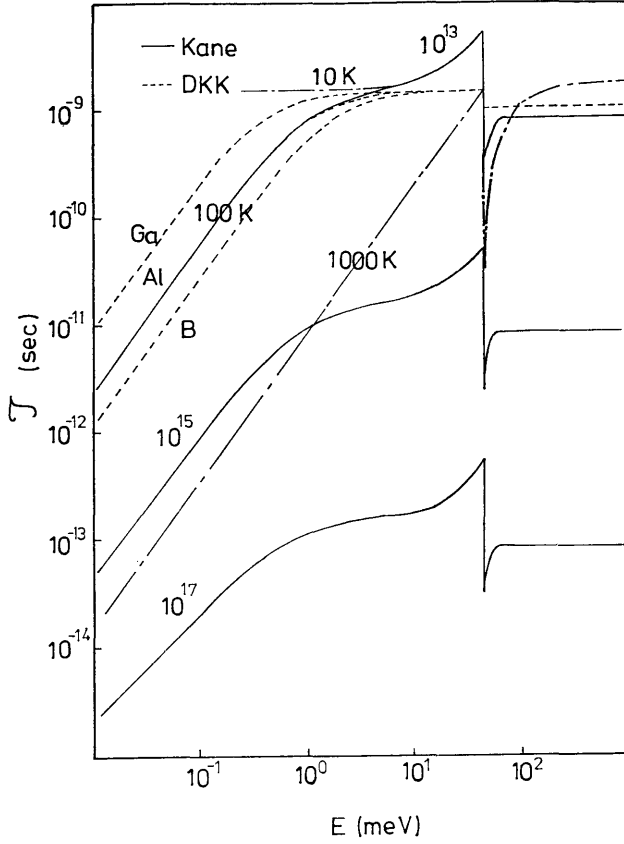


Fig. 8. Relaxation times due to impurity scattering including the effects of both ionized impurity and neutral impurity with varying impurity concentrations (10^{13} , 10^{15} and 10^{17} cm^{-3}). We have used the BH theory for ionized impurity scattering. The solid lines show the variation of the relaxation time of 10^{13} cm^{-3} impurity concentration with varying temperatures (10, 100 and 1000 K). We also show the relaxation time calculated from the DKK model with various acceptors (Ga, Al and B).

According to Erginsoy [14], the relaxation time by neutral center scattering is given as,

$$\frac{1}{\tau_N^i} = 20 N_n \frac{\kappa \hbar^3}{m_i^{*2} e^2}, \quad (20)$$

We show the relaxation time by ionized impurity scattering involving the neutral center scattering in Fig. [8].

Neglecting the effect of the neutral center scattering, one finds that the magnitude of the relaxation time due to ionized impurity scattering increases against the energy of holes particularly in higher impurity concentrations (Fig. 6) so that the mobility in the lower temperature increases [21], which is inconsistent

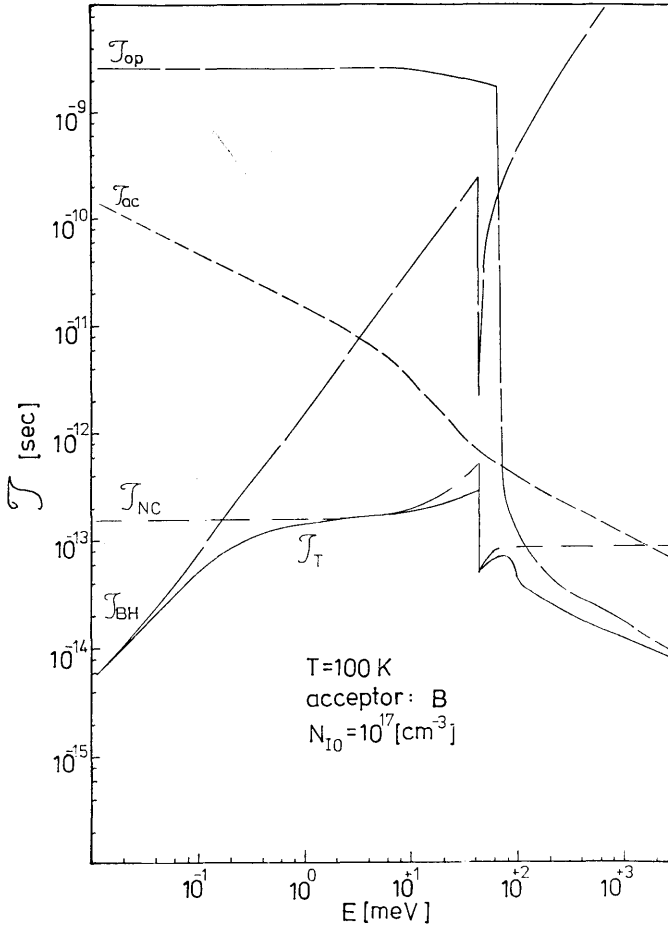


Fig. 9. Energy dependence of mixed relaxation time of silicon. We considered in the figure the lattice scattering involving non-polar optical phonon scattering and the impurity center scattering both the effects of ionized and neutral center. The density of impurity center N_{10} is taken to be 10^{17} cm^{-3} .

with experimental results. This contradiction seems to occur from the following two reasons. The first is that in the BH (or CW) theory one assumes the screening distance as the Debye length (or the average spacing) which would be correct only the lower concentration of the ionized impurities. In higher concentrations one should obtain the screening distance self-consistently from Poisson's equation. The second is that at very low temperatures (low energy) one should strictly consider the effect of the neutral center scattering. All of the mixed relaxation time associated with acoustic and non-polar optical phonon scattering and the impurity scattering including both effects of ionized and neutral centers is shown in Fig. 9.

4. Conclusion

(1) Density of States

The effect of the interaction between subbands becomes remarkable near the split-off energy Δ and prompts for the energy dependence of the density of states to deviate from $E^{0.5}$ power law. Particularly in silicon, this affects considerably the relaxation time and mobility on account of its smaller split-off energy.

(2) Acoustic Phonon Scatterig and its Anisotropy

Since the $E^{-0.5}$ power law of the energy dependence of the relaxation time due to acoustic phonon scattering is valid only below 10 *meV* (Si), the interaction between subbands has a significant effect of the acoustic phonon scattering which predominates other scattering processes in silicon at about 100 K.

Mixing the intra- and inter-subband transition, the anisotropy of the total relaxation time would vanish so far as the k -dependence of the overlap integral is neglected.

(3) Non-Polar Optical Phonon Scattering

The effect of the subband-interaction appears to be different for silicon and germanium; for silicon ($\Delta < \hbar\omega_0$), the subband-interaction is too significant to be neglected (silicon type), while for germanium ($\Delta > \hbar\omega_0$) that is considerably small (germanium type).

(4) Ionized Impurity Scattering

The BH theory is more appropriate for higher impurity concentrations than CW theory. Over 10^{17} cm^{-3} of the impurity concentration one should, however, consider both the neutral center scattering and the accurate screening distance calculated self-consistently using Poisson's equation.

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