

Title	Screening distance and ionized impurity scattering for holes in the warped and non-parabolic band
Sub Title	
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Publisher	慶應義塾大学理工学部
Publication year	1982
Jtitle	Keio Science and Technology Reports Vol.35, No.10 (1982. 12) ,p.169- 184
JaLC DOI	
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Notes	
Genre	Departmental Bulletin Paper
URL	https://koara.lib.keio.ac.jp/xoonips/modules/xoonips/detail.php?koara_id=KO50001004-00350010-0169

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SCREENING DISTANCE AND IONIZED IMPURITY SCATTERING FOR HOLES IN THE WARPED AND NON-PARABOLIC BAND

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(Received September 7, 1982)

ABSTRACT

The screening distance for the ionized impurity potential surrounded by holes in the warped and non-parabolic valence band is obtained by using Dingle's self-consistent method.

By comparing this distance with the previously and commonly used distances R_{CW} and R_{BH} , we can discuss the relation of the two ionized impurity scattering theories i. e., the theory proposed by Conwell and Weisskopf (the CW model) and that proposed by Brooks and Herring (the BH model). We have investigated the validity for each model.

The calculated drift mobility, in which the lattice scattering including the effect of non-polar optical phonons and the impurity scattering due to both ionized and neutral centers are taken into account, shows a good agreement with experimental results so far if the existence of three subbands and the interaction between those subbands would be considered.

1. Introduction

The scattering mechanisms of electrons due to ionized impurity centers have been discussed theoretically by Conwell and Weisskopf [1] (the CW model in this paper) or Brooks [2] and Herring [3] (the BH model) and also Dingle [4]. They have treated this scattering problem by introducing the cut-off Coulomb potential (the CW model) or the screened Coulomb potential (the BH model). Many workers have developed these theoretical model and applied to several cases of electrons and holes. In these treatments, however, they used the simple band model for the actual valence band. In order to investigate the scattering phenomena for holes, it may be possible only in very low temperature to use such a simple parabolic and isotropic band for the valence band. When the temperature increases and the effect of the interaction between subbands becomes significantly, it would be impossible to use such a simple band model. Particularity in silicon, whose split-off energy Δ is relatively small, the warping and the non-parabolicity of equi-energy surfaces play important role in rater low energy states.

It has not, however, been unfortunately discussed the screening distance for holes with considering the effects of both the existence of three subbands and the interaction between those subbands. By using Dingle's self-consistent method, we have calculated in this paper the screening distance for ionized impurity surrounded by holes which occupy those complicated valence band. By comparing the resulting screening distance with the original ones (R_{BH} and R_{CW}), we discuss in this paper the validity of the two scattering models proposed by Brooks-Herring and Conwell-Weisskopf and further verify the reason why at low temperature the CW model could describe more accurately the ionized impurity scattering than the BH model when the ionized impurity concentration is not so high.

2. Theory

2-1. Fermi-Dirac integral for warped and non-parabolic band

The Fermi-Dirac integral for free carrier model is defined as,

$$F_{1/2(\eta)} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{\sqrt{x}}{e^{x-\eta} + 1} dx, \quad \text{where } \eta = \frac{\zeta}{k_B T} \quad \zeta: \text{Fermi energy} \quad (1)$$

By using this Fermi-Dirac integral, the number of holes p in the valence band is given as,

$$p = \frac{1}{4\pi^{3/2}} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} (k_B T)^{3/2} F_{1/2(\eta)}, \quad (2)$$

where m_0 , \hbar , k_B and T are the electron mass, Planck's constant divided by 2π , Boltzmann's constant and temperature, respectively.

The band structure near the valence band edge of IV-group semiconductors has been most thoroughly discussed by Dresselhaus et al. [5] and Kane [6] using the $\hat{k} \cdot \hat{p}$ method including the spin-orbit interaction. Dresselhaus, Kip and Kittel (DKK in this paper) have neglected the interaction between subbands as known as heavy, light and split-off hole bands, whereas Kane has considered that effect. We call in this paper the former band structure as the DKK model and the latter as the Kane model.

The Fermi-Dirac integrals for these two band model are given as follows; for the DKK model

$$F_{1/2(\eta)}^H = \frac{H}{4\pi} \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{\sqrt{x}}{e^{x-\eta} + 1} dx, \quad (3)$$

$$F_{1/2(\eta)}^L = \frac{L}{4\pi} \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{\sqrt{x}}{e^{x-\eta} + 1} dx, \quad (4)$$

and

$$F_{1/2(\eta)}^S = \frac{S}{4\pi} \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{\sqrt{x}}{e^{x + d/k_B T - \eta} + 1} dx, \quad (5)$$

where the constants H , L and S are modified coefficient, which represents the anisotropy of the equi-energy surfaces and defined with the band parameters A , B and C (DKK notation) as [7],

$$H = \int \frac{d\Omega}{(-A - \sqrt{B^2 + C^2\mu})^{3/2}}, \quad (6)$$

$$L = \int \frac{d\Omega}{(-A + \sqrt{B^2 + C^2\mu})^{3/2}}, \quad (7)$$

and

$$S = \int \frac{d\Omega}{(-A)^{3/2}}, \quad (8)$$

with

$$\mu = \sin^2 \theta (\sin^2 \theta \cos^2 \phi \sin^2 \phi + \cos^2 \theta),$$

and for the Kane model, the Fermi-Dirac integrals are given as,

$$F_{1/2(\eta)}^i = \frac{1}{4\pi\sqrt{k_B T}} \frac{2}{\sqrt{\pi}} \int \frac{u_i^{1/2}(k_B T x, \theta, \phi) u_i'(k_B T x, \theta, \phi)}{e^{x-\eta} + 1} d\Omega dx, \quad (9)$$

and

$$F_{1/2(\eta)}^{S} = \frac{1}{4\pi\sqrt{k_B T}} \frac{2}{\sqrt{\pi}} \int \frac{u_S^{1/2}(k_B T x, \theta, \phi) u_S'(k_B T x, \theta, \phi)}{e^{x+A/k_B T-\eta} + 1} d\Omega dx, \quad (10)$$

where u_i is given by Arsche et al. [8] as,

$$k_i^2 = \frac{2m_0}{\hbar^2} u_i(E, \theta, \phi). \quad (11)$$

We distinguish three subbands by indices i ($=H, L$ and S). The derivative of u_i is also defined as,

$$u_i'(E, \theta, \phi) = \frac{\partial u_i}{\partial E}. \quad (12)$$

From eqs. (9) and (10), one can obtain the Fermi-Dirac integral for holes whose equi-energy surface is warped and non-parabolic.

2-2. Self-consistent Field and Screening Distance

For a simplicity, we assume that the ionized acceptor are singly charged centers and whose concentration is not so high, i. e. we consider the non-degenerate p-type semiconductors with shallow acceptor levels; these are applicable to p-type Ge and Si whose acceptor concentration is nearly $10^{13} \sim 10^{17} \text{ cm}^{-3}$.

The electrostatic potential energy $\phi_{(r)}$ of a free hole distance r from the ionized acceptor is given as the Coulomb potential under the simplest approach of

the H-atom approximation. This, however, cause the inconsistent results for the scattering cross section of holes with large impact parameters. Conwell and Weisskopf [1] have firstly introduced the concept of the cut-off distance of the Coulomb potential of the ionized charge, and they have taken the cut-off distance as half of the mean distance of the scattering centers. Wherease Brooks [2] and Herring [3] have proposed the screening potential of the ionized charge surrounded by free carriers and they have introduced the Debye length as the screening distance with considering the distribution of holes with thermal energy. Dingle [4] has developed further these theory to obtaine the more accurate screening distance, and found a comprehensive form for $\phi_{(r)}$, particulary where r is large, taking explicit account of the screening of the negatively charged acceptor ion by the surrounding hole cloud.

The theory proposed by Dingle shows that when the acceptors are negatively charged, they induce the localized electric field and then those electric fields are screened by surrounding free holes, and that the relationship between this screening potential $\phi_{(r)}$ and the screening hole is connected by Poisson's equation. The number of screening hole p is, however, represented by using the Fermi-Dirac integral determined by the term of the screening potential $\phi_{(r)}$. In this way the screening potential of the charged acceptor is the self-consistent one, and therefore it must be self-consistently determined from Poisson's equation, as follows.

Let $\phi_{(r)}$ represent the potential of a singly negatively ionized acceptor screened by hole cloud. When the acceptor is negatively charged, the Fermi energy must be replaced from ζ_p to $\zeta_p - e\phi_{(r)}$, where ζ_p represents the customary space independent Fermi energy. Therefore the hole number $p_i (i=H, L \text{ and } S)$ near the ionized acceptor is given as follows.

$$p_{(r)}^i = \frac{1}{4\pi^{3/2}} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} (k_B T)^{3/2} F_{1/2}^i(\eta_p - e\phi/k_B T), \quad (13)$$

with

$$\eta_p = \zeta_p / k_B T.$$

We are now interesting in the screening potential far from the ionized acceptor, where the effect of the screening by the free carrier cloud is sufficiently significant and the magnitude of those potential is enough small. One can therefore expand the Fermi-Dirac integral $F_{1/2}^i(\eta_p - e\phi/k_B T)$ using the relation,

$$\frac{\partial}{\partial \eta} F_{1/2}^i(\eta) = F_{-1/2}^i(\eta). \quad (14)$$

From equation (2) and (13), the excess number of i -th holes surrounding the ionized acceptor is given as,

$$\begin{aligned} \delta p_{(r)}^i &= p_{(r)}^i - p^i = \frac{1}{4\pi^{3/2}} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} (k_B T)^{3/2} [F_{1/2}^i(\eta_p - e\phi/k_B T) - F_{1/2}^i(\eta_p)] \\ &\simeq \frac{1}{4\pi^{3/2}} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} (k_B T)^{1/2} F_{-1/2}^i(\eta_p) \phi_{(r)}. \end{aligned} \quad (15)$$

Thus the total screening charge of three type holes surrounding the charged acceptor is,

$$\rho_{(r)}^T = \sum_i \rho_{(r)}^i = \frac{e}{4\pi^{3/2}} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} (k_B T)^{1/2} \left[\sum_i F_{-1/2}^i(\eta_p) \right] \phi_{(r)}. \quad (16)$$

Assuming the screening potential [4] as,

$$\phi_{(r)} = \frac{e}{\kappa T} e^{-r/R_T}, \quad (17)$$

and from the Poisson's equation, the screening distance R_T is given as eq. (18),

$$\frac{1}{R_T^2} = \frac{e}{\kappa \sqrt{\pi}} \left(\frac{2m_0}{\hbar^2} \right)^{3/2} (k_B T)^{1/2} \left[\sum_i F_{1/2}^i(\eta_p) \right] \equiv \sum_i \frac{1}{R_i^2}, \quad (18)$$

where R_i is the screening distance due to i -th hole only, and κ is the dielectric constant of the semiconductor. In calculations, we have divided the equi-energy surfaces into 1152 elements and performed the integration by Simpson's method. The energy integration was also carried out by using the Gauss-Laguerre 32 polynomials.

2-3. Relaxation Time and Mobility for Holes

Next we have obtained the relaxation times for holes which exist in the warped and non-parabolic valence band. The scattering mechanisms considered here are those due to lattice vibration including the non-polar optical phonon and the ionized impurities. We have already discussed about the lattice scattering in reference [9]. In this paper we calculate the relaxation time due to ionized impurity and obtained the total relaxation time to deduce the mobility of holes.

The two theories of the BH and CW model are used to represent the ionized impurity scattering. According to them the relaxation time due to the ionized impurity is given as,

$$\frac{1}{\tau^{ij}} = \frac{N_I}{\kappa^2} \left(\frac{\hbar^2}{2m_0} \right)^{1/2} \int G_{ij} H_i d\Omega_j, \quad (19)$$

where τ^{ij} and N_I are the relaxation time from i -th state to j -th state and the net concentration of impurities, respectively. The symbols G_{ij} and H_i are determined as follows. Since the scattering potential by ionized impurity doesn't depend on the band structure, we can represent [10] the anisotropy of the scattering due to the symmetry property of both initial and final wave functions by the overlap function G_{ij} , which has a dependence only on the scattering angle θ and not on wave vector k because of the scattering with small momentum changes. Thus we use the next two relations of G_{ij} as [11].

$$G_{ij} = \frac{1}{4} (1 + 3 \cos^2 \theta) \quad \text{for inter-subband transition,} \quad (20)$$

$$G_{ii} = \frac{3}{4} \sin^2 \theta \quad \text{for intra-subband transition.} \quad (21)$$

The symbols H_i is determined from the scattering matrix element using S-wave function and defined as follows,

$$H_i = \frac{u'_i}{u_i^{3/2}} \frac{1 - \cos \Theta}{[(1 - \cos \Theta) + 1/2k^2 R^2]^2} \quad (22)$$

where Θ and k are the scattering angle and the wave vector for holes.

The difference between the BH model and CW model is represented in terms of the screening distance R as,

$$R_{\text{BH}} = (\kappa k_B T / e^2 N_I)^{1/2} \quad \text{for the BH model,} \quad (23)$$

$$R_{\text{CW}} = N_I^{-1/3} / 2 \quad \text{for the CW model.} \quad (24)$$

Since the valence band is composed by three subbands, we treat the intra- and inter-subband transition for each subband holes by ionized impurity scattering as follows. It is reasonable to assume that the scattering process by this center occurs elastically with small change of the crystal momentum of hole, therefore we consider that both the intra- and inter-subband transitions can occur for heavy and light holes because these two subbands degenerate at zone center. We consider, however, only the intra-subband transition (S-S) for split-off hole because this subband begins to appear at higher energy state than those other two subbands by Δ .

Carrying on the integration defined in eq. (19) over the all possible final states, we calculate the relaxation time for each subband hole.

We have moreover considered the effect of the neutral center scattering. According to Erginsoy [12], the relaxation time by those center scattering is given as,

$$\frac{1}{\tau^i} = 20 N_n \frac{\kappa \hbar^3}{e^2 m_i^{*2}}, \quad (25)$$

where N_n is the concentration of the neutral impurities. The symbol m_i^* ($i=H, L$ and S) is the effective mass and defined as,

$$\frac{m_i^*}{m_0} = \left[\frac{\int u_{i(E, \theta, \phi)}'^2 u_{i(E, \theta, \phi)}' d\Omega}{4\pi \sqrt{E}} \right]^{2/3}. \quad (26)$$

After calculating the relaxation times due to both lattice vibration and impurity center scattering, we obtain the drift mobility by the next equation.

$$\mu_D = \frac{\sum_i p_i \mu_D^i}{\sum_i p_i}, \quad (27)$$

where μ_D^i ($i=H, L$ and S) is the drift mobility for each subband holes and given as,

$$\mu_D^i = \frac{e^2}{\hbar^2} \frac{\int (\partial f / \partial E) \tau_{(E)}^T (\partial E / \partial k_j^i)^2 d\mathbf{k}}{\int f d\mathbf{k}}, \quad (28)$$

where f is the hole distribution function.

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

Table 1. 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 $\epsilon^2=2$ system.

Parameter		Unit	Si	ref.	Ge	ref.
BAND PARA- METER	A	ATOMIC UNIT	-4.42		-13.27	
	B		-0.79	13	-8.63	14
	C		4.78		12.4	
MODI- FIED COEFFI- CIENT	H	ATOMIC UNIT	4.92		2.59	
	L		0.78	7	0.11	7
	S		1.45		0.26	
ρ	g/cm^3	2.329	15	5.32	16	
U_l	cm/sec	9.04×10^5	15	5.4×10^5	16	
T_{opt}	K	735	15	430	16	
κ	ϵ_0	11.7	15	16.0	16	
Δ	meV	44.0	17	295	20	
E_{eff}	eV	5.3	18	5.3	14	
$D_l K$	eV/cm	6.6×10^8	19	9.1×10^8	14	

3. Results and Discussion

3-1. Fermi-Dirac Integral

We show the resulting Fermi-Dirac integral of $F_{1/2}^i$ in Fig. 1. Clearly from eqs. (3)~(5), the Fermi-Dirac integral $F_{1/2}^i$ for the DKK model is independent of the temperature except for split-off hole. On the other hand, that for the Kane model has the dependence of the temperature because the Kane model has the non-parabolic relation between E and \hbar . Since the above two band models have good agreements in the lower energy states than the split-off energy Δ , one can find that the Fermi-Dirac integral calculated from the Kane model converge to that calculated from the DKK model when the temperature is enough low (for silicon at several ten kelvin).

In Fig. 2, we also show the Fermi-Dirac integral of $F_{-1/2}^i$ form in the analogous way as in Fig. 1.

3-2. Screening Distances and Relaxation Time

According to eqs. (2) and (18), and also using the Fermi energy η_p as a parameter, we replotted the relation between the hole number p and the screening distance R , in which the non-parabolicity and the warping of the valence band are carefully considered. A certain good linearity between $\log(p)$ and $\log(R)$ is

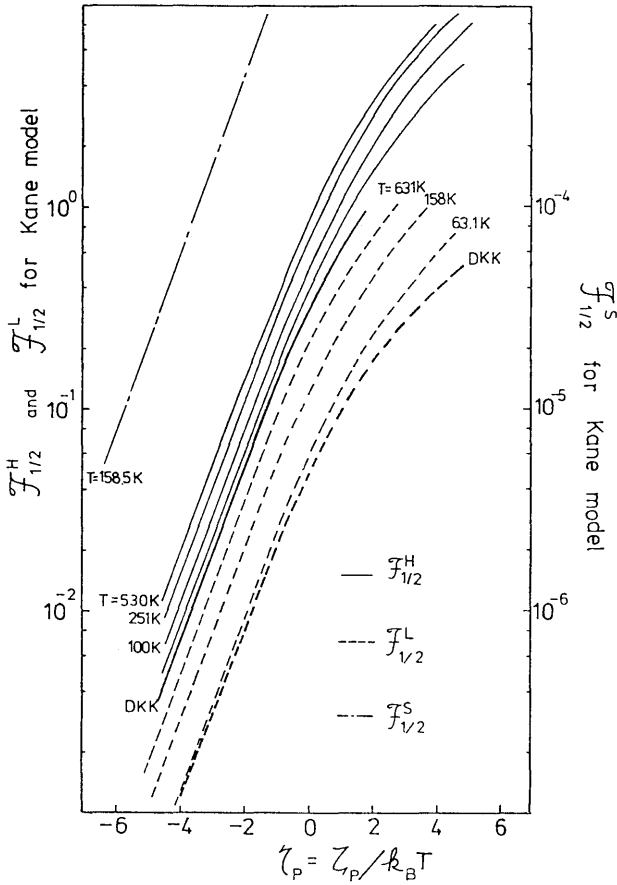


Fig. 1. Fermi-Dirac integral $F_{1/2(\zeta_p)}^i$ for warped and non-parabolic valence band of Si with varying temperature. The symbols $F_{1/2(\zeta_p)}^H$, $F_{1/2(\zeta_p)}^L$ and $F_{1/2(\zeta_p)}^S$ means the values for heavy, light and split-off holes, respectively. We show also the values calculated from the DKK model in the same figure. The values of $F_{1/2}^S$ is shown here only for the case of $T=158.5$ K because the split-off subbands begins to appear higher than the other two subbands by Δ .

found particularly in the lower impurity concentration (under 10^{15} cm^{-3}) or in the higher temperature region. The screening distance R is approximately proportional to both the inverse of the root of the carrier number p and the root of the temperature T . Moreover in such a region mentioned above, the screening distances for each type holes (R_H and R_L) have a good agreement each other (Fig. 3). One can, however, find the discrepancy of the screening distance for the each type holes (R_H and R_L) when the impurity concentration increases. Particularly at low temperature (for a example 15.8K), one can recognize the deviation between R_H (by the heavy holes) and R_L (by the light holes) even at the intermediate impurity concentration as 10^{16} cm^{-3} .

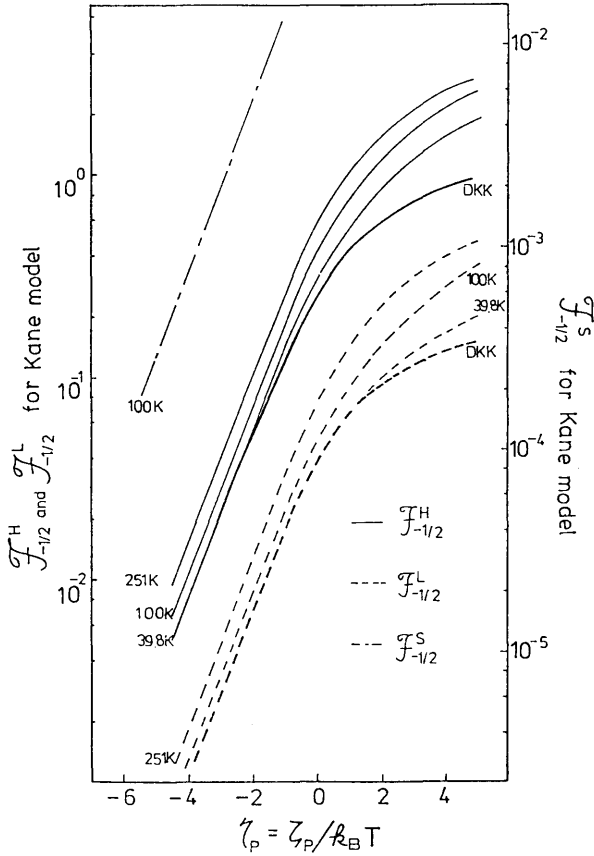


Fig. 2. Fermi-Dirac integral $F_{-1/2}^L$. The symbols are same as in Fig. 1.

Now in order to estimate the validity of the two scattering models (the BH and CW model), we compare the original screening distance proposed by Conwell and Weisskopf (R_{CW}) or Brooks and Herring (R_{BH}) shown in Fig. 4 with our resulting distance R_{Kane} shown in Fig. 3. The cut-off distance R_{CW} defined in the CW model does not involve the effect of the spatial broadening of free holes based on the thermal excitation because in the CW model one assume that the impurities distribute uniformly in the crystal and have the average spacing as the cut-off distance R_{CW} . Therefore R_{CW} is independent of the temperature. This produces the large discrepancy of R_{CW} from R_{Kane} when the temperature increases. For the semiconductors in which the ionized impurities are intermediately doped, the screening distance from the BH model (R_{BH}) show the more accurate value than that from the CW model (R_{CW}). Thus we can confirm that the BH model describes more accurately the phenomena of the ionized impurity scattering in the intermediately doped semiconductors ([21] and [22]).

On the contrary, it is said that the CW model is far more superior than the BH model when the temperature is rather low and the concentration of the ionized

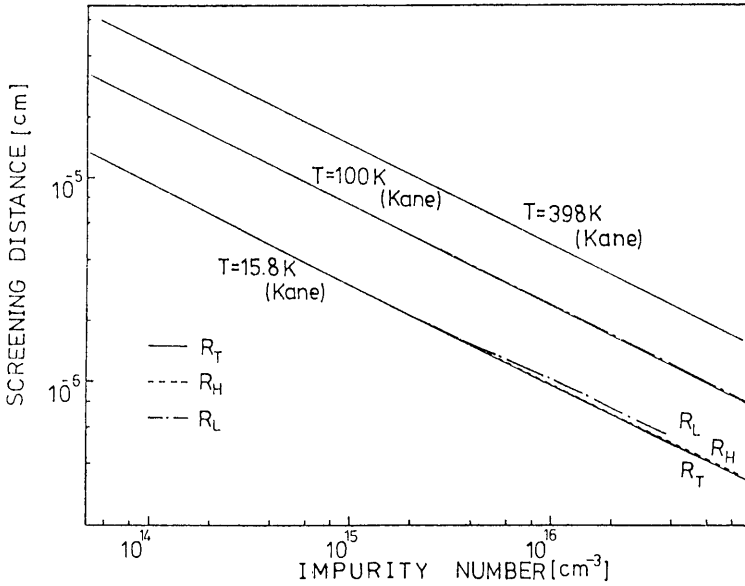


Fig. 3. Screening distance calculated from the Kane model with varying temperature using eq. (18). The symbols R_T , R_H , and R_L are the total screening distance, the screening distance by heavy holes and light holes, respectively. Owing to the separation of the split-off hole subband by Δ , R_S does not appear in the same figure.

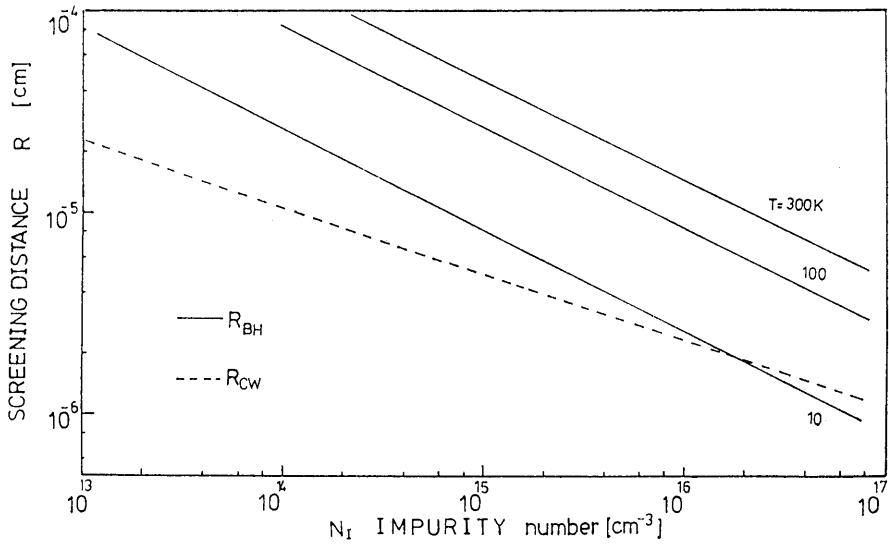


Fig. 4. Screening distance originally proposed by the CW and BH model.

impurities is considerably low. In such a condition the BH model fails and the CW model becomes the only viable replacement [21]. Nextly we point out this reason. Let us consider the screening distance at the low temperature, where the ionized impurity scattering acts most predominantly. In the case of the low concentration of ionized impurities R_{CW} shows amazingly the rather accurate value of the screening distance than R_{BH} (comparing Fig. 3 and Fig. 4).

$$R_{CW} \simeq R_{\text{Kane}} < R_{BH}$$

In such a low temperature and low ionized impurity concentration (several kelvin

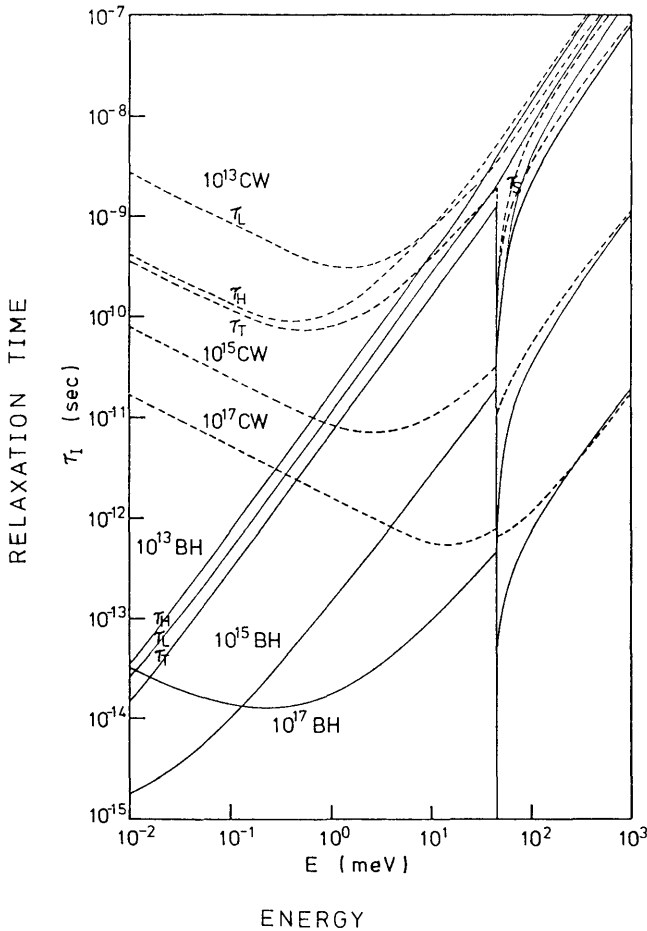


Fig. 5. Energy dependence of relaxation time due to ionized impurity centers for the Kane model calculated from the CW or BH model. The symbols τ^H , τ^L and τ^S are the relaxation time due to heavy light and split-off holes and also τ^T is the total relaxation time. We have calculated those values at $T=100 \text{ K}$ with varying the net impurity concentration $N_I=10^{13}\sim 10^{17} \text{ cm}^{-3}$.

and nearly 10^{13} cm^{-3}), the influence of the spatial broadening of thermally excited free holes around the ionized acceptors is considerably small, so that if the Debye length is taken as the screening distance (R_{BH}), one overestimates the effect of the spatial broadening of free holes. According to eq. (17), the effective region of the screening potential is determined by the screening distance. Since R_{BH} is longer than the actual value R_{Kane} , the effect of electrostatic potential of the BH model is inconsistently widely spread. Therefore in the region of both low temperature and low ionized impurity concentration, the scattering probability calculated by the CW model will be expected to be more proper than that by the BH model. Considering these points, under the condition mentioned above the relaxation time due to the ionized impurity scattering from the BH model will be smaller than that from the CW model, and this deduces that the mobility calculated from the BH model is expected to be inconsistently smaller than the actual values.

In Fig. 5, we show the energy dependence of the relaxation times due to ionized impurities calculated from the BH and CW model. As we predicted above, the resulting relaxation time calculated from the CW model is greater than that from the BH model. The typical energy dependence as $E^{1.5}$ obtained from the

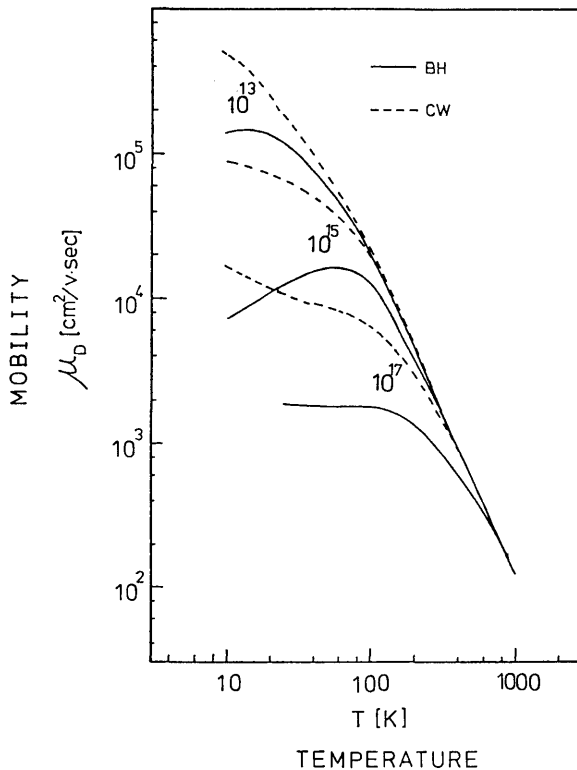


Fig. 6. Temperature dependence of hole drift mobility (Ge) calculated from the Kane model with using two scattering model as the BH and CW model and varying the net concentration of the ionized impurities.

simple isotropic and parabolic band model is found no longer except only in the BH model under sufficiently low impurity concentration (10^{13} cm^{-3}).

3-3. Mobility for holes in the warped and non-parabolic valence band

The resulting drift mobility for holes is shown in Fig. 6. As the temperature becomes lower, the difference of the drift mobility based on the above two ionized scattering models becomes remarkably. When the ionized impurity concentration increases, one can find the following points. The mobility calculated from the BH model show the typical temperature dependence such as the considerable decrease of the mobility due to the ionized impurity scattering at several ten kelvin and also the appearance of its maximum value, which are experimentally found in the intermediately doped semiconductors. The calculated value from the

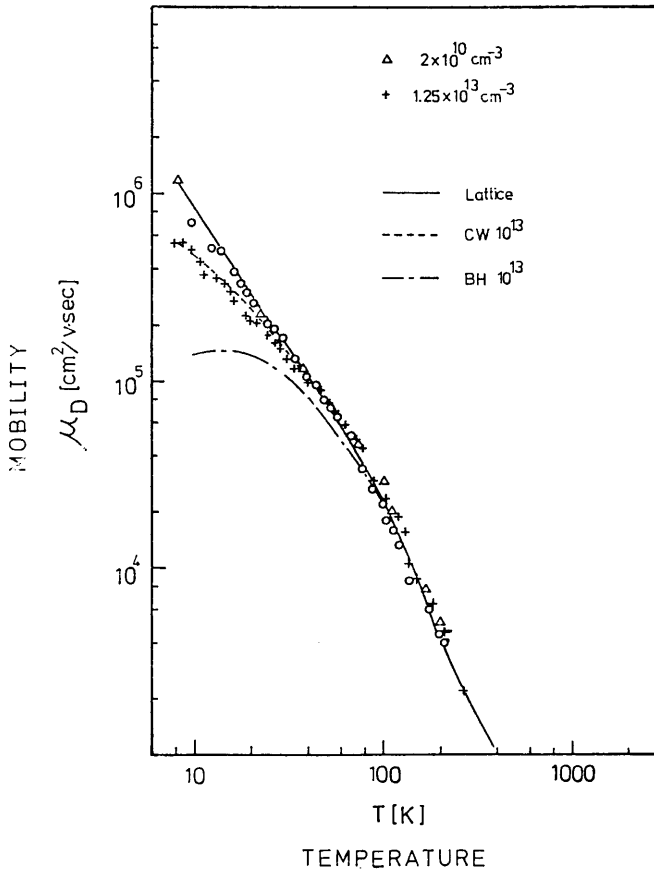


Fig. 7. Comparison of calculated drift mobility with the reported values of Ge. The data were quoted from Brown et al. [22] (+), Ottaviani et al. [23] (Δ) and De Laet et al. [24] (\circ). In the case of lattice scattering dominant, the solid curve is well agree with Ottaviani's data.

CW model, however, does not show these typical temperature dependence of the mobility.

On the other hand, when the impurity concentration decreases, the excess-lowering of the mobility calculated from the BH model is found. Owing to the effect of the screening by free holes mentioned in sec. 3-2, the screening distance R_{BH} is longer than R_{CW} and this causes the excess scattering probability due to ionized acceptors if the BH model is adapted. Thus the values calculated from the CW model represents the more suitable ones than those from the BH model in the low impurity concentration.

Finally we compare the values of drift mobility from the above calculated results with that obtained experimentally in Fig. 7 (for Ge) and in Fig. 8 (for Si). Considering the existence of three subbands and the interaction between those,

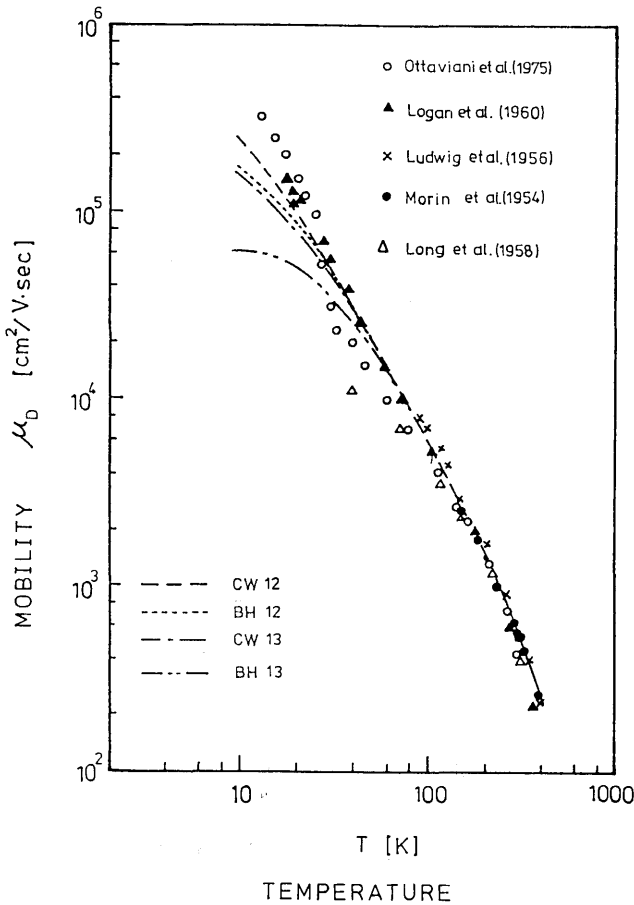


Fig. 8. Comparison of calculated hole drift mobility with the reported values of Si. The data are quoted from Ottaviani et al. [15] (○), Logan et al. [25] (▲), Ludwig et al. [26] (×) and Morin et al. [27] (●). Δ means the Hall mobility from Long et al. [18].

i. e., anisotropy and non-parabolicity of equi-energy surfaces, the calculated drift mobility shows a excellent agreement of the temperature dependence with the experimental values in the CW model.

4. Conclusion

- 1). Comparing the screening distance by Dingle's method considered with both the existence of three subbands and the interaction between those subbands with original screening distance or cut-off distance, we may conclude the BH model describe the appropriate scattering process than the CW model in the intermediately doped semiconductors. On the other hand in the case of sufficiently low impurity concentration and low temperature the CW model tends to show the more actual ionized impurity scattering phenomenon than the BH model because R_{CW} shows the more accurate value than R_{BH} .
- 2). Considering the several scattering mechanisms due to acoustic, non-polar optical phonon, ionized impurity and also neutral impurity centers, the temperature dependence of the calculated hole mobility has a excellent agreement with experimental values if one considers the subband-interaction.

Acknowledgement

The authors wish to thank Prof. M. Fukuchi for his constructive suggestions and stimulating discussion on many aspects of the subject. The Computer facilities were kindly provided by the Computer Center of Keio University. The authors would like to express their thanks to Mr. H. Taki for his kindly checking over the manuscript.

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