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Effect of valence dielectric screening on ionized-impurity-scattering-limited mobility in GaAs

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The effect of valence dielectric screening on ionized-impurity-scattering-limited mobility is studied for *n*-type gallium arsenide at different temperatures and for different impurity concentrations. The screened ionized impurity potential is found by appropriate Fourier transformation of the potential in *k* space. The screening parameter is adjusted to satisfy the Friedel sum rule. The relaxation time is calculated using the Born phase shifts. The mobilities computed are compared with earlier published work.

I. INTRODUCTION

There has been renewed interest in the scattering of charge carriers by ionized impurities in doped semiconductors.[1] We have studied in an earlier paper[2] the effect of valence dielectric screening on ionized impurity scattering and found the effect to be significant in computing relaxation times for high-impurity concentrations. The screened ionized-impurity potential was chosen by appropriate Fourier transformation of the potential in **k** space, with the scattering parameter adjusted to satisfy the Friedel sum rule. The relaxation time was obtained for the Fermi wave vector K_F by computing the Born phase shifts in Si, Ge, and GaAs at 300 K for impurity concentration of 10^{21} cm^{-3}.

In this paper we have extended our work and present our results of electron mobility in *n*-type GaAs as a function of impurity electron density for three different temperatures and compare these results with earlier published work.

II. CALCULATION OF MOBILITY

The Born phase shift for the *l*th partial wave and a given wave vector **K** as a result of a scattering potential $V(r)$ is given by[3]

$$\delta_l^B=-\frac{2m^*K}{\hbar^2}\int_0^\infty j_l^2(Kr)V(r)r^2dr\ , \tag{1}$$

where $j_l(Kr)$ is the spherical Bessel function of order l and m^* the electron effective mass.

We choose the scattering potential energy due to an impurity of charge Ze to be[4]

$$V(r)=-\frac{2Ze^2}{\pi r}\int_0^\infty\frac{\sin(kr)}{k\epsilon_{\text{eff}}(k)}dk\ , \tag{2}$$

where

$$\epsilon_{\text{eff}}(k)=\epsilon(k)+K_0R^{-2}k^{-2}\ . \tag{3}$$

In Eq. (3), K_0 is the static dielectric constant, $\epsilon(k)$ the k-dependent dielectric function for GaAs,[2] and R, the screening length, chosen in order to satisfy the Friedel sum rule expressed by[1]

$$Z=\frac{-1}{\sqrt{\pi}}\left[\frac{2m^*}{\hbar^2}\right]^{3/2}(k_BT)^{1/2}F_{-1/2}(\eta)\int_0^\infty V(r)r^2dr \tag{4}$$

where the Fermi integral $F_j(\eta)$ is defined by[5]

$$F_j(\eta)=\frac{1}{j!}\int_0^\infty\frac{x^jdx}{\exp(x-\eta)+1}\ , \tag{5}$$

with $\eta=E_F/k_BT$, the reduced Fermi energy.

It is easy to see that $V(r)$ in Eq. (2) becomes the Dingle potential given by[5]

$$V_D(r)=-\frac{Ze^2}{K_0r}e^{-r/R_D}\ , \tag{6}$$

if we use K_0 in place of $\epsilon(k)$ and R_D in place of R in Eq. (3). In Eq. (6), R_D is the Dingle screening length given by[5]

$$R_D^{-2}=\frac{4\pi ne^2}{K_0k_BT}\frac{F_{-1/2}(\eta)}{F_{1/2}(\eta)}\ , \tag{7}$$

where n is the carrier concentration.

Substituting for $V(r)$ in Eq. (1) from Eqs. (2) and (6), respectively, one obtains the following Born phase shifts:

$$\delta_l^{BE}=\frac{m^*Ze^2}{\hbar^2K}\int_0^{2K}\frac{P_l(1-k^2/2K^2)}{k\epsilon_{\text{eff}}(k)}dk\ , \tag{8}$$

where $P_l(x)$ are the Legendre functions of the first kind;

$$\delta_l^B=\frac{m^*Ze^2}{\hbar^2K_0K}Q_l\left[1+\frac{1}{2K^2R_D^2}\right]\ , \tag{9}$$

where $Q_l(x)$ are Legendre functions of the second kind.

The total momentum cross section, given by[6]

$$\sigma_T=\frac{4\pi}{K^2}\sum_{l=0}^\infty(l+1)\sin^2(\delta_l-\delta_{l+1}) \tag{10}$$

gives immediately the inverse relaxation time

$$\tau^{-1}=n\left[\frac{\hbar K}{m^*}\right]\sigma_T\ . \tag{11}$$

For isotropic parabolic bands, the drift mobility is

$$\mu = e\langle\tau\rangle / m^* \; , \tag{12}$$

where

$$\langle\tau\rangle = \frac{4}{3\pi^{1/2}F_{1/2}(\eta)} \int_0^\infty x^{3/2} f_0(x)[1-f_0(x)]\tau(x)dx \; , \tag{13}$$

with $f_0(x)$, the Fermi distribution function, given by $1/[\exp(x-\eta)+1]$ and $x = E/k_B T$. In the Brooks-Herring (BH) theory[7] the scattering cross section (obtained using the potential in Eq. (6) in the first Born approximation) turns out to be

$$\sigma_T^{\mathrm{BH}} = \frac{\pi}{2K^2 y^2}\left[\ln(1+b) + \frac{b}{(1+b)}\right] , \tag{14}$$

where $b = 4K^2R_D^2$, $y = \frac{1}{2}Ka_0$, and $a_0 = \hbar^2 K_0 / m^* e^2$.

It may be remarked that the value of effective mass m^* in GaAs is energy dependent.[8] It would be interesting to see, at least qualitatively, the effect of an energy-dependent m^* on the electron mobility. A convenient energy could be the Fermi energy E_F. The energy-dependent m^* is given by

$$m^*(E) = m^*(0) + (0.0436E + 0.236E^2 - 0.147E^3) \; , \tag{15}$$

where $m^*(0)$ is the constant effective mass ($0.0681m_0$) and E is the energy in electron volt. The Fermi energy is now given by

$$E_F = \hbar^2 k_F^2 / 2m^*(E_F) \; . \tag{16}$$

Equations (15) and (16) are solved self-consistently to find E_F and $m^*(E_F)$ for various concentrations.

III. RESULTS AND DISCUSSION

The mobilities are evaluated for GaAs at 10, 80, and 300 K for the concentrations from 10^{18} to 10^{21} cm^{-3}. The material parameters used are (K_0, m^*, Z) = (13.2, $0.0681m_0$, 1). The ratio μ_E/μ_D is presented in Table I for different concentrations and temperatures. μ_D is the mobility on the basis of Eq. (11) with Born phase shifts (δ_l^B) used. μ_D is found to be nearly the same if one uses the BH formula, Eq. (14), in Eq. (11). This observation, already[2] made for one concentration at one temperature, is found to be the same for the range of concentrations and temperatures used in the present work. μ_E is the mobility based on Eqs. (8), (10), and (12). The tabular data show that μ_E and μ_D are appreciably different when the concentration is high and nearly equal at lower concentration ($\sim 10^{18}$ cm^{-3}). This behavior is nearly independent of the temperature. The ratio μ_E/μ_D is monotonically increasing with decrease of concentration for all three temperatures considered, reaching the value 1 at lower concentration. Qualitatively this variation is similar to the one reported by Scarfone and Richardson[9] based on BH theory with a modified Dingle potential. As was mentioned in our earlier work,[2] Ref. 9 has been criticized.[10,11] Moreover, Ref. 9 does not take into consideration the Friedel sum rule. Detailed comparison with experimental results entails the usual difficulty of the interplay of different scattering mechanisms which decide the carrier mobilities.

TABLE I. Variation of mobilities with concentration at (a) 10 K, (b) 80 K, and (c) 300 K. μ_D is the drift mobility computed using δ_l^B, μ_E is the drift mobility computed using δ_l^{BE}.

Concentration n (cm^{-3})	μ_D (cm^2/V sec)	μ_E (cm^2/V sec)	μ_E/μ_D
	(a) 10 K		
10^{21}	2081.97	1553.53	0.7462
5×10^{20}	2220.13	1829.46	0.8240
10^{20}	2621.56	2437.77	0.9299
5×10^{19}	2840.19	2708.79	0.9537
10^{19}	3507.03	3447.29	0.9830
5×10^{18}	3890.94	3848.53	0.9891
10^{18}	5156.33	5137.48	0.9963
	(b) 80 K		
10^{21}	2082.00	1553.52	0.7462
5×10^{20}	2220.20	1829.51	0.8240
10^{20}	2622.25	2438.37	0.9299
5×10^{19}	2842.04	2710.46	0.9537
10^{19}	3525.37	3464.98	0.9829
5×10^{18}	3940.56	3896.99	0.9889
10^{18}	5469.17	5446.61	0.9959
	(c) 300 K		
10^{21}	2081.04	1553.93	0.7467
5×10^{20}	2220.32	1830.15	0.8243
10^{20}	2630.87	2446.26	0.9298
5×10^{19}	2866.46	2732.68	0.9533
10^{19}	3714.10	3646.10	0.9817
5×10^{18}	4416.98	4360.07	0.9871
10^{18}	9320.66	9251.24	0.9926

If we consider the energy-dependent effective mass, Eq. (11), which contains the energy-dependent τ, will have to be reexamined. For the phase shifts δ_l we had obtained, σ_T in Eq. (10) will depend on $m^*(E)$ as $[m^*(E)]^2$, and thus $\tau(E)$ will involve $m^*(E)$ as $1/m^*(E)$. Thus the mobility at a given energy would be smaller if $m^*(E)$ is larger than $m^*(0)$. We have calculated $m^*(E_F)$ with increasing E_F (with increase in concentration) and found that $m^*(E_F)$ reaches a value of $0.1416m_0$ at $E_F = 2.08$ eV which corresponds to a concentration of 10^{20} cm^{-3}. For energies higher than this the formula in Eq. (15) is not applicable. However, we can extrapolate our calculated values of $m^*(E_F)$ for higher E_F corresponding to concentrations of the value 10^{21} cm^{-3}. Since the mobility involves $m^*(E)$ as $[1/m^*(E)]^2$, the mobility will be reduced by a factor of $\gamma = [m^*(0)/m^*(E)]^2$ from the mobility calculated with constant effective mass. For the concentration of 10^{20} cm^{-3}, γ turns out to be about 4. Even though the mobility will be reduced with increased effective mass, the ratio μ_E/μ_D will not be affected.

It should be mentioned that a more accurate treatment of the effect of the variation of m^* with energy would use the full expression for σ_T (instead of approximating $\sin\delta_l$ by δ_l) and the averaging of $\tau(E)$ to be carried out in Eq. (13). Our discussion above gives qualitatively the effect of energy-dependent effective mass on mobility.

In summary, we find that the effect of spatial variation of the dielectric function of GaAs on the ionized-impurity limited mobility is significant at high carrier densities at all temperatures. At lower concentration, the valence dielectric screening is not important, even at low temperatures. An energy-dependent effective mass reduces the value of the mobility from its value calculated with constant effective mass.

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