Effect of the energy-dependent effective mass on ionized-impurity-scattering-limited mobility in gallium arsenide

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The effect of the energy-dependent effective mass on ionized-impurity-scattering-limited mobility is studied for *n*-type gallium arsenide at different temperatures and for various impurity concentrations. The spatial variation of the dielectric function is also included in the screened impurity-ion potential. The screening parameter is adjusted to satisfy the Friedel sum rule. The relaxation time is calculated using Born phase shifts. The mobilities computed are compared with earlier published work.

I. INTRODUCTION

The problem of scattering of charge carriers by ionized impurities in semiconductors has been widely studied in terms of the Brooks-Herring (BH) theory[1] which uses the Born approximation. The ionized-impurity scattering strongly affects the electron mobility in semiconductors at low temperature and is also important near room temperature for large doping levels. Several attempts have been made to improve the BH treatment[2] by removing one or more of its simplifying assumption or by allowing for the effects neglected in that theory. An attractive alternative to the BH theory is the partial-wave phase-shift method which yields an essentially exact solution to the scattering problem for a specific potential. Recently Chandramohan and Balasubramanian (CB) (Ref. 3) have examined the effect of valence dielectric screening on ionized-impurity scattering of degenerate electrons in Si, Ge, and GaAs at 300 K for the impurity concentration of 10^{21} cm^{-3}. The relaxation time was obtained by using the Born phase shifts that satisfy the Friedel sum rule.[4] They (CB) did not find much difference between the Born and partial-wave phase shifts in the case of Ge. In a subsequent work, CB (Ref. 5) have examined the effect of valence dielectric screening on ionized-impurity-scattering-limited mobility of *n*-type GaAs at different temperatures and for various concentrations. It was found to be significant at higher concentrations for all temperatures.

The effective mass of electrons in GaAs is energy dependent. It is of great interest to see the effect of the energy-dependent effective mass on ionized-impurity-scattering-limited mobility of electrons in GaAs.

A qualitative treatment of the above problem has been given by CB (Ref. 5) for the impurity concentration of 10^{20} cm^{-3} in GaAs. In the present work, we have examined the effect of energy-dependent effective mass on mobility at different temperatures and for various impurity concentrations in GaAs. The theoretical details are given in Sec. II and the results are given and discussed in Sec. III.

II. THEORETICAL DETAILS

According to Dingle,[6] the potential energy may be written in the form

$$V(r)=\frac{-Ze^2}{K_0 r}e^{-r/R_D}\ , \tag{1}$$

where K_0 is the static dielectric constant. In Eq. (1), the Dingle screening length R_D is given by

$$R_D^{-2}=\frac{4\pi n e^2}{K_0 k_B T}\frac{F_{-1/2}(\eta)}{F_{1/2}(\eta)}\ , \tag{2}$$

where n is the carrier concentration and the Fermi integral of order j is defined by

$$F_j(\eta)=\frac{1}{j!}\int_0^\infty \frac{x^j}{[\exp(x-\eta)+1]}dx\ . \tag{3}$$

The total momentum-transfer cross section in the BH theory turns out to be[7]

$$\sigma_T^{\rm BH}=\frac{\pi}{2K^2y^2}\left[\ln(1+b)-\frac{b}{1+b}\right]\ , \tag{4}$$

where $b=4K^2R_D^2$,

$y=(1/2)Ka_0$,

TABLE I. Energy-dependent effective mass for various concentrations.

Concentrations (cm^{-3})	m^* (a.u.)
5×10^{20}	0.2063
10^{20}	0.1406
5×10^{19}	0.1174
10^{19}	0.0850
5×10^{18}	0.0781
10^{18}	0.0709

TABLE II. Values of mobilities μ_{DM}, μ_{EM}, and the ratio μ_{EM}/μ_{DM} for various concentrations with energy-dependent effective mass at 10 K. The values of the mobilities and their ratio with constant effective mass are given in parentheses.

Concentrations (cm^{-3})	μ_{DM} (cm^2/V sec)	μ_{EM} (cm^2/V sec)	μ_{EM}/μ_{DM}
5×10^{20}	352.22 (2219.94)	278.29 (1832.25)	0.7901 (0.8254)
10^{20}	808.14 (2621.73)	743.27 (2439.63)	0.9197 (0.9305)
5×10^{19}	1183.66 (2840.35)	1122.21 (2708.55)	0.9481 (0.9536)
10^{19}	2486.70 (3506.96)	2440.19 (3439.69)	0.9813 (0.9808)
5×10^{18}	3160.54 (3890.53)	3120.11 (3840.81)	0.9872 (0.9872)
10^{18}	4862.98 (5152.21)	4823.89 (5109.40)	0.9920 (0.9917)

and the effective Bohr radius

$$a_0=\hbar^2K_0/m^*e^2 .$$

The inverse relaxation time is given by

$$\tau^{-1}=n\left|\frac{\hbar K}{m^*}\right|\sigma_T . \quad (5)$$

For isotropic parabolic conduction bands, the drift mobility is

$$\mu=e\langle\tau\rangle/m^* , \quad (6)$$

where

$$\langle\tau\rangle=\frac{4}{3\pi^{1/2}F_{1/2}(\eta)}\int_0^\infty x^{3/2}f_0(x)[1-f_0(x)]\tau(x)dx . \quad (7)$$

In Eq. (7), $f_0(x)$ is the Fermi-Dirac distribution function and $x=E/k_BT$.

In the Born approximation, the phase shifts are given by[8]

$$\delta_l^B=\frac{-2m^*K}{\hbar^2}\int_0^\infty j_l^2(Kr)V(r)r^2dr , \quad (8)$$

where $j_l(x)$ is a spherical Bessel function. If the Born approximation is valid, then the phase shifts for the conventional screened Coulomb potential (Dingle) obey the Friedel sum rule expressed by[2]

$$Z=\frac{-1}{\sqrt{\pi}}\left[\frac{2m^*}{\hbar^2}\right]^{3/2}(k_BT)^{1/2}F_{-1/2}(\eta)\int_0^\infty V(r)r^2dr . \quad (9)$$

This result was pointed out by Stern[9] and also by Krieger and Strauss.[10] If the scattering potential differs from the conventional screened Coulomb one, then the Dingle screening length R_D must be adjusted to satisfy the Friedel sum rule. This approach was used by Chattopadhyay[11] and also by Boardman and Henry.[12]

The total momentum cross section, in terms of the phase shifts, turns out to be[10]

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

The screened impurity ion potential which includes the spatial variation of the dielectric medium is given by[13]

$$V(r)=\frac{-2Ze^2}{\pi r}\int_0^\infty\frac{\sin(kr)}{k[\epsilon(k)+K_0R_D^{-2}k^{-2}]}dk . \quad (11)$$

Substituting for $V(r)$ in Eq. (8) from Eqs. (1) and (11), respectively, one obtains the following Born phase shifts:

$$\delta_l^B=\frac{m^*Ze^2}{\hbar^2K_0K}Q_l\left[1+\frac{1}{2K^2R_D^2}\right] , \quad (12)$$

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

$$\delta_l^{BE}=\frac{m^*Ze^2}{\hbar^2K}\int_0^{2K}\frac{P_l(1-k^2/2K^2)}{k[\epsilon(k)+K_0R_D^{-2}k^2]}dk , \quad (13)$$

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

The expression for the energy-dependent effective mass in GaAs (Ref. 14) is given by

$$m^*(E)=m^*(0)+(0.0436E+0.236E^2-0.147E^3) , \quad (14)$$

where $m^*(0)$ is equal to $0.0681m_0$ and E is the energy in electron volts. The Fermi energy is given by

TABLE III. Values of mobilities μ_{DM}, μ_{EM}, and the ratio μ_{EM}/μ_{DM} for various concentrations with energy-dependent effective mass at 80 K. The values of the mobilities and their ratio with constant effective mass are given in parentheses.

Concentrations (cm^{-3})	μ_{DM} (cm^2/V sec)	μ_{EM} (cm^2/V sec)	μ_{EM}/μ_{DM}
5×10^{20}	352.26 (2219.97)	278.32 (1832.27)	0.7901 (0.8254)
10^{20}	808.54 (2622.03)	743.64 (2439.92)	0.9197 (0.9305)
5×10^{19}	1184.68 (2622.03)	1123.18 (2709.33)	0.9481 (0.9536)
10^{19}	2496.34 (3515.69)	2449.65 (3448.25)	0.9813 (0.9808)
5×10^{18}	3186.62 (3914.95)	3145.85 (3864.91)	0.9872 (0.9872)
10^{18}	5145.90 (5428.40)	5104.54 (5383.30)	0.9920 (0.9917)

TABLE IV. Values of mobilities μ_{DM}, μ_{EM}, and the ratio μ_{EM}/μ_{DM} for various concentrations with energy-dependent effective mass at 300 K. The values of the mobilities and their ratio with constant effective mass are given in parentheses.

Concentrations (cm^{-3})	μ_{DM} (cm^2/V sec)	μ_{EM} (cm^2/V sec)	μ_{EM}/μ_{DM}
5×10^{20}	352.84 (2220.37)	278.78 (1832.60)	0.7901 (0.8254)
10^{20}	813.82 (2626.05)	748.49 (2443.66)	0.9197 (0.9305)
5×10^{19}	1198.28 (2852.16)	1136.07 (2719.80)	0.9481 (0.9536)
10^{19}	2624.33 (3631.58)	2575.26 (3561.92)	0.9813 (0.9808)
5×10^{18}	3532.60 (4238.89)	3487.41 (4184.71)	0.9872 (0.9872)
10^{18}	8900.19 (9093.49)	8828.66 (9017.93)	0.9920 (0.9917)

$$E_F = \hbar^2 K_F^2 / 2m^*(E_F) \ . \tag{15}$$

Equations (14) and (15) 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 the temperatures 10, 80, and 300 K for the concentrations from 10^{18} to 5×10^{20} cm^{-3}. The values of energy-dependent effective mass for various concentrations are given in Table I. The values of the mobilities μ_{DM}, μ_{EM}, and the ratio μ_{EM}/μ_{DM} are presented in Tables II–IV at the temperatures 10, 80, and 300 K, respectively, for various concentrations. In calculating the values of μ_{DM} and μ_{EM} the effective mass is treated as energy dependent. In computing μ_{DM} we use the Dingle potential with static dielectric constant to account for the valence dielectric screening whereas in the calculation of μ_{EM} the spatial variation of the dielectric function is taken care of. The corresponding values (μ_D, μ_E, and μ_E/μ_D) with the constant effective mass are given in parentheses.

From Table II it is found that at 10 K the mobility μ_{DM} deviates from the BH value μ_D when the effective mass is treated as energy dependent. This deviation is more for higher concentration but decreases with decrease in concentration. We are able to observe similar deviation in the values of μ_{EM} from that of μ_E from Table II. Though the value of the mobility decreases when the effective mass of electron is treated as energy dependent there is not much variation between the ratios μ_{EM}/μ_{DM} and μ_E/μ_D, as seen from Table II. The above behavior is independent of temperature as seen from Table III for 80 K and from Table IV for 300 K.

Detailed comparison with experimental results entails the usual difficulty of interplay of different scattering mechanisms which decide the carrier mobilities. In summary, we find that the effect of the energy-dependent effective mass of electrons in GaAs on the ionized-impurity-scattering-limited mobility is significant at higher carrier densities at all temperatures. At lower concentration the energy-dependent effective mass is not important, even at low temperatures.

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