PHYSICAL REVIEW B VOLUME 19, NUMBER 2 15 JANUARY 1979

Electron mobility in semiconductors based on a dielectric-function modification of the Dingle potential

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(Received 22 June 1978)

An alternative ionized-impurity potential, embodying a spatially variable dielectric function, has recently been proposed by Csavinszky. Unlike its predecessor, this potential incorporates the behavior of the dielectric function at the origin. The electron conductivity mobilities, calculated for Si and Ge from these potentials, have been compared numerically with the corresponding prediction of the Dingle theory. In a previous Comment, it was shown that the mobility based on the first potential overestimated this prediction. Here, it is found that the second potential is also questionable because it leads to a gross underestimation. A possible reason for this behavior is suggested.

Calculations of the contribution to electron mobility in semiconductors due to scattering from ionized impurities are, of necessity, dependent upon the impurity-ion potential chosen. The potential traditionally used is one due to Dingle,[1]

$$\phi_0 = (e_0/\kappa_0 r)\exp(-r/R_0) . \quad (1)$$

Here R_0 allows for the screening of the ion by free charge carriers in their respective bands, and κ_0 is the static dielectric constant of the material. The electron mobility derived from ϕ_0 will be referred to as μ_0. It is known, however, that κ_0 is only a constant at distances of the order of a lattice spacing away from the impurity ion. A generalization of Eq. (1) to include the spatial variation of the dielectric constant has recently been proposed.[2] In that development, use was made of an analytical approximation, based on the isotropic Penn model,[3] having the form,[4,5]

$$[\kappa(r)]^{-1} = \kappa_0^{-1} + \exp(-\alpha r) - A\exp(-\beta r) - B\exp(-\gamma r) . \quad (2)$$

Here, α, β, γ, A, and B are constants characteristic of the particular semiconductor. They have been evaluated in Refs. 4 and 5 for Si and Ge, respectively. By making use of an equivalent variational principle to solve the differential equation resulting from the replacement of κ_0 by $\kappa(r)$ in the standard linearized Poisson's equation, a potential,

$$\phi_1 = \phi_0[C\exp(nr/R_0) + (1-C)\exp(-nr/R_0)] , \quad (3)$$

was developed. A term arising in the derivation of the Poisson's equation,[6] involving the derivative of $\kappa(r)$, has been neglected in the calculation of Ref. 2. The parameters n and C are determined within the context of the variational calculation and are dependent upon the medium and upon R_0. Recent papers have utilized Eq. (3) to determine the electron mobility.[7,8] It was found that μ_1, the mobility derived from ϕ_1, was larger than μ_0. For Si, the ratio μ_1/μ_0 was found to range from approximately 1.3 at an impurity concentration of about $10^{19}\,\text{cm}^{-3}$ (see Fig. 1 of Ref. 8). As experimental data generally indicate that theoretical μ_0 values are already an overestimation of the actual mobility, it was felt that results from use of Eq. (3) might be suspect. In a later publication,[9] the statement was made that the boundary condition,

$$\phi(r \to 0) = e_0/\kappa_0 r , \quad (4)$$

might be open to criticism. Since $\kappa(r)$ tends to unity as r approaches zero (the parameters A and B obey the relation, $A+B=\kappa_0^{-1}$), a more plausible boundary condition would be

$$\phi(r \to 0) = e_0/r . \quad (5)$$

In Ref. 9, Eq. (5) was incorporated in another potential,

$$\phi_2 = \phi_0[1 + (\kappa_0 - 1)\exp(-ar)] . \quad (6)$$

Like Eq. (3), Eq. (6) was obtained with the neglect of the $\kappa(r)$-derivative term. Here there is only one parameter, a, to be determined from the variational calculation and this is again dependent upon R_0. An extended table of a versus R_0 for Si and Ge is included in Table I.

It may be noted that ϕ_2, by construction, is ϕ_0 multiplied by a correction factor. This factor approaches unity as the distance from the charged impurity increases. Such asymptotic behavior is physically reasonable since the variation of the dielectric function only occurs at distances close to the impurity center and, thus, the correction factor should be less important at large values of r. In addition, as can be seen from the behavior of the parameter a, the distance at which the correction factor will approximate unity increases with R_0. This trend anticipates the result that ϕ_2

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TABLE I. Variational parameter a appearing in the impurity-ion potential ϕ_2 vs the Dingle screening length R_0 for Si and Ge.

R_0 (a.u.)	a(Si) (10^{-4} a.u.$^{-1}$)	a(Ge) (10^{-4} a.u.$^{-1}$)
5	2575.0	2076.0
10	467.1	251.8
15	140.2	70.19
20	59.43	28.99
25	30.69	14.72
30	17.92	8.484
35	11.39	5.340
40	7.690	3.572
45	5.438	2.506
50	3.999	1.826
55	3.018	1.372
60	2.335	1.057
65	1.843	0.8385
70	1.482	0.6702
75	1.209	0.5443
80	0.9989	0.4480
85	0.8351	0.3733
90	0.7053	0.3143
95	0.6011	0.2671
100	0.5165	0.2290
105	0.4520	0.1977
110	0.3933	0.1719
115	0.3444	0.1505
120	0.3033	0.1324
125	0.2685	0.1171
130	0.2388	0.1041
135	0.2134	0.0930
140	0.1915	0.0834
145	0.1724	0.0750
150	0.1559	0.0678
155	0.1414	0.0614
160	0.1286	0.0558
165	0.1173	0.0509
170	0.1073	0.0466
175	0.0985	0.0427
180	0.0905	0.0392
185	0.0834	0.0361
190	0.0771	0.0333
195	0.0713	0.0308
200	0.0661	0.0286
205	0.0614	0.0266
210	0.0572	0.0247
215	0.0533	0.0230
220	0.0498	0.0215
225	0.0466	0.0201
230	0.0436	0.0188
235	0.0409	0.0176
240	0.0384	0.0165
245	0.0361	0.0156
250	0.0340	0.0146

will show more divergence from ϕ_0 for nondegenerate (high-R_0) doping than for degenerate doping.

A numerical comparison of ϕ_0, ϕ_1, and ϕ_2 is displayed in Fig. 1. The curves are for Si at $R_0 = 15$ a.u. On the scale shown ϕ_0 and ϕ_1 are

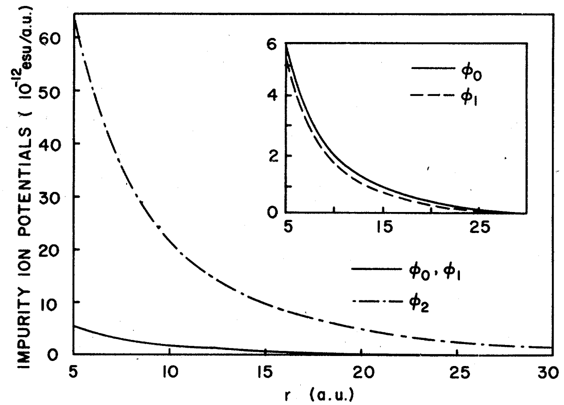

FIG. 1. Impurity-ion potentials ϕ_0, ϕ_1, and ϕ_2 as a function of distance r from the origin. The curves are for Si with the Dingle screening length R_0 equal to 15 a.u.

nearly identical. The inset reveals that ϕ_1 remains slightly less than ϕ_0 throughout the region considered. On the other hand, ϕ_2 is a full order of magnitude larger than either ϕ_0 or ϕ_1. As mentioned before, ϕ_2 does approach ϕ_0 for large r. However, ϕ_1 decreases much more slowly than ϕ_0 with increasing r and, thus, does not limit to ϕ_0.

Using ϕ_2, it is an easy calculation to show that the corresponding electron mobility can be expressed as the proportionality

$$\begin{aligned}\mu_2^{-1} \propto\ & \ln(1+4k^2R_0^2) - 4k^2R_0^2/(1+4k^2R_0^2) \\ & + (\kappa_0-1)^2[\ln(1+4k^2R_3^2) - 4k^2R_3^2/(1+4k^2R_3^2)] \\ & + (\kappa_0-1)\{\ln[16k^4R_0^2R_3^2 + 4k^2(R_3^2+R_0^2)+1] \\ & - [(R_0^2+R_3^2)/(R_0^2-R_3^2)] \\ & \times \ln[(1+4k^2R_0^2)/(1+4k^2R_3^2)]\} \equiv Q_2\,. \end{aligned} \quad (7)$$

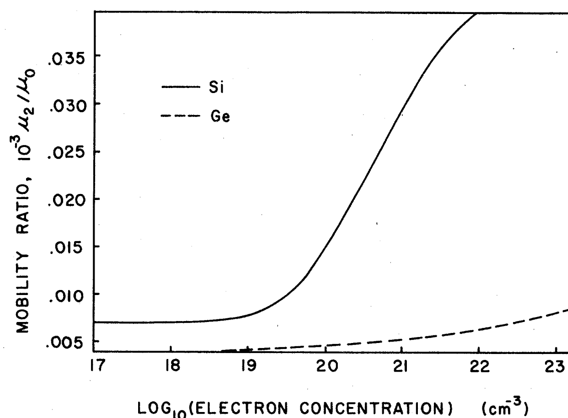

FIG. 2. Ratio of electron mobilities μ_2/μ_0 as a function of electron concentration. The calculations for Si and Ge are shown at room temperature.

Here k is the electron wave number and R_3 is an abbreviation for $R_0/(1+aR_0)$. Similarly, the Dingle potential yields

$$\mu_0^{-1} \propto \ln(1+4k^2R_0^2) - 4k^2R_0^2/(1+4k^2R_0{}^2) \equiv Q_0 \,. \quad (8)$$

The proportionality constant being identical for both μ_0 and μ_2, it follows that

$$\mu_2/\mu_0 = Q_0/Q_2 \,. \quad (9)$$

The ratio of mobilities in Eq. (9) is shown in Fig. 2 as a function of electron concentration for both Si and Ge at room temperature.

As had been expected from the form of ϕ_2, this ratio is largest in the degenerate region and approaches a smaller value asymptotically as the density decreases. That is, the effect of ϕ_2 on the mobility is more pronounced in the nondegenerate region. The mobility calculated using ϕ_1, on the other hand, showed greater departure from the Dingle mobility in the degenerate region. In comparison to μ_0, application of ϕ_2 decreases the mobility by more than two orders of magnitude. Again, this is in contrast to the effect of ϕ_1, which was to increase the calculated mobility. Finally, it is noted that, at any given electron concentration, the ratio μ_2/μ_0 is further from unity for Ge than for Si, whereas the ratio μ_1/μ_0 showed greater divergence from unity for Si than for Ge (see Fig. 1 of Ref. 8).

In Fig. 3, the electron mobility has been plotted as a function of electron density for Si at room temperature. The three curves represent the theoretical mobilities μ_0, μ_1, and μ_2. For reference, the triangular points are experimental data taken from Gränacher and Czaja.[10] The difference between μ_1 and μ_0 is only evident for electron concentrations greater than 10^{18} cm^{-3}. The curve representing μ_2, however, lies significantly below μ_0, μ_1, and the experimental points for all concentrations shown. These lower mobility values are a direct consequence of the large increase in the value of ϕ_2 over that ϕ_0. Additionally, if other scattering mechanisms, such as lattice scattering or scattering by neutrals, were included in this calculation, the total mobility, including μ_2, would drop to still lower values.

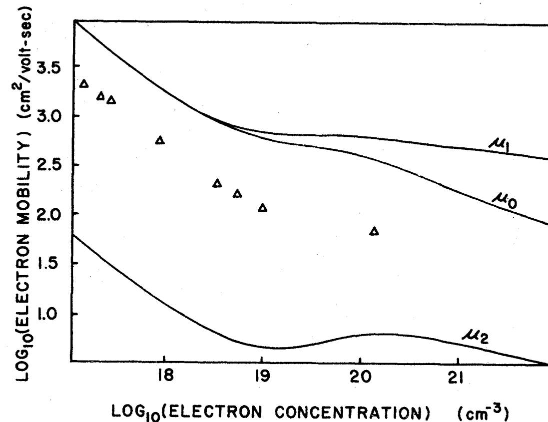

FIG. 3. Electron-conductivity mobility as a function of electron concentration. The experimental points Δ are taken from Ref. 10. The curves are for Si at room temperature.

From these results, we conclude that recent impurity-ion potentials[2,9] embodying the spatial variation of the dielectric function yield electron conductivity mobilities which either overestimate or grossly underestimate the mobility based on the Dingle potential. It is not clear why the inclusion of this effect has not improved the mobility calculation. We think that this failure is due to the behavior of the potential. It seems physically reasonable that ϕ_2 should closely resemble ϕ_0 in the region where $\kappa(r)$ has become equal to κ_0, yet ϕ_2 fails to do this. This point, among others, is currently under investigation.

ACKNOWLEDGMENTS

The authors are grateful to the University of Vermont for an institutional grant and for making available the resources of its academic computing center. This paper is an outgrowth of work initiated under contract with the IBM Corporation, Essex Junction, Vermont, and we are indebted to Dr. E. E. Gardner for his interest and support. Thanks are also due to H. A. Slack and T. A. Fennell for computational assistance.

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