Corrections to the impurity-ion potential characterized by a spatially variable dielectric function; corresponding electron-conductivity mobility in silicon and germanium

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(Received 6 October 1978)

The complete linearized Poisson equation for the potential of impurity ions in a semiconductor, including the spatial variation of the dielectric function, is solved numerically by an equivalent variational principle, incorporating a functional recently proposed by Brownstein. The resulting potential is compared and contrasted with previous formulations which neglect a term involving the derivative of the dielectric function. In the region where this function becomes a constant, the chosen potential approximates that of Dingle, while at the impurity site it is greater than the latter by a multiplicative factor equal to the dielectric constant. Within the linear approximation, the present potential is believed to contain the correct embodiment of spatial variation in the dielectric function in a self-consistent manner. The electron-conductivity mobility, in the Born approximation, is also determined with this potential. Comparison with analogous calculations and with some typical experimental data as reference is made. It is found that the present theory of ionized-impurity-limited mobility yields a significant improvement over the Dingle theory and over prior treatments of this problem.

The present paper is a continuation of a series[1-3] concerning the contribution of ionized-impurity scattering, in the Born-approximation theory of Brooks and Herring,[4] to the electron-conductivity mobility in a semiconductor. The mobility has been calculated using an impurity-ion potential derived from the linearized Poisson equation where the static dielectric constant κ_0 in that equation, is replaced by a spatially varying dielectric function $\kappa(r)$. The familiar impurity-ion potential, due to Dingle,[5]

$$\phi_0 = (e_0/\kappa_0 r)e^{-r/R_0}, \quad (1)$$

follows from the linearized Poisson equation with the uniform dielectric constant. In Eq. (1), e_0 denotes the magnitude of the electronic charge and R_0 is a screening length characteristic of the electron density, the temperature, and the particular semiconductor in question. In the following, μ_0 will designate the mobility calculated by use of ϕ_0.

The generalization of ϕ_0 to include the spatial variation of the dielectric function has recently been proposed by Csavinszky.[6] The potential was chosen arbitrarily to be a linear combination of two screened Coulomb potentials,

$$\phi_1 = \phi_0[Ce^{nr/R_0} + (1-C)e^{-nr/R_0}]. \quad (2)$$

The advantage of this form is the subsequent applicability of ϕ_1 to any theories of ionized-impurity scattering based on the Dingle-type potential. The constants n and C in ϕ_1 are parameters which must be calculated numerically for each semiconductor and for each desired value of R_0 by means of an equivalent variational-principle approach which is described fully in Ref. 6.

In Ref. 2, the ratio of the mobility μ_1, calculated using ϕ_1, to μ_0 was presented as a function of the free-electron concentration for both Si and Ge and of the temperature, for Si only. It was found that μ_1 was greater than μ_0 for degenerate doping and approached μ_0 for nondegenerate doping. As the Dingle mobility μ_0 is already known to be an overestimation of the measured quantity, this result was not entirely satisfactory.

An alternative potential, also due to Csavinszky,[7] in which a more physically accurate boundary condition was used, was the subject of Ref. 3. This potential has the form

$$\phi_2 = \phi_0[1 + (\kappa_0 - 1)e^{-ar}]. \quad (3)$$

Here a is the parameter to be determined numerically from the variational calculation. It was found that μ_2, the mobility calculated with ϕ_2, drastically under estimated both μ_0 and some typical experimental points.[8] As our calculation of μ_2 only takes ionized-impurity scattering into account, and inclusion of other scattering mechanisms would bring the total mobility to even lower values, this result was not promising either. Examination of ϕ_2 reveals that it remains significantly larger than ϕ_0 at distances much greater than a lattice constant away from the impurity ion (see Fig. 2 of Ref. 3). However, this does not seem to correspond physically with the behavior of the dielectric function. This function,

$$\kappa(r)^{-1} = \kappa_0^{-1} + e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r}, \quad (4)$$

which is an analytic approximation based on the isotropic Penn model,[9] was formulated by Azuma

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and Shindo[10] for Si and by Okuro and Azuma[11] for Ge. The parameters α, β, γ, A, and B are constants specific to a given semiconductor and are tabulated in Refs. 10 and 11. (There appear to be two misprints in Ref. 10. See Ref. 6, footnote 8 for details.) The function $\kappa(r)$ reaches its uniform value κ_0 at a distance of the order of a lattice constant away from the impurity ion. Therefore, we would expect that a ratio of the modified potential ϕ_2 to ϕ_0 would approach unity within a distance of this order of magnitude. Obviously, ϕ_2 does not have this behavior. In the present paper, we formulate an impurity-ion potential ϕ which we believe to be the correct embodiment of the spatial variation of the dielectric function in the linearized Poisson-equation approximation. The electron mobility μ is calculated with this potential and we discuss the relationship of μ to μ_0, μ_1, and μ_2 and to some typical experimental data.

Incorporation of the spatial behavior of the dielectric function into the derivation of a more complete linearized Poisson equation has been discussed in detail elsewhere.[6] The electric displacement $\vec{D}(r)$ which is defined by

$$\vec{D}(r) = \kappa(r)\vec{E}(r), \tag{5}$$

is introduced into the Maxwell equation

$$\nabla \cdot \vec{D} = 4\pi\rho, \tag{6}$$

where ρ denotes the screening-charge density. By writing the electric field as the negative gradient of the potential, and treating ϕ and κ as functions only of r, Eq. (6) becomes

$$\phi'' + \frac{2}{r}\phi' + \frac{4\pi\rho}{\kappa(r)} = -\frac{\kappa'(r)}{\kappa(r)}\phi'. \tag{7}$$

Upon expanding the Fermi-Dirac integral of order $\frac{1}{2}$, $\mathfrak{F}_{1/2}$, which occurs in the exact expression for the charge density, to linear order in $e_0\phi(r)/k_BT$, ρ takes on the form

$$\rho = -\frac{4\pi e_0^2 m^{*3/2}(2\pi k_B T)^{1/2}}{h^3}\mathfrak{F}_{-1/2}(\eta_\nu)\phi(r). \tag{8}$$

Here m^* is an isotropic effective electron mass, η_ν is the reduced Fermi level, and the other symbols take on their usual meanings. The Fermi-Dirac integrals are defined in Eq. (2) of Ref. 6. Additionally, by defining the screening length R_0

$$R_0^{-2} = \frac{16\pi^2 e_0^2 m^{*3/2}(2\pi k_B T)^{1/2}}{\kappa_0 h^3}\mathfrak{F}_{-1/2}(\eta_\nu), \tag{9}$$

using Eq. (8), and making the substitution $\psi(r) = (\kappa_0 r/e_0)\,\phi(r)$, Eq. (7) is transformed into

$$\psi'' - R_0^{-2}\psi - \kappa_0 R_0^{-2}\psi(e^{-\alpha r} - Ae^{-\beta r} - Be^{-\gamma r})$$
$$= -\kappa(r)(\alpha e^{-\alpha r} - A\beta e^{-\beta r} - B\gamma e^{-\gamma r})(\psi' - \psi/r). \tag{10}$$

The term on the right-hand side of Eq. (10), which, for convenience, shall be called S, has been neglected in previous impurity-ion-potential calculations.[6,7] The magnitude of this term has been discussed in several references.[6,12,13] In Ref. 6, S is considered in terms of ϕ rather than ψ. As it is the ψ equation which will be solved using the variational principle, this argument may be misleading.

In Ref. 12, it is noted that S is very small at large distances from the impurity ion. For this reason, it is set equal to zero in order to find the solution of the asymptotic form of the linearized Poisson equation. In Ref. 13, S is treated as the inhomogeneous part of a second-order differential equation and a particular solution is achieved using the two solutions to the corresponding homogeneous equation, derived in Ref. 6, with the approximation that $\kappa(r) = \kappa_0$. The final result is that the particular solution contains terms which are negligible in comparison with the homogeneous solution in the limit of very large r. Therefore, it is concluded that the asymptotic validity of the impurity-ion potential of Ref. 6 is established.

As discussed in Ref. 3, however, it is not the asymptotic behavior of the impurity-ion potential which is disturbing but the behavior near the origin. The expansion of the Fermi-Dirac integral, leading to Eq. (8), is strictly only valid for large r, but the nonphysical behavior of ϕ_2, everywhere but in the asymptotic limit, leads us to consider the small-r behavior further. It should be apparent that, in the region of small r, S is not negligible with respect to the rest of Eq. (10). Specifically, for Si, at $R_0 = 30$ a.u., and using the potential ϕ, defined below in Eq. (16), the ratio of S to the left-hand side of Eq. (10) ranges from approximately 1.4–665 as r decreases from 5.0–0.1 a.u. As it is in this region where the most variation of $\kappa(r)$ occurs, we feel that is it essential to seek a solution of Eq. (10) which would include the previously neglected term.

As indicated above, Eq. (10), without the right-hand side, has already been solved[6,7] by means of an equivalent variational principle. In those cases, the functional chosen was

$$F_C = -\tfrac{1}{2}(\psi')^2 - \tfrac{1}{2}\kappa_0 R_0^{-2}[1/\kappa(r)]\psi^2. \tag{11}$$

In order to solve the full Eq. (10) by the variational method, a new functional, which will yield Eq. (10) upon its substitution into the Euler-Lagrange equation, must be devised. Such a functional has been proposed by Brownstein,[14] namely,

$$F_B = \frac{\kappa}{2}\left(-(\psi')^2 + \frac{4\pi G}{\kappa}\psi^2\right) - \frac{\kappa'\psi^2}{2\,r} + \frac{\kappa'}{2}\left(\frac{\kappa(0)}{\kappa}\right)^4\frac{1}{r}. \tag{12}$$

Here, κ is understood to refer to $\kappa(r)$ and G is an

abbreviation for $-\kappa_0 R_0^{-2}/4\pi$. Because the correct boundary condition at the origin is

$$\psi(r \to 0) = \kappa_0 \,, \tag{13}$$

rather than

$$\psi(r \to 0) = 1 \,, \tag{14}$$

Eq. (12) has been altered slightly to read

$$F = \frac{\kappa}{2}\left(-(\psi')^2 + \frac{4\pi G}{\kappa}\psi^2\right) - \frac{\kappa'}{2}\frac{\psi^2}{r} + \frac{\kappa'}{2}\kappa_0^2\left(\frac{\kappa(0)}{\kappa}\right)^4 \frac{1}{r}. \tag{15}$$

The trial function, ψ, used in the variational calculation and the corresponding ϕ have the forms

$$\psi = e^{-r/R_0}[1 + (\kappa_0 - 1)e^{-pr}]$$
$$\phi = \phi_0[1 + (\kappa_0 - 1)e^{-pr}] \,, \tag{16}$$

satisfying Eq. (13), where p is the variational parameter. The term in square brackets can be viewed as a correction to the Dingle potential ϕ_0. This term can be seen to approach unity at large r. This is physically reasonable as the dielectric function approaches a constant value, the value used to produce ϕ_0, in this limit. The question remains, however, of how rapid this approach to ϕ_0 should be. As was discussed in Ref. 3, the values of parameter a, (analogous to our p) that are obtained using Eq. (11) with the boundary condition, Eq. (13), are such as to cause the potential produced ϕ_2 to remain significantly greater than ϕ_0 at distances much larger than a lattice spacing. Remembering that $\kappa(r)$ reaches its uniform value at a distance of the order of a lattice spacing away from the ion, this behavior is not acceptable.

Figure 1 shows curves of the parameter p as a function of the screening length R_0 for both Si and Ge. The only appreciable deviation from a constant value occurs in the low-R_0 (high-degeneracy) range. It is interesting to note that p levels off at approximately the distance of a lattice spacing. For Si, the value of p varies only from 0.3127–0.3491 as R_0 increases from 10–250 a.u. Over the same R_0 span, the variation in p for Ge is 0.5314 to 0.5802. For comparison with the previous parameter, a, for Si at $R_0 = 30$ a.u., $a = 0.0018$ whereas $p = 0.3233$. Thus the correction term of Eq. (16) reaches unity much faster than it did in the case of ϕ_2.

The actual behavior of the impurity-ion potentials may be seen explicitly in Fig. 2, where we have plotted ϕ_0, ϕ_1, ϕ_2, and our ϕ, for Si at $R_0 = 15$ a.u. It can be seen that ϕ approximates ϕ_0 at a much lower value of r than does ϕ_2. The distance at which ϕ approximates ϕ_0 is of the order of magnitude of the distance at which $\kappa(r) = \kappa_0$ (see Fig. 2 of Ref. 10). Thus, the small change in $\kappa(r)$ from the uniform κ_0 value, which occurs near the origin, is translated into a small variation in the impurity-ion potential from the Dingle potential. We note that, as defined by the boundary condition, ϕ is κ_0 times greater than ϕ_0 at the origin.

In the first Born approximation, we determine the mobility arising from ϕ to be expressed by the proportionality

$$\mu^{-1} \propto \ln(1 + b_0^2) - \frac{b_0^2}{1 + b_0^2} + (\kappa_0 - 1)^2\left(\ln(1 + b_3^2) - \frac{b_3^2}{1 + b_3^2}\right) + (\kappa_0 - 1)\left[\ln(b_0^2 b_3^2 + b_3^2 + b_0^2 + 1) - \left(\frac{R_0^2 + R_3^2}{R_0^2 - R_3^2}\right)\ln\left(\frac{1 + b_0^2}{1 + b_3^2}\right)\right] \equiv Q \,. \tag{17}$$

Here we have defined $b_0 = 2kR_0$ and $b_3 = 2kR_3$, where k is the electron wave number and $R_3 = R_0/(1 + pR_0)$.

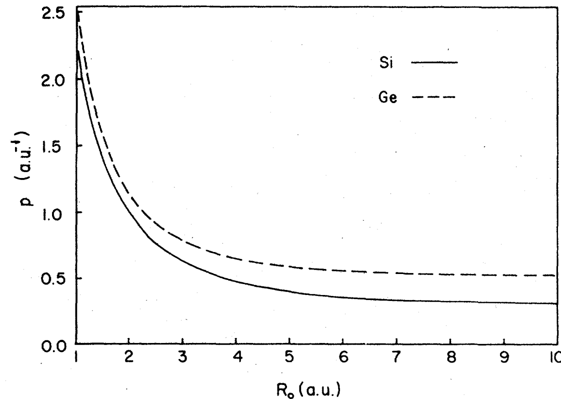

FIG. 1. Values of the parameter p occurring in Eq. (16), as a function of the Dingle screening length R_0 for Si and Ge.

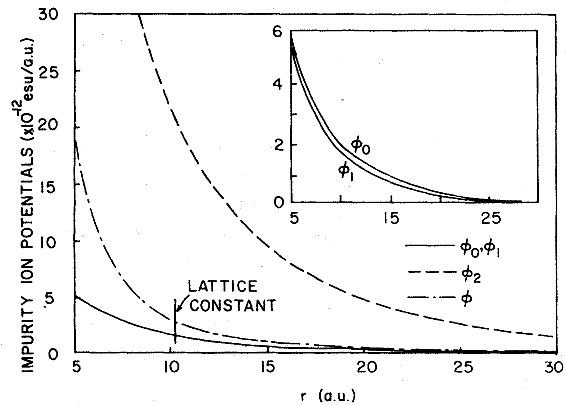

FIG. 2. Impurity-ion potentials ϕ, ϕ_0, ϕ_1, and ϕ_2 as functions of distance r from the origin. The curves are for Si with the Dingle screening length $R_0 = 15$ a.u. The lattice constant for Si (10.3 a.u.) is displayed for reference.

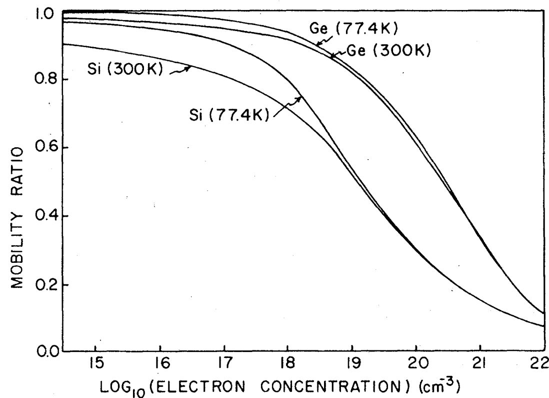

FIG. 3. Ratio of electron-conductivity mobilities μ/μ_0 as a function of electron concentration. The calculations for Si and Ge are shown for $T = 77.4$ °K and $T = 300$ °K.

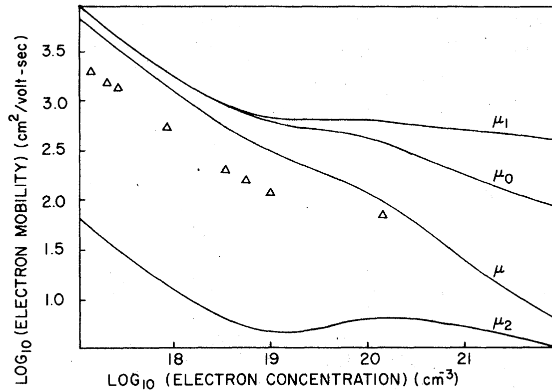

FIG. 4. Electron-conductivity mobilities μ, μ_0, μ_1 and μ_2 as functions of electron concentration. The experimental points, Δ, are taken from Ref. 8. The curves are for Si at room temperature.

Similarly, the electron mobility calculated using ϕ_0 is

$$\mu_0^{-1} \propto \ln(1 + b_0^2) - b_0^2/(1 + b_0^2) \equiv Q_0 . \tag{18}$$

The proportionality constant is the same in Eqs. (17) and (18) and, thus, the ratio of the new mobility to the Dingle mobility will be given by

$$\mu/\mu_0 = Q_0/Q . \tag{19}$$

Figure 3 contains graphs of μ/μ_0 as a function of electron concentration for Si and Ge at temperatures of 300 and 77.4 °K. The new mobility μ shows the greatest deviation from μ_0 in the degenerately doped region. The ratio levels off to approximately 0.89 and 0.97 for Si and Ge, respectively, at a concentration of 10^{15} cm^{-3} and 300 °K. Therefore, even for dilute doping, μ/μ_0 is still significantly different from unity for both Si and Ge. The temperature change makes virtually no difference in the mobility ratio in the degenerate region, for both Si and Ge, but, in the nondegenerate region, the lower temperature is associated with a higher mobility ratio. That is, the lower the temperature, the closer μ is to μ_0.

In Figure 4, we display the concentration dependence of the various mobilities μ, μ_0, μ_1, and μ_2, calculated for Si at 300 °K, and also some experimental points[8] for reference. It can be seen that μ lies below μ_0 but above μ_2 and also above the experimental points. The effect on the electron mobility of the new potential is, thus, in the proper direction and does not overshoot the experimental points as μ_2 does. It is to be expected that, were the contributions from other scattering mechanisms taken into account, μ would lie even closer to the experimental points. Therefore, the effect of taking the spatial variation of the dielectric constant into account in the formation of an impurity-ion potential is to lower the electron mobility. This is what one would expect from the form of $\kappa(r)$ and also accords physically with the experimental data.

Some cautions as to the applicability of this potential should be noted. First, as the concentration of atoms in undoped Si,[5] for example, is 5×10^{22} cm^{-3}, it is possible that, for high impurity concentrations, the assumption that the dielectric function of the doped semiconductor is identical to that of the undoped material may be untenable. For this reason, we consider the calculations in the heavily-doped regime to be the least reliable. A useful extension of this work would be to consider the problem of a concentration-dependent dielectric function. Additionally, the linear approximation made in arriving at Eq. (8) for the charge density is strictly only valid for large values of r.[6] Since our primary interest has proved to be in the small-r region, it would be elucidative to consider more terms in this expansion, i.e., to consider the nonlinear Poisson equation. An approach to this problem has recently been proposed by Csavinszky.[15]

The present calculations are being extended to other semiconductors, such as GaAs or ZnSe, by formulating their dielectric functions in terms of Eq. (4). We have already begun such work with the aid of the Walter and Cohen[16] dielectric function curves. Alternatively, one could use the dielectric function of Schulze and Unger.[17] The resulting potentials should also be useful in other calculations of the equilibrium and transport properties of doped semiconductors. Applications are currently under way.

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 International Business Machines Corp., Essex Junction, Vt., and we are indebted to Dr. E. E. Gardner for his interest and support. Thanks also are due to H. A. Slack, T. A. Fennell, and L. J. Bauch for computational assistance.

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