Numerical solution to the nonlinear Poisson's equation including a spatially variable dielectric constant

J. R. Meyer
Naval Research Laboratory, Washington, D. C. 20375
(Received 12 February 1979; revised manuscript received 16 April 1979)

Numerical solutions to both the nonlinear and linearized Poisson's equations have been obtained for the case of a spatially variable dielectric constant. It is found that the model potentials employed in several recent mobility calculations are physically unreasonable. It is also found that in most cases where the spatial dependence of the dielectric constant is important, the use of the linearized form of Poisson's equation is questionable.

A number of investigators have recently sought to improve the usual Brooks-Herring result for electron mobility in a semiconductor due to scattering by ionized impurities through the use of scattering potentials which take into account the spatial dependence of the dielectric constant. In this article, the various approximate analytic potentials which have been employed in these calculations are tested by comparing them with the results of a numerical solution to the generalized, linearized Poisson's equation. The nonlinear Poisson's equation has also been solved numerically, in order to test the soundness of potentials derived from the linear formulation.

Generalization of Poisson's equation to incorporate the spatial dependence of the dielectric constant, $\kappa(r)$, leads to the form[1]

$$\nabla^2\phi(r) = \frac{-4\pi\rho(r)}{\kappa(r)} - \frac{\vec{\nabla}\kappa(r)\cdot\vec{\nabla}\phi(r)}{\kappa(r)} \quad , \tag{1}$$

where $\phi(r)$ is the electrostatic potential due to a positive point charge, and the boundary conditions are $\phi(r\to 0) = e/r$ and $\phi(r\to\infty) = 0$.[2]

The screening charge, $\rho(r)$, is given by[3]

$$\rho(r) = -e[n(r) - n] = \frac{-e\nu}{4}\left(\frac{2m^*k_BT}{\pi\hbar^2}\right)^{3/2}\left[\mathfrak{F}_{1/2}\left(\eta + \frac{e\phi}{k_BT}\right) - \mathfrak{F}_{1/2}(\eta)\right] \quad , \tag{2}$$

where n is the electron density, ν is the number of degenerate electron valleys, η ($\equiv E_F/k_BT$) is the reduced Fermi energy, $\mathfrak{F}_k$ is the Fermi integral[4] of order k, and parabolic, isotropic electron bands have been assumed. Using the relation $\mathfrak{F}_k'(\eta) = \mathfrak{F}_{k-1}(\eta)$, the "linearized" screening charge is obtained by expanding $\mathfrak{F}_{1/2}(\eta + e\phi/k_BT)$ in a Taylor series, which is terminated after the second term,

$$\rho_{\text{linear}} = -e^2\nu\left(\frac{m^*}{\pi\hbar^2}\right)^{3/2}\left(\frac{k_BT}{2}\right)^{1/2}\phi(r)\mathfrak{F}_{-1/2}(\eta) \quad . \tag{3}$$

Poisson's equation can be solved analytically if two simplifying approximations are made: the linear expression for the screening charge is used [Eq. (3)] and the dielectric constant is assumed to be independent of r [i.e., $\kappa(r)\to\kappa_0$, where κ_0 is the static dielectric constant of the semiconductor]. One then obtains the screened Coulomb potential due to Dingle[3] and Mansfield[5]

$$\phi_0(r) = (e/\kappa_0 r)e^{-r/R_0} \quad , \tag{4}$$

where R_0 is the degeneracy-dependent screening length[3]

$$R_0^{-2} = \left(\frac{4\pi ne^2}{\kappa_0 k_BT}\right)\frac{\mathfrak{F}_{-1/2}(\eta)}{\mathfrak{F}_{1/2}(\eta)} \quad . \tag{5}$$

In order to generalize this result by removing one of the simplifying approximations, Csavinszky has employed an equivalent variational principle to solve the linearized form of Eq. (1).[1] For germanium and silicon, he used the spatially dependent dielectric functions due to Okuro and Azuma[6], and Azuma and Shindo[7]

$$\kappa(r) = [e^{-\alpha r} + A(1 - e^{-\beta r}) + B(1 - e^{-\gamma r})]^{-1} \tag{6}$$

which are based on the Penn model.[8] The parameters[6,7] α, β, γ, A, and B satisfy the conditions that $\kappa(r\to 0) = 1$ and $\kappa(r >> a_0) = \kappa_0$, where a_0 is the lattice constant. Using a model potential of the form

$$\phi(r) = (e/\kappa_0 r)[Ce^{-r(1-n)/R_0} + (1 - C)e^{-r(1+n)/R_0}] \tag{7}$$

values for the variational parameters C and n were obtained. In this early calculation the second term of Eq. (1) was ignored, an approximation which has since been shown to be invalid.[9,10] Csavinszky has also noted that an incorrect boundary condition at small r had been used in obtaining this result.[11] Nonetheless, the potential of Ref. 1 has been employed in the calculation of ionized-impurity-

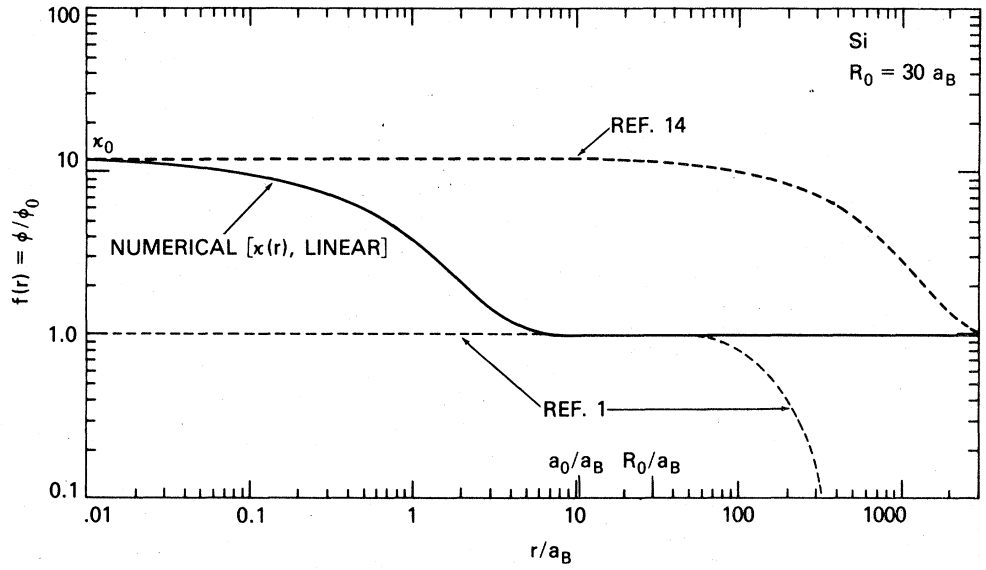

FIG. 1. Ratio of potentials which include the effects of a spatially variable dielectric constant to the potential of Eq. (4) vs r in atomic units. The solid curve represents the numerical solution to the generalized, linearized Poisson's equation, while the dashed curves are potentials obtained variationally by Csavinszky in Refs. 1 and 14.

scattering mobilities.[12,13]

The tabulated results of Ref. 1 are shown in Fig. 1 for the case of silicon at $R_0 = 30a_B$, where a_B is the Bohr radius. The function plotted is $f(r) \equiv \phi(r)/\phi_0(r)$, the ratio of the potential which includes the spatial dependence of the dielectric constant to the form given by Eq. (4). Also shown is a solution to the generalized, linearized Poisson's equation which was obtained numerically by computer. The behavior of this result agrees with what is expected intuitively. The boundary condition at small r requires that $\phi(r \to 0) = e/r$, which means that $f(r \to 0) = \kappa_0$ since Eq. (4) reduces to $\phi_0(r \to 0) = e/\kappa_0 r$. At large r for which $\kappa(r) \to \kappa_0$, the form of Eq. (4) is regained and $f(r) \approx 1$. The crossover occurs in the region where $\kappa(r)$ is changing, namely, when r is slightly less than the lattice constant a_0. The third curve of Fig. 1 represents a solution to the linearized form of Eq. (1) which was obtained by Csavinszky using a model potential of the form[14]

$$\phi(r) = \frac{ee^{-r/R_0}}{\kappa_0 r}[1 + (\kappa_0 - 1)e^{-ar}] \ , \tag{8}$$

where a is the only variational parameter. Although the asymptotic behavior at $r = 0$ and $r = \infty$ is now correct, the crossover from $f(r) \approx \kappa_0$ to $f(r) \approx 1$ occurs at r nearly three orders of magnitude too large when compared to the numerical result. The reason is probably that, as in Ref. 1, the second term of Eq. (1) was ignored. The potential of Ref. 14 has also been employed to obtain electron mobilities.[15]

Very recently, a solution to the generalized, linearized Poisson's equation has been obtained by Csavinszky and Morrow[11] which is in good qualitative agreement with the numerical result shown in Fig. 1.

For the purpose of calculating mobilities, the spatial dependence of the dielectric constant can be ignored if $f(r) \approx 1$ in the region where scattering by the potential is most important, namely, $r \approx R_0$. This will be the case when

$$\Delta_1 \equiv a_0/R_0 << 1 \ , \tag{9}$$

$$\Delta_1 \underset{\eta << 0}{=} 0.13(n/10^{18})^{1/2}(T/300)^{-1/2}(\kappa_0/12)^{-1/2}(a_0/10.2a_B) \ \text{(nondegeneracy)} \ , \tag{10a}$$

$$\Delta_1 \underset{\eta >> 0}{=} 0.42(n/10^{18})^{1/6}(\kappa_0/12)^{-1/2}(m_{ds}{}^*/0.3m_0)^{1/2}(\nu/6)^{1/3}(a_0/10.2a_B) \ \text{(extreme degeneracy)} \ , \tag{10b}$$

where m_{ds}^* is the density-of-states effective mass and m_0 is the free-electron mass. The normalization values shown for the material parameters are typical of n-type silicon.[16]

The second approximation made in obtaining Eq. (4) is that the expansion[17] of $\rho(r)$ in powers of

$z \equiv e\phi/k_B T$,

$$\mathfrak{F}_{1/2}(\eta+z) \rightarrow \mathfrak{F}_{1/2}(\eta) + z\mathfrak{F}_{-1/2}(\eta) + \frac{z^2}{2!}\mathfrak{F}_{-3/2}(\eta) + \frac{z^3}{3!}\mathfrak{F}_{-5/2}(\eta) + \cdots \quad (11)$$

was truncated after the second term. The relation

$$\Delta_\rho(r) \equiv \frac{\rho - \rho_{\text{linear}}}{\rho} = \frac{\mathfrak{F}_{1/2}(\eta+z) - \mathfrak{F}_{1/2}(\eta) - z\mathfrak{F}_{-1/2}(\eta)}{\mathfrak{F}_{1/2}(\eta+z) - \mathfrak{F}_{1/2}(\eta)} > 0 \quad (12)$$

holds for all values of η and positive z, indicating that the linear screening charge always underestimates the nonlinear ρ. It can be shown that $\Delta_\rho(r) << 1$ if and only if the third term of Eq. (11) is small compared to the second. With $\phi(r)$ replaced by $\phi_0(R_0)$ from Eq. (4) this ratio, denoted Δ_2, becomes

$$\Delta_2 = \frac{e^2 \exp(-1)}{2\kappa_0 R_0 k_B T} \frac{\mathfrak{F}_{-3/2}(\eta)}{\mathfrak{F}_{-1/2}(\eta)} \quad (13)$$

and the linear Poisson's equation should be adequate for use in the calculation of mobilities when $\Delta_2 << 1$. In the limits of small and large η

$$\Delta_2 \underset{\eta << 0}{=} 0.21(n/10^{18})^{1/2}(T/300)^{-3/2}(\kappa_0/12)^{-3/2}$$

(nondegeneracy), (14a)

$$\Delta_2 \underset{\eta >> 0}{=} 2.4(n/10^{18})^{-1/2}(\kappa_0/12)^{-3/2}(m_{ds}^*/0.3m_0)^{3/2}(\nu/6)$$

(extreme degeneracy). (14b)

It is seen that $\Delta_2 > \Delta_1$ for most reasonable values of n and T, indicating that in most regions where the spatial dependence of the dielectric constant is important, use of the linearized form of Poisson's equation is questionable. As an example, for silicon at $n = 7.5\times10^{18}$ cm^{-3} and $T = 300$ °K which corresponds to $\eta \approx -1.1$ and $R_0 = 30\ a_B$ (the same as in Fig. 1), $\Delta_2 \approx 0.6$, which indicates that use of the linear Poisson's equation is probably not a good approximation under these conditions.

Numerical solutions to the nonlinear Poisson's equation obtained for the parameters listed above are shown in Fig. 2. Along with the linear result already discussed, nonlinear potentials are given for dielectric constants with and without spatial dependence. In either case, the ratio of the linear potential to the nonlinear one is on the order of a factor of 2 at $r \approx R_0$. Csavinszky[18] and Adawi[19] have dealt with

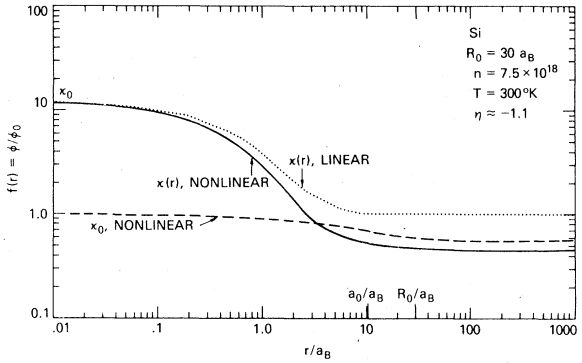

FIG. 2. Ratio of potentials obtained numerically in various limits to the potential of Eq. (4) vs r in atomic units. Linear or nonlinear refers to whether the linearized form of the screening charge represented by Eq. (3) was employed, while κ_0 or $\kappa(r)$ refers to whether the spatially dependent dielectric constant was incorporated.

the nonlinear equation using approximate analytic methods. Adawi correctly predicted that even though the linear approximation to $\rho(r)$ is valid at large r, the potential there is weaker than the linear result. This can be understood if one considers the consequences of the implicit requirement that the total

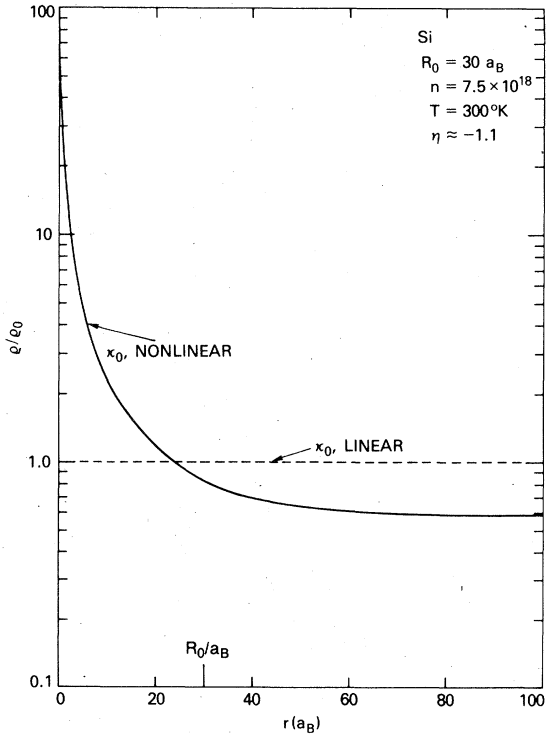

FIG. 3. Ratio of the screening charges vs r in atomic units, where ρ and ρ_0 were obtained from the nonlinear and linear solutions to Poisson's equation, respectively, both ignoring the spatial dependence of the dielectric constant.

screening charge integrated over all r must be equal in magnitude and opposite in sign to the test charge. For the case in which the spatial dependence of the dielectric constant is ignored, Fig. 3 shows the behavior of $\rho(r)/\rho_0(r)$, where

$$\rho_0(r) = -(e/4\pi r R_0^2) e^{-r/R_0}$$

is the screening charge corresponding to the linear solution [Eq. (4)]. Since both the linear and nonlinear potentials are fixed by the boundary condition that $\phi(r \to 0) = e/\kappa_0 r$, it follows from Eq. (12) that $\rho(r)$ must be larger than $\rho_0(r)$ at small r. The condition that $4\pi \int \rho(r) r^2 \, dr$ must be equal for the two cases then requires that $\rho(r)$ be smaller than $\rho_0(r)$ in some other region, namely, at large r. Because the linearization of ρ is valid at large r, a smaller $\rho(r \to \infty)$ implies a smaller $\phi(r \to \infty)$. Thus

$$\phi(r \to \infty) = A\,(e/\kappa_0 r) e^{-r/R_0} \,, \tag{15}$$

where $A < 1$. For the example given, the numerical result is $A \approx 0.58$, which can be compared with the value $A \approx 0.69$ obtained from substitution of the same parameters into the approximate expression of Adawi.[19] Under conditions for which the linearized Poisson's equation is expected to be valid [$\Delta_2 << 1$], the factor A approaches unity.

Summarizing, it is concluded that the calculated mobilities of Refs. 12, 13, and 15 are unreliable since they are based on potentials which are physically unreasonable. It is further concluded that in most cases where the spatial dependence of the dielectric constant is important, use of the linear form of Poisson's equation is questionable.

---

[1]P. Csavinszky, Phys. Rev. B 14, 1649 (1976).

[2]If the spatial dependence of the dielectric constant is ignored, the first boundary condition becomes $\phi(r \to 0) = e/\kappa_0 r$.

[3]R. B. Dingle, Philos. Mag. 46, 831 (1955).

[4]J. S. Blakemore, *Semiconductor Statistics* (Pergammon, New York, 1962).

[5]R. Mansfield, Proc. R. Soc. London Sect. B 69, 76 (1956).

[6]S. Okuro and M. Azuma, J. Phys. Soc. Jpn. 20, 1099 (1964).

[7]M. Azuma and K. Shindo, J. Phys. Soc. Jpn. 19, 424 (1964).

[8]D. R. Penn, Phys. Rev. 128, 2093 (1962).

[9]K. R. Brownstein, Phys. Rev. B 15, 5073 (1977).

[10]P. Csavinszky, Bull. Am. Phys. Soc. 22, 266 (1977).

[11]P. Csavinszky and R. A. Morrow, Bull. Am. Phys. Soc. 24, 277 (1979).

[12]M. A. Paesler, Phys. Rev. B 17, 2059 (1978); M. A. Paesler, D. E. Theodorou, and H. J. Queisser, Phys. Rev. B 18, 5895 (1978).

[13]L. M. Richardson and L. M. Scarfone, Phys. Rev. B 18, 5892 (1978).

[14]P. Csavinszky, Int. J. Quantum Chem. 13, 221 (1978).

[15]L. M. Richardson and L. M. Scarfone, Phys. Rev. B 19, 925 (1979).

[16]M. Neuberger, *Handbook of Electronic Materials* (Plenum, New York, 1971), Vol. 2.

[17]P. Csavinszky, Int. J. Quantum Chem. 12, 335 (1977).

[18]P. Csavinszky, Philos. Mag. 10, 231 (1964); Phys. Rev. B 14, 4483 (1976); Phys. Rev. B 17, 3177 (1978).

[19]I. Adawi, Philos. Mag. 13, 331 (1966).