

**Spatially variable dielectric functions in semiconductors and ionized-impurity-limited mobility**

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(Received 28 April 1978)

Recently, the ionized-impurity-limited mobility has been calculated by Paesler in terms of a scattering potential based on a spatially variable dielectric function. We demonstrate that the relaxation time used in his treatment does not reduce to the expected form in the nondegenerate limit. This discrepancy casts doubts upon the correctness of the resulting mobility curves. An alternative expression for the relaxation time is presented along with new curves and their interpretation.

Ionized-impurity scattering in doped semiconductors has been investigated primarily in terms of the traditional Brooks-Herring<sup>1</sup> (BH) theory which represented the first attempt in semiconductor physics to allow directly for the fact that carriers may collect around an impurity center and partly screen its Coulomb potential. The actual derivation and requisite assumptions of this theory have been given by Falicov and Cuevas.<sup>2</sup> Strictly speaking, we are interested here in the treatment of Dingle<sup>3</sup> and Mansfield,<sup>4</sup> who make the assumption that all impurities are ionized, whereas the BH theory includes the concentration of neutrals as well as ionized centers in the screening.

The BH theory assumes that the first Born approximation applies, the relaxation time is a scalar, the constant-energy surfaces are spheres, the impurities scatter the carriers independently, perturbing effects of the impurities on the carrier energy levels and wave functions are negligible, carrier-carrier interactions are unimportant, impurity-cell effects can be ignored, and the carriers are scattered by a screened Coulomb potential scaled by the static dielectric constant  $\kappa_0$  of the semiconducting medium. Various workers have aimed at removing one or more of these restrictions and a recent effort, due to Csavinszky,<sup>5</sup> attempts to generalize Dingle's treatment by replacing  $\kappa_0$  by the spatially variable dielectric function  $\kappa(r)$  of the medium.

The analytical form for  $\kappa(r)$  follows from the analysis of Azuma and Shindo<sup>6</sup> for silicon and from Okuro and Azuma<sup>7</sup> for germanium. These authors base their wave-vector-dependent dielectric function on the formula given by Penn,<sup>8</sup> who used a model isotropic semiconductor. The result of Csavinszky's calculations is an impurity-ion potential  $\phi(r)$  consisting of a linear combination of two exponentially screened Coulomb potentials scaled by  $\kappa_0$ . In detail,

$$\phi(r) = (e/\kappa_0 r) [C e^{-r/R_1} + (1 - C) e^{-r/R_2}]. \tag{1}$$

Here,  $e$  is the magnitude of the electronic charge,  $C$  is a dimensionless parameter characteristic of the material, while  $R_1$  and  $R_2$  act as screening lengths. Of course, interest in constructing scattering potentials having the screened Coulomb form lies in the usefulness they afford in Born-type expansions for the transition rate. In the nondegenerate limit,  $R_1$  and  $R_2$  are equal to the Dingle screening length  $R_0$ ,  $C$  becomes 0.5, and  $\phi(r)$  reduces to the Dingle potential,

$$\phi_0(r) = (e/\kappa_0 r) e^{-r/R_0}. \tag{2}$$

Therefore, one would expect that any quantity calculated in terms of  $\phi(r)$  should reduce to the same quantity calculated in terms of  $\phi_0(r)$  in this limit. In Ref. 5, it is shown that the new potential is most important in the case of heavy doping.

In order to study the effects of introducing a spatially dependent dielectric function into the BH theoretical treatment of carrier mobility, Paesler<sup>9</sup> used  $\phi(r)$  to develop an expression for the relaxation time  $\tau$  for ionized impurity scattering. We have noted his calculation with interest as it parallels our own work on this problem.<sup>10</sup> However, we believe there to be an inconsistency in his form for  $\tau$  which, if corrected, would considerably alter his stated conclusions. In Eq. (7) of Ref. 9 we are given the relationship (we assume an obvious misprint in that his  $\tau$  should read  $\tau^{-1}$ ):

$$\begin{aligned} \tau^{-1} \propto C^2 & [\ln(1 + \beta_1^2) - \beta_1^2/(1 + \beta_1^2)] \\ & + (1 - C)^2 [\ln(1 + \beta_2^2) - \beta_2^2/(1 + \beta_2^2)] \\ & + 4C(1 - C) \{ \ln[(1 + \beta_1^{-2} + \beta_2^{-2} + \beta_1^{-2}\beta_2^{-2})/(\beta_1^{-2}\beta_2^{-2})] \\ & + [\beta_1^{-2}\beta_2^{-2}/(\beta_1^{-2} - \beta_2^{-2})] \\ & \times \ln[\beta_2^{-2}(1 + \beta_1^{-2})/\beta_1^{-2}(1 + \beta_2^{-2})] \}. \end{aligned} \tag{3}$$

Here,  $\beta_1$  and  $\beta_2$  are abbreviations for  $2kR_1$  and  $2kR_2$ , respectively. In the nondegenerate limit, Eq. (3) becomes

$$\begin{aligned} \tau^{-1} \propto \frac{1}{2} & [\ln(1 + \beta_0^2) - \beta_0^2/(1 + \beta_0^2)] \\ & + 2 \ln(1 + \beta_0^2) - (1 + \beta_0^2)^{-1}, \end{aligned} \tag{4}$$

where  $\beta_0 = 2kR_0$ . Because the square-bracketed term in Eq. (4) is itself proportional to the inverse relaxation time  $\tau_0^{-1}$  found with the Dingle potential, it is obvious that Eq. (3) fails to fulfill the previously stated consistency requirement. Numerically, Paesler's  $\tau$  is approximately 0.4 of  $\tau_0$  in the nondegenerate limit. This discrepancy would explain why his curves (Fig. 1 of Ref. 9) asymptote out to, again, nearly 0.4 instead of unity.

Within the same BH framework, our calculation of the modified relaxation time yields

$$\begin{aligned} \tau^{-1} \propto & C^2 [\ln(1 + \beta_1^2) - \beta_1^2/(1 + \beta_1^2)] \\ & + (1 - C)^2 [\ln(1 + \beta_2^2) - \beta_2^2/(1 + \beta_2^2)] \\ & + C(1 - C) \{ \ln[(1 + \beta_1^{-2} + \beta_2^{-2} + \beta_1^{-2}\beta_2^{-2})/\beta_1^{-2}\beta_2^{-2}] \\ & \quad + [(\beta_1^{-2} + \beta_2^{-2})/(\beta_1^{-2} - \beta_2^{-2})] \\ & \quad \times \ln[\beta_2^{-2}(1 + \beta_1^{-2})/\beta_1^{-2}(1 + \beta_2^{-2})] \}. \end{aligned} \quad (5)$$

$\equiv Q.$

Comparison of the right-hand side of Eqs. (3) and (5) shows immediately that one difference between them occurs in the third term where a prefactor of 4 appears in the former equation, in place of unity in the latter. The other difference is seen in the second part of the third term where Eq. (3) shows  $\beta_1^{-2}\beta_2^{-2}$ , as opposed to  $\beta_1^{-2} + \beta_2^{-2}$  in Eq. (5). It can readily be shown that Eq. (5) does reduce to the Dingle form in the nondegenerate limit.

The ratio of the calculated mobility to the BH mobility is given by

$$\mu/\mu_{\text{BH}} = [\ln(1 + \beta_0^2) - \beta_0^2/(1 + \beta_0^2)]/Q. \quad (6)$$

In Fig. 1, we have plotted this ratio as a function of the carrier density for Si and Ge at room temperature. The most noteworthy feature of these

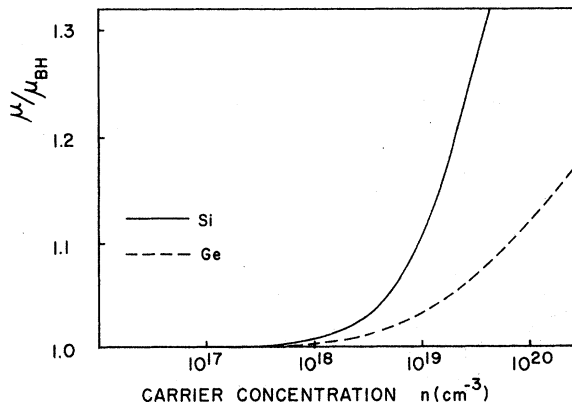


FIG. 1. Ratio of the calculated mobility to the Brooks-Herring mobility as a function of carrier concentration. The calculations for Si (solid line) and Ge (dashed line) are shown at room temperature ( $T=300$  K).

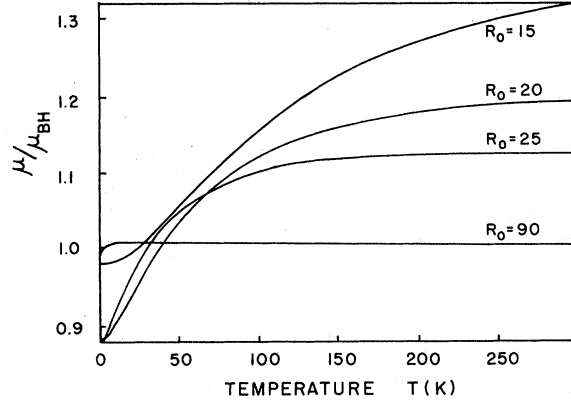


FIG. 2. Ratio of the calculated mobility to the Brooks-Herring mobility as a function of temperature. The calculations are for Si only and are displayed for four different values of the Dingle screening length  $R_0$ .

curves is that they asymptote to unity at low carrier concentration  $n$  in contrast to Fig. 1 of Ref. 9. It can be seen that, in the high- $n$  region, the calculated mobility is larger than that predicted by the BH theory. The incorporation of the spatially variable dielectric function in the impurity-ion potential increases the effectiveness of the screening and hence, due to the increase in the relaxation time, the carriers will have a greater mobility. We may also note that, while Fig. 1 of Ref. 9 shows a greater deviation from the asymptotic value for Ge than for Si, our curves show the opposite result. That is, for a given  $n$ , the mobility ratio is closer to unity for Ge than for Si. We feel that ours is a more reasonable result in view of the behavior of the  $n$  (not to be confused with the carrier concentration) and  $C$  parameters which characterize the potential used. As can be seen from Tables II and III of Ref. 5, for a given value of  $R_0$ , the  $n$  and  $C$  values for Ge are closer to their nondegenerate values (0 and 0.5) than are those for Si. Thus we would expect that quantities calculated for Ge will deviate less from the same quantities calculated using the Dingle potential than would those quantities calculated for Si.

In Fig. 2 we have plotted the mobility ratio as a function of temperature for several values of the screening length  $R_0$ . It can be seen that the most interesting variation occurs for low values of  $R_0$ . The higher the screening length, the more rapidly the mobility ratio levels out. For  $R_0=90$  and for all higher values of  $R_0$ , the variation with temperature will be negligible, with the ratio keeping a fairly constant profile at unity. In the higher-temperature region, the ratio can be seen to decrease with increasing  $R_0$  for a constant temperature. This is to be expected since, as  $R_0$  increases at fixed temperature, the carrier density will be

decreasing and we have seen in Fig. 1 that, under these conditions, the mobility ratio also will decrease. In the low-temperature region, the general trend is also toward decreasing ratio with increasing  $R_0$  but, as the curve crossing shows, there are competing effects which complicate the analysis. We have plotted only Si in our Fig. 2 because Ge, remaining in the degenerate region throughout the considered temperature range, shows virtually no temperature dependence. It is apparent that, if we were to plot our actual mobility values  $\mu$  on a curve similar to that of Fig. 2 of Ref. 9, our values would lie slightly above the  $\mu_{BH}$  curve of that graph. This difference between  $\mu$  and  $\mu_{BH}$  would be an increasing function of temperature. Another version of Csavinsky's potential,<sup>11</sup> in which a more plausible boundary condition at  $r=0$  is used, will provide refinements on the above results. We are presently considering this potential.

In conclusion, it has been shown that the effect

of taking the spatial variation of the dielectric constant of the semiconducting medium into account is to enhance the screening around the impurity ions so that the carrier mobility is increased. This increase is concentration dependent, being largest in the heavily doped region. The mobility ratio has also been shown to increase with temperature for a given value of the screening length.

#### 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 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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