

Ionized impurity scattering in semiconductors with spatially variable dielectric functions

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A spatially-dependent dielectric function $\epsilon(r)$ based on the Penn model is incorporated into existing theories of ionized impurity scattering. For the case of Si (Ge) it is shown that such an incorporation lowers the calculated mobility by a factor of 2.5 (3.0) at low-impurity concentrations. At high-impurity concentrations, the effect of introducing $\epsilon(r)$ into the formalism is to lower the calculated mobility by as much as several orders of magnitude. We conclude that analysis of mobility data may thus be used as a sensitive probe of the spatial dependence of the dielectric function.

Theoretical treatments of ionized impurity scattering all depend on the choice of the ionized impurity potential used in the matrix element for scattering. In a recent paper¹ Csavinszky points out that no treatments to date appear to incorporate the spatial dependence (or, alternatively, the wave-vector dependence) of the dielectric function $\epsilon(r)$ into the scattering potential. He suggests that this might be done and proceeds to derive an expression for the scattering potential $\phi'(r)$ which is based on the Penn model.² What is outlined below is a recalculation of the traditional Brooks-Herring³ (BH) mobility μ_{BH} incorporating the analytical form of $\phi'(r)$ derived by Csavinszky. Then, in considering the special cases of Si and Ge, we show how incorporation of this scattering potential affects the calculated mobility. Finally, we emphasize how analysis of mobility data may be used as a sensitive probe of the dielectric function in the vicinity of an ionized impurity. In the literature $\epsilon(r)$ has been introduced to properly account for energy levels of excitons⁴ and bound carrier states near impurities.⁵ Analysis of scattering near impurities is here proposed as another means of obtaining information on $\epsilon(r)$.

The analytical expression for the spatial dielectric function obtained on the basis of the Penn model is¹

$$\epsilon(r)^{-1} = e^{\alpha r} + A(1 - e^{-\beta r}) + B(1 - e^{-\gamma r}), \quad (1)$$

where A , B , α , β , and γ are material constants that have been tabulated for Si and Ge.^{6,7} By putting $\epsilon(r)$ into Poisson's equation, Csavinszky⁸ derives the following expression for the scattering potential:

$$\phi'(r) = \left(\frac{Z |e|}{4\pi\kappa_0\kappa r} \right) [C e^{-r/R_1} + (1 - C) e^{-r/R_2}]. \quad (2)$$

Here $Z |e|$ is the charge on the ionized impurity, κ and κ_0 are the material and free space dielectric constants, and r is the radial distance from the scattering center. C is a dimensionless constant

characteristic of the material considered, and R_1 and R_2 play the role of screening lengths in Csavinszky's paper [see Eqs. (43) and (44) of Ref. 1].

Standard treatments of impurity scattering⁹ employ a scattering potential $\phi(r)$ given by

$$\phi(r) = (Ze/4\pi\kappa_0\kappa r) e^{-r/R_0}, \quad (3)$$

where R_0 is the screening length.

In the following, we use the potential developed by Csavinszky to determine the charge carrier mobility μ . Using the potential $\phi'(r)$, in the matrix element for scattering

$$H_{kk'} = \int \Psi_k^* |e| \phi'(r) \Psi_{k'} d^3r, \quad (4)$$

one solves for the scattering cross section

$$\sigma(\theta) = |H_{kk'}|^2 \quad (5)$$

and then calculates the momentum relaxation time

$$\tau^{-1} \propto \int \sigma(\theta) (1 - \cos\theta) \sin\theta d\theta \quad (6)$$

to obtain the mobility. Here Ψ_k and $\Psi_{k'}$ are the incident and scattered charge-carrier wave functions.

In the spirit of the BH treatment³ the integration indicated in expression (6) can be performed to yield in our case

$$\begin{aligned} \tau \propto C^2 \left(\ln(1 + \beta_1^{-2}) - \frac{\beta_1^2}{1 + \beta_1^2} \right) \\ + (1 - C)^2 \left(\ln(1 + \beta_2^{-2}) - \frac{\beta_2^2}{1 + \beta_2^2} \right) \\ + 4C(1 - C) \left[\ln \left(\frac{1 + \beta_1^{-2} + \beta_2^{-2} + \beta_1^{-2}\beta_2^{-2}}{\beta_1^{-2}\beta_2^{-2}} \right) \right. \\ \left. + \left(\frac{\beta_1^{-2}\beta_2^{-2}}{\beta_1^{-2} - \beta_2^{-2}} \right) \ln \left(\frac{\beta_2^{-2}(1 + \beta_1^{-2})}{\beta_1^{-2}(1 + \beta_2^{-2})} \right) \right] \equiv M. \quad (7) \end{aligned}$$

In this expression β_i is associated with R_i via $\beta_i = 2\kappa R_i$. The calculated mobility μ is then re-

lated to the BH mobility by

$$\frac{\mu}{\mu_{\text{BH}}} = \left(\ln(1 + \beta_{\text{BH}}^2) - \frac{\beta_{\text{BH}}^2}{1 + \beta_{\text{BH}}^2} \right) / M. \quad (8)$$

In this expression β_{BH} is the screening factor initially appearing in the BH papers. We will now analyze Eq. (8) which is our principal analytical result.

To understand how this expression behaves, in Fig. 1 we have plotted μ/μ_{BH} for Ge and Si using the material parameters as calculated by Csavinsky. We plot μ/μ_{BH} as a function of charge carrier concentration n with temperature T as a parameter. Note that the effect of introducing a spatially dependent dielectric function is to decrease the calculated mobility by at least a factor of 2.5 (3.0) for Si (Ge). As n increases, the decrease becomes quite dramatic, changing the predicted mobility by several orders of magnitude. We see in Fig. 1 that the slower moving (i.e., colder) charge carriers are more strongly affected by the introduction of $\epsilon(r)$ than faster (i.e., hotter) charge carriers. As the carrier concentration n at a given T (and thus the number of scattering centers) decreases, the relative weight of the far field increases. That is, the carriers "see" more of the statically screened potential and hence $\mu/\mu_{\text{BH}} \rightarrow 1$ for small n . For large carrier concentrations, on the other hand, the increased number of ionized impurities leads to an increase in the relative amount of time spent by a free carrier in the vicinity of a scattering center, and μ/μ_{BH} turns strongly away from unity at high n .

Perhaps the most striking result demonstrated in Fig. 1 is the fact that μ/μ_{BH} does not approach unity as n gets vanishingly small. This implies that even for an extremely dilute concentration of impurities, the corrections made by the introduction of $\phi'(r)$ into the matrix element for scattering are significant.

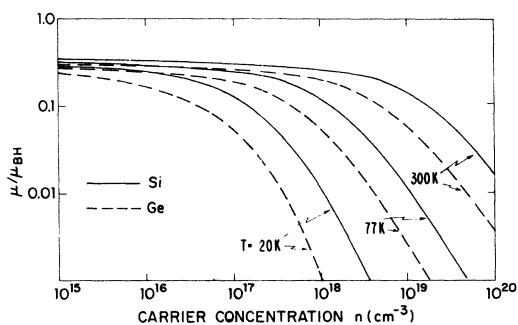


FIG. 1. Ratio of the calculated mobility to the Brooks-Herring mobility as a function of carrier concentration. The calculations for Si (solid lines) and Ge (dashed lines) are shown for three different temperatures.

The differences in the temperature dependence of the mobilities calculated by various techniques is illustrated in Fig. 2. Here we use a plot for Si prepared by Blatt¹⁰ to compare the temperature dependence of μ , μ_{BH} and the mobility calculated using a partial-wave scattering approach μ_{PW} . The dashed line is μ (as calculated above) translated to higher values by a factor of 2.7, while the dash dotted line is proportional to $T^{3/2}$. These data are for $n = 2 \times 10^{16} \text{ cm}^{-3}$, independent of T . If we were to treat the more likely case where $n = n(T)$ we would expect *all* calculated mobilities to more closely follow a $T^{3/2}$ dependence. We present the data of Fig. 2 to demonstrate that the T dependence of the mobilities as calculated by the various methods may be used to ascertain the validity of the calculation employed.

Experimental studies of Hall mobility in the ionized impurity-scattering conduction regime may be used as a test of our inclusion of $\phi'(r)$ into the theory. In an early study, Brown and Bray¹¹ examined a family of p -Ge samples and found that their results "attested to the increasing inadequacy of the impurity scattering treatment at lower temperatures and for higher impurity concentrations. When the theory began to fail, it consistently *overestimated* the mobility." Although the discrepancy between BH and experiment as measured by Brown and Bray was never larger than a factor of 0.5, their conclusions are in direct qualitative agreement with our Fig. 1 where the discrepancy between μ_{BH} and our μ is shown to be an increasing function of im-

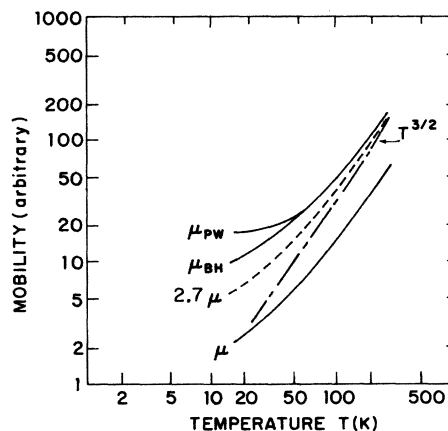


FIG. 2. Mobility as a function of temperature T for several means of calculation. The mobility determined in the present work μ is persistently below all other calculated values. To emphasize the T dependence of the various mobilities, we plot 2.7μ and thereby note that μ more closely follows a $T^{3/2}$ dependence than do either the Brooks-Herring mobility μ_{BH} or the partial-wave mobility μ_{PW} .

purity concentration and a decreasing function of temperature.

In a series of six *n*-Ge samples with impurity concentrations between 2×10^{15} and 10^{16} cm⁻³, Cuevas and Falicov^{12,13} find that on the average the BH theory overestimates the measured mobility by a factor of 0.8. They find, however, that the overestimation is a decreasing function of the density of impurities with the largest overestimation (a factor of 0.3) existing for their lowest impurity concentration. They attribute the overestimation of the BH and other theoretical treatments to an oversimplification of the pair-correlation function.

In a study of Cu-doped Ge samples, Norton and Levinstein¹⁴ measured μ as a function of N_I and found excellent agreement between the data and the BH theory. They point out, however, that a three parameter fit was used to analyze the data. The adjustable parameters include the donor density, a scale factor multiplying the neutral-impurity-scattering time and a third parameter to account for any error in measuring the sample dimensions. A comprehensive investigation such as Norton and Levinstein's (with better control over these three factors so that they do not enter as free parameters) would lend more insight into the applic-

ability of the BH treatment and its assumption of a spatially independent dielectric function.

In conclusion, if one uses the Penn-model-based Csavinszky scattering potential $\phi'(r)$ in a treatment of ionized impurity scattering, one is led to a calculated mobility appreciably smaller than that obtained with the standard Brooks-Herring treatment. In addition, the mobility thus calculated more closely follows a $T^{3/2}$ dependence than do the Brooks-Herring or the partial-wave mobilities. The differences seen in mobility due to the introduction of $\phi'(r)$, stress the fact that mobility measurements in the ionized impurity-scattering conduction regime are a sensitive probe of the spatial dependence of the potential of an ionized impurity.

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to account for the small- r behavior of $\phi'(r)$ where the authors of Refs. 6 and 7 have shown that the dielectric constant tends to unity. For the purposes of our calculation, we use the form of the potential given by our Eq. (2).

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