Angular dependence of impurity scattering in nonparabolic semiconductors

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The probability of scattering by ionized impurities has been calculated as function of the scattering angle for various energy values of the electrons in indium antimonide at 77 K. It is found that for electron energies higher than 0.1 eV, almost-zero angle scatterings are most prevalent. [S0163-1829(98)08419-7]

I. INTRODUCTION

The probability of scattering of electrons with ionized impurities under high-field condition is a complicated function of the polar angle between the wave vectors before and after collision. While calculating the high-field conductivity characteristics of semiconductors by the Monte Carlo technique, this dependence has been variously taken into consideration by different authors. Some have calculated the scattering angle by generating random numbers using the von Neumann technique,[1] while others have used a numerical solution of the scattering integral to find out a scattering angle in terms of a random number.[2,3]

It is of interest to study the dependence of the scattering rate on the polar angle between the electron wave vectors before and after the collision. In this paper we present the dependence of the scattering rate on the polar angle and the electron energy for different amounts of ionized impurity concentration.

II. THEORY

The probability of an electron being scattered from the state $\mathbf{k}$ is given by

$$S(\mathbf{k}) = V_c/(4\pi^2\hbar)\int |M(\mathbf{k},\mathbf{k}')|^2\delta(E_{\mathbf{k}}-E_{\mathbf{k}'})d\mathbf{k}', \quad (1)$$

where V_c is the crystal volume. The material is assumed to be nondegenerate, i.e., it is assumed that the final state $\mathbf{k}'$ is empty. The density of states in $\mathbf{k}'$ space is $(1/2\pi)^3$ because it is assumed that the spin is not altered due to scattering by ionized impurities.

The matrix element for ionized impurity scattering which takes place without the assistance of phonons and is assumed elastic, is given by[4]

$$|M(\mathbf{k},\mathbf{k}')|^2 = [A(|\mathbf{k}-\mathbf{k}'|)]^2 G(\mathbf{k},\mathbf{k}'), \quad (2)$$

where

$$[A(|\mathbf{k}-\mathbf{k}'|)]^2 = [(Ze^2)/(\varepsilon V_c)][(|\mathbf{k}-\mathbf{k}'|^2+\lambda^{-2})]^{-1}$$

where λ is the Debye screening length being given by $\lambda = [(ne^2)/(\varepsilon k_B T)]^{1/2}$ for n-type nondegenerate materials.

The screening of the wave function has been taken into consideration to avoid the mathematical singularity that would otherwise creep in the expression. $G(\mathbf{k},\mathbf{k}')$ is the overlap integral and is given by $G(\mathbf{k},\mathbf{k}') = a + b\cos\theta + c\cos^2\theta$, where θ is the polar angle between the wave vectors before and after collision. The coefficients a, b, and c are evaluated[4] in terms of the band gap E_g, the nonparabolicity factor α and the spin-orbit splitting energy Δ.

Substituting for the matrix element and carrying out the integration over the azimuthal angle ϕ and $\mathbf{k}'$ and noting that for elastic scattering the integrand is nonzero only when $E_{\mathbf{k}} = E_{\mathbf{k}'}$, one gets, from Eq. (1), for the total scattering rate,

$$S_{\text{imp}}(\mathbf{k},\lambda) = C_{\text{imp}}\gamma'(E_k)k^{-3}F_{\text{imp}}(\mathbf{k},\lambda), \quad (3)$$

where

$$C_{\text{imp}} = (Z^2e^4N_i m^*)/(8\pi\varepsilon^2\hbar^3),$$

$\gamma'(E_k) = \partial\gamma(E_k)/\partial E_k$, $\gamma(E_k) = (\hbar^2k^2)/(2m^*)$ is the energy parameter for nonparabolic band and is given by $\gamma(E_{\mathbf{k}}) = E_{\mathbf{k}}(1+\alpha E_{\mathbf{k}})$ for the case of simple nonparabolicity, $\alpha = 1/E_g$, and

$$\begin{aligned} F_{\text{imp}}(k,\lambda) &= \int_0^{\pi}[O_i(\cos\theta)\sin\theta\, d\theta][1-\cos\theta \\ &\quad + (2k^2\lambda^2)^{-1}]^{-2} \\ &= \int_0^{\pi} f_{\text{imp}}(\mathbf{k},\lambda,\theta)d\theta, \end{aligned} \quad (4)$$

where $O_i(x) = a + bx + cx^2$.

We note that the dependence of the scattering rate upon the polar angle between $\mathbf{k}$ and $\mathbf{k}'$ is given exclusively by Eq. (4). The probability that the electron will be scattered through an angle θ is given by

$$P(\theta) = \left[\int_0^{\theta} f_{\text{imp}}(\mathbf{k},\lambda,\theta)d\theta\right] \Big/ \left[\int_0^{\pi} f_{\text{imp}}(\mathbf{k},\lambda,\theta)d\theta\right] \quad (5)$$

and this integral can be evaluated analytically.

We note that if screening is neglected, the expression for $f_{\text{imp}}(\mathbf{k},\lambda,\theta)$ presents a singularity at $\theta=0$. In the presence of screening, however, the singularity is removed but low-angle scatterings are still favored, unless the electron energy is very low or the free electron concentration is too large to produce any considerable effect due to screening.

III. RESULTS

We have calculated the values of $P(\theta)$ for various values of θ for indium antimonide at 77 K using the following val-

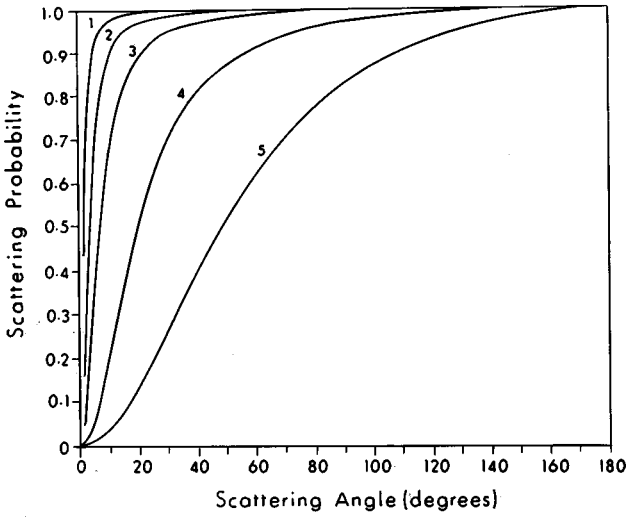

FIG. 1. Variation of the scattering probability with the angle of scattering in InSb at 77 K for different values of the electron energy. The ionized impurity concentration is 10^{13} cm^{-3}, (1) 3.9 $\times 10^{-3}$ (2) 9.8×10^{-4} (3) 2.4×10^{-4} (4) 3.0×10^{-5} (5) 3.0 $\times 10^{-6}$.

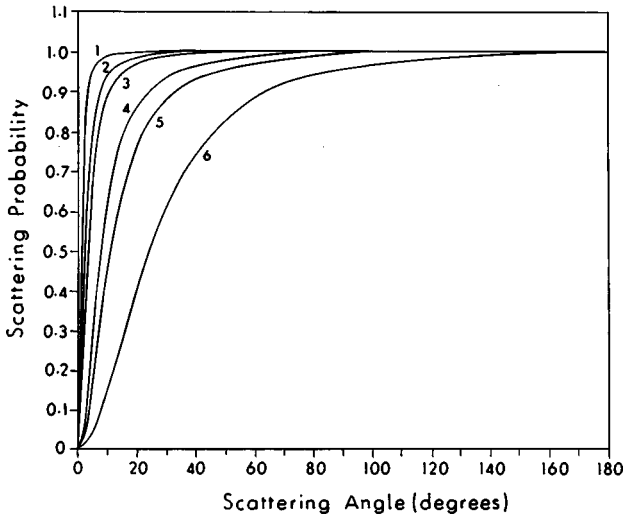

FIG. 2. Variation of the scattering probability with the angle of scattering in InSb at 77 K for different values of ionized impurity concentration. The average electron energy is 0.01 eV for all the curves. (1) 1×10^{13} (2) 5×10^{13} (3) 1×10^{14} (4) 5×10^{14} (5) 1×10^{15} (6) 5×10^{15}.

ues of the material parameters:

$$m^* = 0.0145 m_0, \quad \varepsilon = 17.54 \varepsilon_0 \quad E_g = 0.21218 \text{ eV},$$

$$\Delta = 0.09 \text{ eV}.$$

In Fig. 1 we have plotted the values of $P(\theta)$ versus θ for different values of the electron energy taking the free electron as well as ionized impurity concentration to be 10^{13} cm^{-3}. It is seen from the calculations that for higher values of electron energy ($E > 0.01$ eV), the scattering probability reaches the value of 1 sharply and the curves for various energies become indistinguishable indicating that only extremely low angle scatterings ($\theta < 0.1°$) occur in this energy range. For electron energies less than 0.01 eV, however, the scattering probability varies almost linearly with the logarithm of the angle and the curves become almost equispaced for equal changes in energy. Almost 90% of the scatterings, however, takes place within an angle of 15° for energies down to 10^{-5} eV. When these results are compared with those obtained by using simple expressions[5] that neglect the effect of overlapping of the s- and p-type wave functions, it is seen that the results do not differ by more than 5%. This indicates that the overlap integral does not contribute significantly to the angular dependence of the probability of scattering by ionized impurities in indium antimonide.

In Fig. 2 we have plotted the variation of the scattering probability for different values of the ionized impurity concentration taking the electron energy to be 0.01 eV. The free carrier concentration in all these cases have been taken to be equal to the ionized impurity concentration. We note that large-angle scatterings increase with increasing carrier concentration due to increase in the contribution of screening.

The usefulness of these graphs becomes evident when we consider simulation of the electron trajectory by the Monte Carlo technique, which has now become an important tool for the calculation of high-field conductivity in semiconductors. In this technique, a random number is generated to determine θ, the polar angle between the wave vectors before and after scattering. Equation (5) is then made use of to find θ, i.e., given a random number r, uniformly distributed between 0 and 1, one has to find θ such that the right-hand side of Eq. (5) becomes equal to r. This can be done either by solving Eq. (5) numerically or by an elaborate two-dimensional table lookup arrangement. During an actual simulation, however, this becomes painstakingly difficult and time consuming, because the values of the integrals depend upon energy and the electron passes through a very wide range of energy during its course of motion.

On the other hand the nature of the graphs presented here shows that $P(\theta)$ and θ can be related by some empirical relationship. Such empirical relation may be effectively used for faster and simpler implementation of the Monte Carlo technique without considerable loss in accuracy.

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