Calculation of ionized impurity-scattering probability with scattering angles in GaN

P.S. Mallick, Janardan Kundu, and C.K. Sarkar

Abstract: The probability of scattering by ionized impurities has been calculated as function of the scattering angle for various energy values of the electrons in gallium nitride at 77 K. It is found that for electron energies higher than 0.1 eV, almost-zero angle scatterings are most prevalent.

PACS Nos.: 72.10.−d, 72.20.Fr

Résumé : Nous avons calculé en fonction de l'angle de diffusion la probabilité de diffusion d'électrons à différentes énergies par des impuretés ionisées dans du nitrure de Gallium à 77 K. Nous trouvons qu'aux énergies au delà de 0.1 eV, l'angle prévalent de diffusion est 0 degrés.

[Traduit par la Rédaction]

1. Introduction

Gallium nitride, a direct band gap semiconductor, has emerged as an important material for high-power, optoelectronic as well as for high-temperature devices because of its large band gap (3.4 eV), strong bond strength (2.3 eV/bond), and high breakdown voltage (3×10^6 V/cm) [1]. Recently, the material has become more popular because of several new applications including blue-light-emitting diodes and blue-laser diodes [2]. Theoretical studies of the electrical conductivity characteristics of gallium nitride have been carried out in great detail over the past two decades using analytical methods where one has to solve the Boltzmann transport equation (BTE) taking the various scattering mechanisms for the charge carriers into account. Solution of the Boltzmann equation is beset with many complications, particularly under a large applied electric field. To obviate these difficulties, one has to have recourse to a numerical techniques such as the Monte Carlo simulation technique that has now become an important tool for studying electron transport in semiconductors as well as device simulation. In this technique, the motion of the electron through the semiconductor is simulated in a digital computer by using random numbers and taking into account the probabilistic nature of the various electron–lattice collision processes. The motion of a single electron is followed through a large number of collisions, and the principle of ergodicity is invoked to obtain the ensemble average from the time average of a single particle. The electron transport parameters in GaN have already been obtained using the Monte Carlo simulation technique [3–5]. Study of the polar angle between the wave vectors before and after scattering is very useful for simulating the trajectory of the electron. The probability of scattering of electrons with ionized impurities under high-field conditions is a complicated function of the polar angle. While calculating the high-field conductivity characteristics of semiconductors using 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 [6], while others have taken recourse to a numerical solution of the scattering integral to find out a scattering angle in terms of a random number [7, 8]. 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 note, we present the dependence of the scattering rate on the polar angle and the electron energy for different amounts of ionized impurity concentration in gallium nitride. Recently, we obtained similar results in some II–VI compound semiconductors such as ZnO, CdS, and CdTe [9] where we have shown that almost 80% of the scatterings take place within an angle of 20° but here in the case of GaN we have found that 90% of the scatterings take place within an angle of 15°.

Received 19 September 2007. Accepted 13 February 2008. Published on the NRC Research Press Web site at http://cjp.nrc.ca/ on 12 August 2008.

P.S. Mallick.[1] School of Electrical Sciences, VIT University, Vellore 632 014, Tamilnadu, India.
J. Kundu. Department of Electronics and Communication Engineering, Kodaikanal Institute of Technology, Tamilnadu 624 104, India.
C.K. Sarkar. Department of Electronics and Telecommunication Engineering, Jadavpur University, Kolkata 700 032, India.

[1] Corresponding author (e-mail: psmallick@vit.ac.in).

2. Theory

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

$$S(k) = \frac{V_c}{4\pi^2\hbar}\int \left|M(k,k')\right|^2 \delta(E_K - E_{K'})\mathrm{d}k' \qquad (1)$$

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

The evaluation of the scattering probability requires the complete expressions of the matrix element, $M(\boldsymbol{K}, \boldsymbol{K}')$ and the expressions are different for different kinds of scattering. The matrix element for the ionized impurity scattering that takes place without the assistance of phonons and is assumed to be elastic

 doi: 10.1139/P08-027

is given by [10]

$$\left|M\left(k,k'\right)\right|^2 = \left[A\left(\left|k-k'\right|\right)\right]^2 G\left(k,k'\right) \tag{2}$$

where,

$$\left[A\left(\left|k-k'\right|\right)\right]^2 = \left[\frac{Z\,e^2}{\varepsilon V_c}\right]\left[\left(\left|k-k'\right|^2+\lambda^{-2}\right)\right]^{-1}$$

Z is the degree of ionization of the impurity atoms and assumed to be unity and λ is the Debye screening length given by [10]

$$\lambda = \left[\frac{n\,e^2}{\varepsilon k_B T}\right]^{-1/2}$$

for n-type nondegenerate materials, where n is the concentration of electrons.

Substituting the appropriate matrix element and carrying out the integration in (1), we find the rate of scattering by ionized impurity atoms to be

$$S_{\rm imp}(\boldsymbol{k}) = \frac{V_c}{4\pi^2\hbar}N_i V_c \int \frac{Z^2\,e^4}{V_c^2\varepsilon^2}\left[\left|\boldsymbol{k}-\boldsymbol{k}'\right|^2+\lambda^{-2}\right]^{-2} \times G(\boldsymbol{k},\boldsymbol{k}')\delta\left(E_{\boldsymbol{k}}-E_{\boldsymbol{k}'}\right)\,\mathrm{d}k'$$

We note that $\mathrm{d}\boldsymbol{k}' = \boldsymbol{k}'^2\sin\theta\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}\boldsymbol{k}'$ where θ is the polar angle between $\boldsymbol{k}$ and $\boldsymbol{k}'$, and ϕ is the azimuthal angle. Also, $\boldsymbol{k}'^2\,\mathrm{d}\boldsymbol{k}'$ may be expressed in terms of E_k' as

$$k'^2\,\mathrm{d}k' = 0.5\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\left[\gamma(E_{\boldsymbol{k}'})\right]^{1/2}\gamma'(E_{\boldsymbol{k}'})\,\mathrm{d}E_{\mathbf{k}'}$$

where,

$$\gamma'\left(E_k\right) = \frac{\partial\gamma\left(E_k\right)}{\partial E_k}$$

$\gamma\left(E_k\right) = \left(\hbar^2k^2\right)/\left(2m^*\right)$ is the energy parameter for the nonparabolic band and is given by $\gamma(E_k) = E_k(1+\alpha E_k)$ for the case of simple nonparabolicity, $\alpha = 1/E_g$.

The screening of the wave function has been taken into consideration to avoid the mathematical singularity that would otherwise creep in the expression. $G(\boldsymbol{k},\boldsymbol{k}')$ is the overlap integral and is given by $G(\boldsymbol{k},\boldsymbol{k}') = a+b\cos\theta+c\cos^2\theta$, where θ is the polar angle between the wave vectors before and after collision. The coefficients a, b, and c are evaluated [10] in terms of the band gap E_g and the nonparabolicity factor α as

$$a = \left(\frac{1+\alpha E}{1+2\alpha E}\right)\left(\frac{1+\alpha E'}{1+2\alpha E'}\right) \cong 1-\alpha\left(E+E'\right)+\alpha^2\left(EE'+2E^2+2E'2\right)$$

$$b = 2\frac{(1+\alpha E)^{1/2}\left(1+\alpha E'\right)^{1/2}\left(\alpha^2EE'\right)^{1/2}}{(1+2\alpha E)\,(1+2\alpha E')} \cong 2\left(\alpha^2EE'\right)^{1/2}$$

$$c = \frac{\alpha^2EE'}{(1+2\alpha E)\,(1+2\alpha E')} \cong \alpha^2EE'$$

The integral over E_k' is evaluated straight away using the fact that for elastic scattering the integrand is nonzero only when $E_k = E_k'$. The integration is thus performed by replacing k' by k in the integrand since E_k' depends only on the magnitude of k'. We thus get for $S_{\rm imp}(k)$,

$$S_{\rm imp}\left(k,\lambda\right) = C_{\rm imp}\gamma'\left(E_k\right)k^{-3}F_{\rm imp}\left(k,\lambda\right) \tag{3}$$

where

$$C_{\rm imp} = \frac{Z^2\,e^4N_im^*}{8\pi\varepsilon^2\hbar^3}$$

$$F_{\rm imp}\left(k,\lambda\right) = \int_0^\pi\left[O_i\left(\cos\theta\sin\theta\right)\right] \times\left[1-\cos\theta+\left(2k^2\lambda^2\right)^{-1}\right]^{-2}\mathrm{d}\theta = \int_0^\pi f_{\rm imp}\left(k,\lambda,\theta\right)\,\mathrm{d}\theta \tag{4}$$

where $O_i(x) = a+bx+cx^2$, N_i is the impurity concentration.

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

$$P\left(\theta\right) = \frac{\int_0^\theta f_{\rm imp}\left(k,\lambda,\theta\right)\,\mathrm{d}\theta}{\int_0^\pi f_{\rm imp}\left(k,\lambda,\theta\right)\,\mathrm{d}\theta} \tag{5}$$

and this integral can be evaluated analytically.

We note that if screening is neglected, the expression for $f_{\rm imp}\left(\boldsymbol{k},\lambda,\theta\right)$ 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.

3. Results

We have calculated the values of $P(\theta)$ for various values of θ for gallium nitride at 77 K using the following values of the material parameters:

$$m^* = 0.19m_0, \qquad \varepsilon = 9.5\varepsilon_0,\ E_g = 3.5\ \mathrm{eV}$$

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 the ionized impurity concentration to be 10^{13} cm^{-3}. It can be seen from the calculations that for higher values of the electron energy ($E > 0.01$ eV), the scattering probability

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

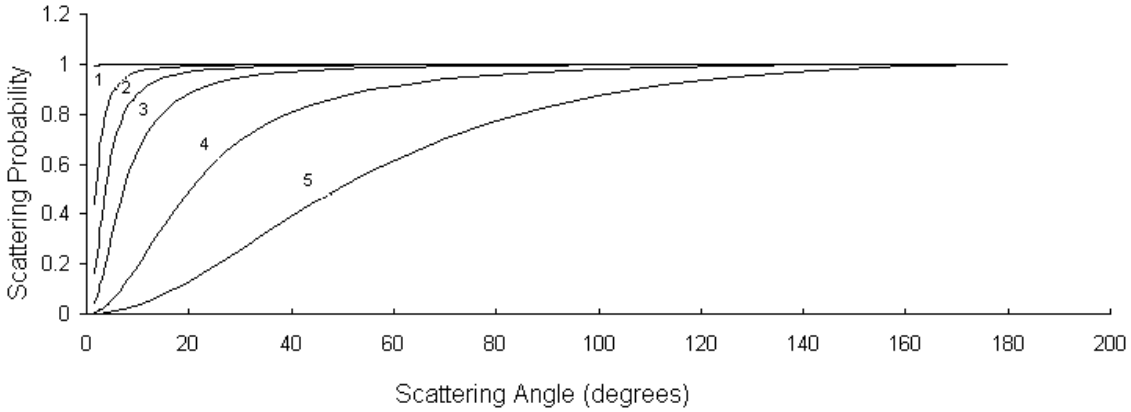
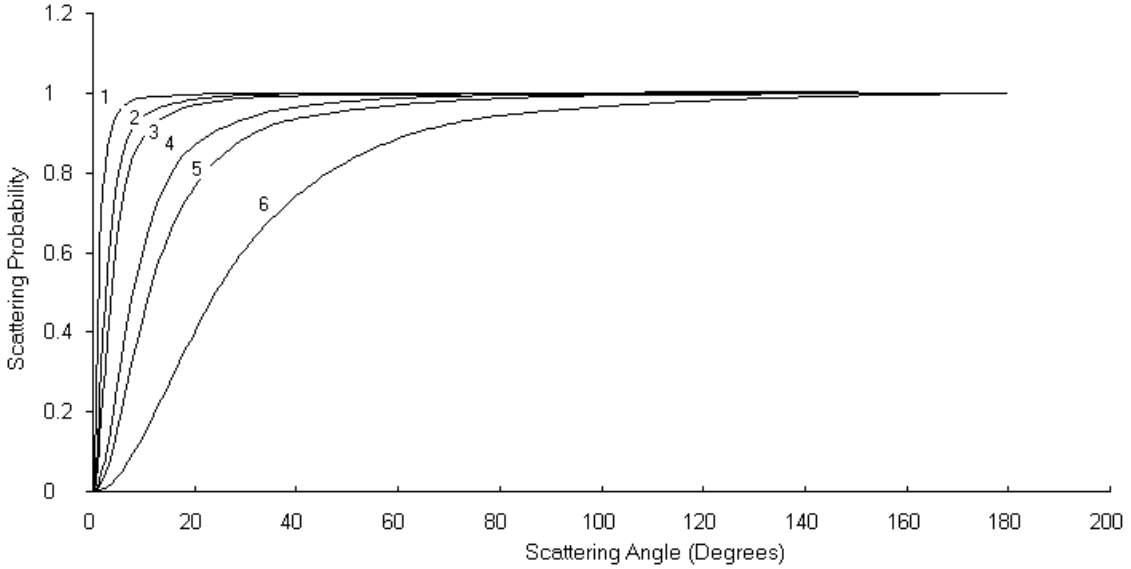


Fig. 2. Variation of the scattering probability with the angle of scattering in GaN at 77 K for different values of ionized impurity concentration. The average electron energy is 0.01 eV for all the curves. (1) 1×10^{13} cm^{-3}, (2) 5×10^{13} cm^{-3}, (3) 1×10^{14} cm^{-3}, (4) 5×10^{14} cm^{-3}, (5)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



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 [11] 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 gallium nitride.

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 has 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 the screening.

The usefulness of these graphs becomes evident when we consider simulation of the electron trajectory by the Monte Carlo technique. 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 used 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 (5) becomes equal to r. This can be done either by solving (5) numerically or by an elaborate two-dimensional table look-up 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 rela-

tionship. Such an 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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