

Research Article

Effect of Scattering Angle in Electron Transport of AlGa_N and InGa_N

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The scattering angle between electrons plays a very important role for the calculation of scattering probability. The probability of scattering is an essential parameter for the simulation of electron paths. In this work, we calculated the scattering probability with scattering angle in AlGa_N and InGa_N at 77 K and found that the lower angle scatterings only dominate.

1. Introduction

The wide bandgap materials, AlGa_N and InGa_N, have received much attention for the design of optoelectronic devices in the visible to ultraviolet spectral regions [1, 2] and for high-power microwave devices [3]. The energy bandgap of these compounds is large as compared to Si or GaAs. Therefore, these compound semiconductors have a larger breakdown voltage too. The saturation drift velocity of these compounds is also slightly higher. Thus, the high-electric field and high frequency devices made from both compound semiconductors would have better characteristics [4–7]. Therefore, it will be interesting to study the characteristics of these ternary compound semiconductors.

Study of electrical conductivity of AlGa_N, InGa_N, and other larger bandgap ternary compounds were not carried out in detail. The BTE Equation solution considering different scattering mechanisms into account is a tedious process, specifically in the presence of a strong applied electric field. The MC simulation technique is now a vital numerical technique for studying electron transport. The MC simulation technique is used. The motion of the electron is simulated by using random numbers. It considers the probabilistic character of different electron-lattice scattering mechanisms. When electrons move in an electric field, an

abundance of scattering occurs, as well as the ergodic principle can be used to obtain the ensemble average derived from a single electron's time average. Electron mobility and other transport properties of AlGa_N and InGa_N were obtained earlier using the Monte Carlo simulation technique by Maziar Farahmand et al. [4]. The mobility of electrons was also calculated by our group for other optoelectronic materials using the same numerical technique [5]. It is important to know the wave vectors' polar angles prior to and following collision to simulate the trajectory of the particle. In the presence of a strong electric field, the scattering probability of electrons is always a function of the polar angle. Researchers have been considering this dependence when calculating the high field conductivity properties using the Monte Carlo technique. Some of them studied the angle of scattering by using a random number generator through the von Neumann technique [5], and others considered numerical solutions to determine the scattering angle using random numbers [6–8]. Study of the relationship between the scattering rate and the before and after collision polar angle of electron wave vectors is a point of interest. The reliance of the impurity scattering rate as a function of polar angle is studied for both AlGa_N and InGa_N. We obtained similar results in gallium nitride earlier where it was shown that about 90% of the scatterings occur

within an angle of 15° [9], but now for InGaN, we have obtained slightly different results. We have found almost the same results in AlGaIn, but for InGaIn, it is that nearly 95% of scatterings occur within a 10° angle.

2. Modeling

The likelihood of an electron scattering from the state t can be calculated as follows:

$$S(t) = \frac{V_c}{4\pi^2\hbar} \int |M(t, t')|^2 \delta(E_t - E_{t'}) dt', \quad (1)$$

where, V_c is the crystal volume, the final state t' is empty, and the state density in t' space is $(1/2\pi)^3$. Here, the spin is assumed not to be altered as a result of scattering by ionized impurities [10].

The matrix component $M(t, t')$ is obtained by calculating the scattering probability, which necessitates the full matrix element expression. The obtained expressions differ based on the type of scattering. The ionized scattering of impurities phenomenon occurs without the help of phonons and is thought to be elastic, as stated by [10].

$$|M(t, t')|^2 = [A(|t - t'|)]^2 G(t, t'), \quad (2)$$

where,

$$[A(|t - t'|)]^2 = \left[\frac{(Ze^2)}{(\epsilon V_c)} \right] \left[(|t - t'|^2 + \lambda^{-2}) \right]^{-1}. \quad (3)$$

Z is the impurity atoms degree of ionization, assumed unity, and the Debye screening length $\lambda = [(ne^2)/(\epsilon k_B T)]^{-1/2}$ for n -type nondegenerate materials, where n denotes electron concentration [10].

By replacing the relevant matrix element and performing the integration in (1), we obtain the rate at which ionized impurity atoms scatter as [9]

$$S_{\text{imp}}(k) = \frac{V_c}{4\pi^2\hbar} N_i V_c \int \left(\frac{Z^2 e^4}{V_c \epsilon^2} \right) \times \left[|t - t'|^2 + \lambda^{-2} \right]^{-2} G(t, t') \delta(E_t - E_{t'}) dt'. \quad (4)$$

We note that $dt' = t'^2 \sin \theta d\theta d\phi dt'$, where θ is the polar angle between t and t' , and ϕ is the azimuthal angle [9]. Also, $t'^2 dt'$ can be stated in terms of $E_{t'}$ as

$$t'^2 dt' = 0.5 \left(\frac{2m^*}{\hbar^2} \right)^{3/2} (\gamma(E_{t'}))^{1/2} \gamma'(E_{t'}) dE_{t'}, \quad (5)$$

where,

$$\gamma'(E_t) = \frac{\partial \gamma(E_t)}{\partial E_t}. \quad (6)$$

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

The wave function is being screened to avoid the mathematical singularity. Otherwise, the expression would

be distorted. $G(t, t')$ is the overlap integral and is given by $G(t, t') = a + b \cos \theta + c \cos^2 \theta$, where θ is polar angle formed by the collision of two wave vectors. The band gap is used to calculate the coefficients a , b , and c [9] and E_g and the nonparabolicity factor α as

$$\begin{aligned} a &= \left(\frac{1 + \alpha E}{1 + 2\alpha E} \right) \left(\frac{1 + \alpha E'}{1 + 2\alpha E'} \right) \cong 1 - \alpha(E + E') + \alpha^2(EE' + 2E^2 + 2E'^2), \\ b &= 2 \frac{(1 + \alpha E)^{1/2} (1 + \alpha E')^{1/2} (\alpha^2 EE')^{1/2}}{(1 + 2\alpha E)(1 + 2\alpha E')} \cong 2(\alpha^2 EE')^{1/2}, \\ c &= \frac{\alpha^2 EE'}{(1 + 2\alpha E)(1 + 2\alpha E')} \approx \alpha^2 EE'. \end{aligned} \quad (7)$$

It is well known that the integrand for elastic scattering will be nonzero when $E_t = E_{t'}$. Since $E_{t'}$ depends only on the magnitude of t , integration is accomplished through replacement of t' by t in the given integrand. By doing this, $S_{\text{imp}}(t)$ can be obtained.

$$S_{\text{imp}}(t, \lambda) = C_{\text{imp}} \gamma'(E_t) t^{-3} F_{\text{imp}}(t, \lambda), \quad (8)$$

where,

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

$$\begin{aligned} F_{\text{imp}}(t, \lambda) &= \int_0^\pi [O_i (\cos \theta \sin \theta)] \times \left[1 - \cos \theta + (2t^2 \lambda^2)^{-1} \right]^{-2} d\theta \\ &= \int_0^\pi f_{\text{imp}}(t, \lambda, \theta) d\theta, \end{aligned} \quad (9)$$

where $O_i = a + bx + cx^2$, N_i is the concentration of impurities.

Equation (4) shows the scattering angle's dependence on the angle formed by the variables t and t' . Given that the probability of an electron being scattered at an angle θ is given by [12]

$$P(\theta) = \frac{\left[\int_0^\theta f_{\text{imp}}(t, \lambda, \theta) d\theta \right]}{\left[\int_0^\pi f_{\text{imp}}(t, \lambda, \theta) d\theta \right]}. \quad (10)$$

It is understandable that if no screening is carried out, the equation for $f_{\text{imp}}(t, \lambda, \theta)$ presents a singularity at $\theta = 0$. When screening occurs, although the singularity has been removed, low angle scatterings are still taken into account. Unless the electron energy is extremely low or the free electron concentration is too high to produce a significant effect as a result of screening.

3. Results and Discussion

The scattering probability in InGaIn at 77 K varies with electron energy in Figure 1. Concentration of ionized impurities 10^{15} cm^{-3} is assumed. It is observed that the scattering probability will reach a value of 1 exactly and the

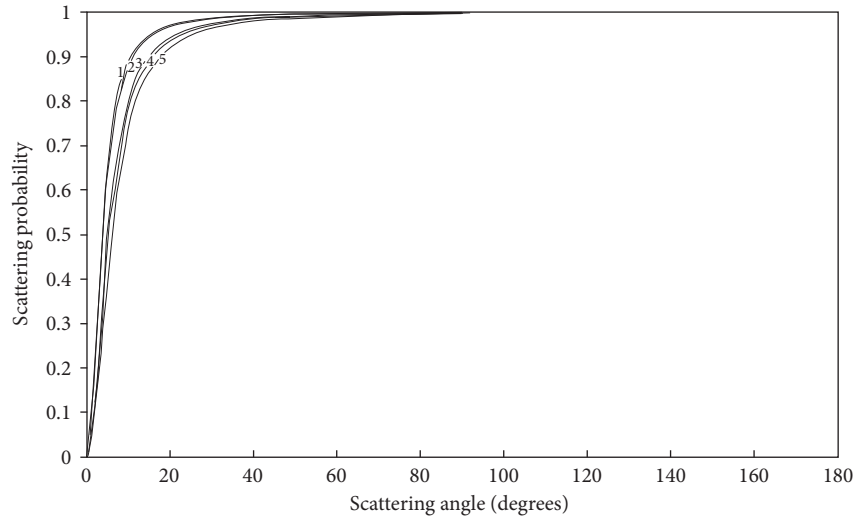


FIGURE 1: Analysis of the scattering angle in InGaN at 77 K. The concentration of ionized impurities is 10^{15} cm^{-3} (1) $3.9 \times 10^{-3} \text{ eV}$ (2) $9.8 \times 10^{-4} \text{ eV}$ (3) $2.4 \times 10^{-4} \text{ eV}$ (4) $3.0 \times 10^{-5} \text{ eV}$ (5) $3.0 \times 10^{-6} \text{ eV}$.

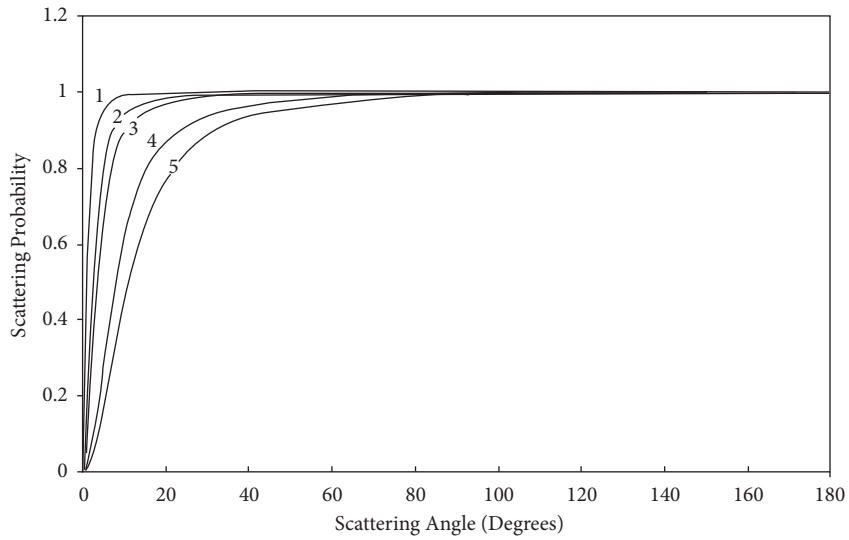


FIGURE 2: The scattering angle in InGaN at 77 K for various ionized impurity concentrations was studied. The average electron energy across all curves is 0.01 eV. (1) $1 \times 10^{13} \text{ cm}^{-3}$ (2) $5 \times 10^{13} \text{ cm}^{-3}$ (3) $1 \times 10^{14} \text{ cm}^{-3}$ (4) $5 \times 10^{14} \text{ cm}^{-3}$ (5) $1 \times 10^{15} \text{ cm}^{-3}$ (6) $5 \times 10^{15} \text{ cm}^{-3}$.

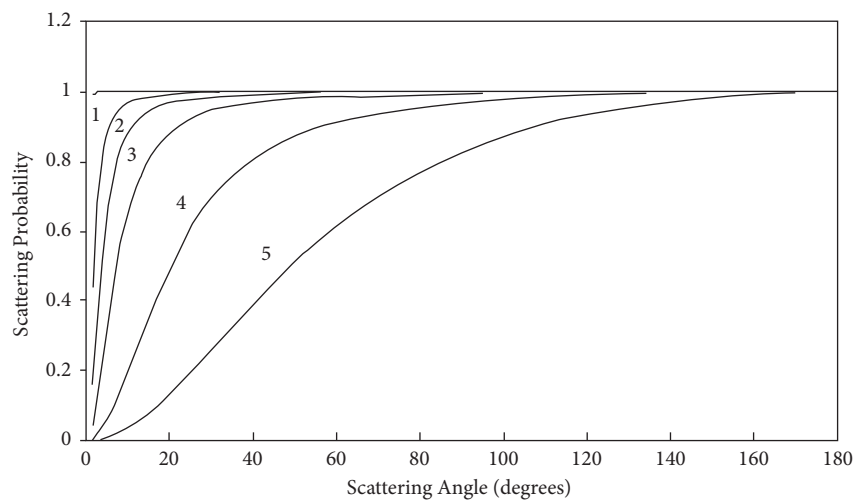


FIGURE 3: The probability of scattering analysis with angle of scattering in AlGaIn at 77 K for various electron energy values. The concentration of ionized impurities is 10^{15} cm^{-3} . (1) $2.0 \times 10^{-3} \text{ eV}$ (2) $7.5 \times 10^{-4} \text{ eV}$ (3) $4.2 \times 10^{-4} \text{ eV}$ (4) $3.0 \times 10^{-5} \text{ eV}$ (5) $5.0 \times 10^{-6} \text{ eV}$.

curves for different levels will become nonidentical by implying that only low scattering angles will occur in the presented energy range [10]. This is the condition for $E > 0.01$ eV. But, for the condition where $E < 0.01$ eV, for equal changes in energy, the scattering likelihood changes almost are linear with the angle's logarithm, and the curves become nearly equispaced. For energies less than 10^{-5} eV, the majority of scatterings will occur within a 10° angle. When these results are compared to previously published papers using simple expressions [11], it is clear that the overlapping of *s*- and *p*-type wave functions has been overlooked. The results also show little variation. This implies that the overlap integral has little effect on the angle of dependence of the scattering probability of ionized impurities in InGaN and AlGaN.

The scattering probability varies with value. Figure 2 depicts the variation of the concentration of ionized impurities. The energy of electrons is assumed to be 0.01 eV. It should be noted that as carrier concentration increases so does the contribution of screening. $P(\theta)$ is calculated for different values of ' θ ' in AlGaN at 77 K. It is found that the majority of the scatterings are taking place within the range of 0 – 10° for the energies down to 10^{-5} eV. The variation with respect to the scattering is shown in Figure 3.

4. Conclusions

The efficacy of the obtained results becomes obvious when we use the MC technique to simulate the electron trajectory. A variable number will be obtained in this technique in order to estimate θ , the polar angle formed by the wave vectors prior to and following scattering. However, in practise, this becomes extremely difficult and takes time as the integral values are energy-dependent, and during its motion, the electron experiences a wide range of energy.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest regarding the publication of this paper.

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