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THE SHORT-RANGE PRINCIPLE IN THE ELECTRON SCATTERING THEORY IN INDIUM NITRIDE

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The processes of the electron scattering on the short-range potential caused by interaction with polar and nonpolar optical phonons, piezoelectric and acoustic phonons, static strain, neutral and ionized impurities in wurtzite InN sample with electron concentration $\sim 6 \times 10^{17}\,\mathrm{cm}^{-3}$ are considered. The temperature dependence of the electron mobility in the temperature range $4.2 - 560\,K$ is calculated.

Key words: transport phenomena, charge carrier scattering, indium nitride

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Introduction

The III-V nitrides are important materials for optoelectronic and for high-temperature and high-power electronic device applications. Recently, there has been an extensive investigation of the electrical [1,2] and optical [3-7] properties of InN thin films. Further progress in the design and optimization of InN-based devices requires a thorough adequate approximation of the material parameters. One of the important material parameter is the charge carrier mobility.

The investigation of the temperature dependence of electron mobility was presented in [1,8-10]. Theoretical analysis of experimental data of electron scattering on various types of crystal defects in InN was carried out by relaxation time approximation [1,8,10] and place Monte-Carlo method [9]. The common feature of these methods is the using of the long-range charge carrier scattering models for the description of the transport phenomena in this semiconductor. In these models it is supposed that either the charge carrier interacts with all the crystal (electron -phonon interaction) or it interacts with the defect potential of the impurity the action radius of which is equal to $\sim 10 - 1000a_0$ (a_0 – lattice constant). However, such an assumption has next contradictions: a) it contradicts the special relativity according to which the charge carrier would interact only with the neighbouring crystal region; b) it contradicts the atomistic hypothesis according to which the charge carrier interacts (and transfers the energy respectively) only with one atom but not simultaneously with many atoms which are situated in different points of space. Besides for defects with the interaction energy $U \approx \frac{1}{r^n}$ $(n = 1, 2)$ on distances $\sim 10a_0$ the potential becomes the magnitude of the second order while all mentioned above scattering models are considered in the first (Born) approximation. From the other side in [11 - 15] the short-range models of charge carrier scattering in $A^{II}B^{VI}$ and $A^{III}B^{V}$ semiconductors were proposed in which the above mentioned shortcomings were absent. It has been supposed there that the carrier interacts with the defect potential only within the limits of one elementary cell. The aim of the present paper is to use this approach for description of the charge carrier scattering processes on the various types of crystal defects in indium nitride.

Theory

According to the short-range scattering models in wurtzite structure semiconductor the carrier transition probability from state $\boldsymbol{k}$ to state $\boldsymbol{k}$ caused by the interaction with polar optical (PO), nonpolar optical (NPO), piezooptic (POP) and piezoacoustic (PAC), acoustic (AC) phonons, static strain (SS) potential, ionized (II) and neutral (NI) impurity looks like [14,15]:

$$W_{\mathrm{PO}}(\mathbf{k},\mathbf{k}') = \frac{a_0^6}{12c_0^2\left(\frac{a_0+c_0}{2}\right)^8}\frac{64\pi^7\gamma_{PO}^{10}e^4}{225\varepsilon_0^2 G}\frac{M_{In}+M_N}{M_{In}M_N}\left\{\frac{1}{\omega_{LO}}\left[N_{LO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{LO}) + \right.\right.$$
$$\left.\left. + \ (N_{LO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{LO})\right] + \frac{2}{\omega_{TO}}\left[N_{TO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{TO}) + (N_{TO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{TO})\right]\right\}; \quad (0.1)$$

$$W_{\mathrm{NPO}}(\mathbf{k},\mathbf{k}') = \frac{1}{\left(\frac{a_0+c_0}{2}\right)^2}\frac{\pi^3 E_{\mathrm{NPO}}^2}{288 a_0^2 G}\frac{M_{In}+M_N}{M_{In}M_N}\left\{\frac{1}{\omega_{LO}}\left[N_{LO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{LO}) + \right.\right.$$
$$\left.\left. + (N_{LO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{LO})\right] + \frac{2}{\omega_{TO}}\left[N_{TO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{TO}) + (N_{TO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{TO})\right]\right\}; \quad (0.2)$$

$$W_{\mathrm{POP}}(\mathbf{k},\mathbf{k}') = \frac{a_0^{10}}{\left(\frac{a_0+c_0}{2}\right)^{10}}\left(\frac{32}{75}\right)^2\frac{\pi^9 e^2 e_{14}^2 \gamma_{PZ}^{10}}{\varepsilon_0^2 G}\frac{M_{In}+M_N}{M_{In}M_N}\left\{\frac{1}{\omega_{LO}}\left[N_{LO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{LO}) + \right.\right.$$
$$\left.\left. + (N_{LO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{LO})\right] + \frac{2}{\omega_{TO}}\left[N_{TO}\delta(\varepsilon'-\varepsilon-\hbar\omega_{TO}) + (N_{TO}+1)\delta(\varepsilon'-\varepsilon+\hbar\omega_{TO})\right]\right\}; \quad (0.3)$$

$$W_{\mathrm{PAC}}(\mathbf{k},\mathbf{k}') = \frac{a_0^{10}}{\left(\frac{a_0+c_0}{2}\right)^8}\frac{128\pi^7 e^2 e_{14}^2 \gamma_{PZ}^{10} k_B T}{225\varepsilon_0^2\hbar G[M_{In}+M_N]}\left(\frac{1}{c_{LO}}+\frac{2}{c_{TO}}\right)^2\delta(\varepsilon'-\varepsilon); \quad (0.4)$$

$$W_{\mathrm{AC}}(\mathbf{k},\mathbf{k}') = \left[4\left(\frac{a_0+c_0}{2}\right)^{-3}\frac{a_0^2 c_0\sqrt{3}}{2}\right]^2\frac{\pi^3 k_B T E_{\mathrm{AC}}^2}{144\hbar G[M_{In}+M_N]}\left(\frac{1}{c_{LO}}+\frac{2}{c_{TO}}\right)^2\delta(\varepsilon'-\varepsilon); \quad (0.5)$$

$$W_{\mathrm{II}}(\mathbf{k},\mathbf{k}') = \left(\frac{a_0+c_0}{2}\right)^4\frac{\pi e^4 Z_i^2 N_{\mathrm{II}}\gamma_{II}^4}{2\varepsilon_0^2\hbar V}\delta(\varepsilon'-\varepsilon); \quad (0.6)$$

$$W_{\mathrm{NI}}(\mathbf{k},\mathbf{k}') = \frac{(a_0+c_0)\gamma_{II}}{4}\frac{20\pi^2 N_{\mathrm{NI}}\hbar^3}{V m^{*2} k'}\delta(\varepsilon'-\varepsilon); \quad (0.7)$$

$$W_{\mathrm{SS}}(\mathbf{k},\mathbf{k}') = \left(\frac{a_0+c_0}{2}\right)^6\frac{2^5 3^4\pi^3 C^2 e^2 e_{14}^2 N_{\mathrm{SS}}}{V\varepsilon_0^2\hbar}\frac{1}{q^2}\delta(\varepsilon'-\varepsilon); \quad (0.8)$$

where M_{In}, M_N – the atom masses; G – the number of unit cells in a crystal volume; ε_0 – the vacuum permittivity; e – the elementary charge; k_B – the Boltzmann constant; $\hbar$ – the Planck constant; N_{LO}; N_{TO} – the number of longitudinal (LO) and transverse (TO) phonons with a frequency ω_{LO} and ω_{TO} respectively (we put $\omega_{LO} = \omega_{TO}$); e_{14} – the component of the piezoelectric tensor; c_{LO}, c_{TO} – the respective sound velocities (we put $c_{LO} = c_{TO} = c$); V – the crystal volume; N_{I}, N_{NI}, N_{SS} – the ionized impurities, neutral impurities and strain centers concentration respectively; Z_i – the impurity charge in electron-charge units; E_{AC}, E_{NPO} – the acoustic and optical deformation potentials respectively; γ_{PO}, γ_{PZ}, γ_{II} – the fitting parameters determining the action radius of short-range potential ($R = \gamma a_0$, $0 < \gamma_{PO}, \gamma_{PZ} \leq \sqrt{1 + a_0^2/c_0^2}/2 = 1.187$, $0 \leq \gamma_{II} \leq (1 + c_0/a_0)/2 = 1.31$); m^* – the carrier effective mass; $q = |\mathbf{k}' - \mathbf{k}|$; $C \approx 0.1$.

In Eq. (0.1) - (0.8) the first multiplier in the right-hand member represents the geometrical factor which takes into account the distinction between the wurtzite and zinc blende structure. It must be noticed that the strong power dependence of parametersγ_{PO}, γ_{PZ}, γ_{II} sharply limits the choice opportunities of their numerical values.

The calculation of the conductivity tensor components was made on the base of the formalism of a precise solution of the stationary Boltzmann equation [16]. Using this formalism one can obtain additional fitting parameter $\gamma_{SS}N_{SS}$ (we put $\gamma_{SS} = 1$) for SS-scattering mode. The parameters of indium nitride used for calculation are listed in Table 1.

Table 1. Parameters of wurtzite InN used in calculations

Material parameter	Value	References
Lattice constant, a_0 (m)	3.545×10^{-10}	[17]
c_0 (m)	5.703×10^{-10}	
Energy gap, E_g (eV)	$0.69 - 0.41 \times 10^{-4} T^2/(T + 454)$	[18]
Electron effective mass, m_n/m_0	0.115	[17]
Density, ρ_0 $(g \cdot cm^{-3})$	6.81×10^3	[9, 19]
Optical deformation potential, E_{NPO} (eV)	41	Estimation
Optical phonon frequency, ω_{LO} $(rad \cdot s^{-1})$	13.527×10^{13}	[17]
Static dielectric constant, ε_s	15.3	[21]
High frequency dielectric constant, ε_∞	8.4	[21]
Acoustic deformation potential, E_{AC} (eV)	7.1	[21, 22]
Sound velocity, c $(m \cdot s^{-1})$	6.24×10^3	[9, 19]
Piezoelectric tensor component, e_{14} $(C \cdot m^{-2})$	0.5	[21]

The next parameter which is unknown for InN is the optical deformation potential $E_{\rm NPO}$ (d_0 – for conduction band electrons). To estimate its value let's use the fact that for conduction band of the zinc blende InP, InAs, InSb it is equal 35.6, 33.3 and 26.8 eV respectively [20]. Therefore for gallium nitride the value $d_0 = 41$ eV was choose.

Comparison of theory and experiment

A comparison of the theoretical temperature dependences of the electron mobility $\mu_n(T)$ was made with the experimental data presented in [10] (electron concentration $\sim 6 \times 10^{17} cm^{-3}$). During the calculations it was assumed that in all the investigated temperature range 4.2 - 560 K the impurity conductivity occurs.The Fermi level was calculated from the charge neutrality equation given by:

$$n = \frac{N_D}{2\exp\left(\frac{F-E_D}{k_B T}\right)+1} - N_A, \qquad (0.9)$$

where the values of donors, acceptors concentration and donor ionization energy were defined in [10]: $N_D = 9 \times 10^{17} cm^{-3}$; $N_A = 5.3 \times 10^{17} cm^{-3}$; $E_D = 0.09$ eV.

The theoretical $\mu_n(T)$ curves are presented in Fig. 1. It is seen that the theoretical curves well agree with experimental data in all investigated temperature range. To estimate the role of the different scattering mechanisms in Fig. 2 the dotted lines represent the appropriate dependences. The solid line represents the dependence calculated on the base of short-range scattering models in the framework of the exact solution of the Boltzmann equation. The obtained electron scattering parameters for different scattering modes are listed in Table 2.

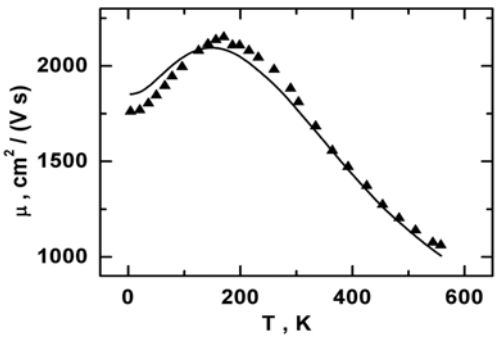

Fig.1. The temperature dependence of electron mobility in InN crystal

Table 2. Parameters γ for different scattering modes

Sample	γ_{PO}	γ_{PZ}	γ_{II}	$\gamma_{SS} N_{SS} \times 10^{-14} cm^{-3}$
1	0.75	0.30	0.22	11.5

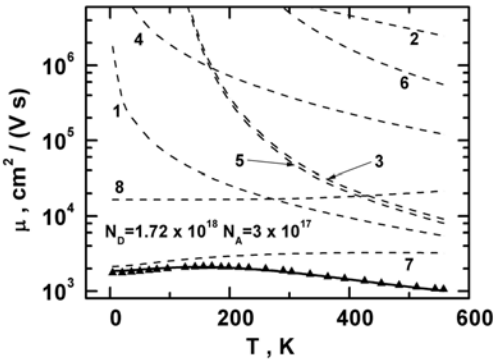

Fig.2. The contribution of different scattering modes into electron mobility in InN. Solid line – mixed scattering mechanism; 1,2,3,4,5,6,7,8 – AC-, II-, NPO-, PAC-, PO-, POP-, SS-, NI- scattering mechanism respectively

It is seen that the main scattering mechanism in all temperature range is the static strain scattering (curve 7). At T¡300 K rather small but not negligible is neutral impurity scattering (curve 8) the influence of which decreases with temperature. At high temperatures (T¿300 K) the contribution of the polar optical (curve 5), nonpolar optical (curve 3) and acoustic phonon (curve 1) scattering becomes dominant. Other scattering mechanisms such as ionized impurity scattering, piezoacoustic and piezooptic phonon scattering, give negligibly small contributions.

Conclusion

On the base of the short-range principle the electron scattering processes on the various types of crystal defects in wurtzite InN are considered. A good agreement between theory and experiment in all investigated temperature range is established.

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ПРИНЦИП БЛИЗКОДЕЙСТВИЯ В ТЕОРИИ РАССЕЯНИЯ ЭЛЕКТРОНОВ В НИТРИДЕ ИНДИЯ

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Россмотрены процессы россеяния электронов на близкодействующем потенциале, обусловленном взаимодействием с полярными и неполярными оптическими фононами, пьезоэлектрическими и акустическими фононами, статической деформации, нейтральной и заряженной примеси в образцах GaN со структурой вюртцита и концентрацией электронов $\sim 6 \times 10^{17}\,см^{-3}$. Рассчитана температурная зависимость подвижности электронов в интервале $4.2 - 560\,K$.

Ключевые слова: явления переноса, рассеяние носителей заряда, нитрид индия.

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ПРИНЦИП БЛИЗЬКОДІЇ В ТЕОРІЇ РОЗСІЯННЯ ЕЛЕКТРОНІВ В НІТРИДІ ІНДІЮ

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Розглянуто процеси розсіяння електронів на близькодіючому потенціалі, обумовленому взаємодією з полярними та неполярними оптичними фононами, п'єзоелектричними та акустичними фононами, полем статичної деформації, іонізованими та нейтральними домішками в зразку InN зі структурою вюртциту та з концентрацією електронів $\sim 6 \times 10^{17}\,\text{см}^{-3}$. Розраховано температурну залежність рухливості електронів в інтервалі $4.2 - 560\,K$.

Ключові слова: явища переносу, розсіяння носіїв заряду, нітрид індію

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