

HOT ELECTRONS IN WURTZITE INDIUM NITRIDE: A NEW NUMERICAL APPROACH

N.A. Masyukov and A.V. Dmitriev

*Department of Low Temperature Physics and Superconductivity, The Faculty of Physics,
Moscow State University, 1/8, Leninskie gory, 119991, Moscow, Russia
E-mail: masniki@gmail.com
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Abstract

For a long time, the band gap width of around 2 eV has been assumed for wurtzite InN. However, recent experimental and theoretical investigations (see [1]) have provided convincing evidence that the band gap of InN is actually close to 0.7 eV. Thus, the alloy $\text{In}_x\text{Ga}_{1-x}\text{N}$ formed of InN and wideband GaN is promising for the use in optoelectronic applications. The problem of electron transport in the bulk InN was studied in papers [2-6] using the Monte-Carlo approach. However, no comparison with experimental data was presented in these papers.

In our paper a new numerical method for solution of the Boltzmann transport equation (BTE) in the isotropic case is introduced and applied to the hot-electron transport in the non-parabolic one-valley model of n -type InN. Applicability of this model is also discussed. Ionized impurity, polar optical phonon (PO) and acoustical phonon (AP) scattering mechanisms are taken into account in the simulations. According to the experiment of [8], we use in our numerical simulation the lattice temperature $T = 77$ K and the free electron concentration $N = 9 \cdot 10^{18} \text{ cm}^{-3}$ so that the electron gas degenerates, the ionized impurity concentration is equal to N . Numerical results agree well with the experimental data of [8].

The main problem and the physical model

The isotropic space-uniform d.c. case is considered. For the conductivity valley the dispersion relation of electron energy ε with the wave vector $\mathbf{k}$ is given by

$$\frac{\hbar^2 k^2}{2m^*} = \varepsilon(1 + \alpha\varepsilon), \quad (1)$$

where α is the nonparabolicity parameter which depends on the band gap $\alpha = \varepsilon_g^{-1}$.

In the isotropic case BTE is an integro-differential equation

$$\frac{\partial f}{\partial t} = -\frac{e\mathbf{E}}{\hbar} \frac{\partial f}{\partial \mathbf{k}} + \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} \quad (2)$$

with the normalizing condition

$$\sum_{\mathbf{k}} f(\mathbf{k}) = NV. \quad (3)$$

Here $\mathbf{E}$ is the applied electric field, $f(t, \mathbf{k})$ is the electron distribution function, $\mathbf{k}$ is the wave vector, e is the electron charge, V is the crystal volume,

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = \sum_{\mathbf{k}'} \left[W(\mathbf{k}' \rightarrow \mathbf{k}) f(\mathbf{k}') (1 - f(\mathbf{k})) - W(\mathbf{k} \rightarrow \mathbf{k}') f(\mathbf{k}) (1 - f(\mathbf{k}')) \right] \quad (4)$$

is the collision integral, and $W(\mathbf{k} \rightarrow \mathbf{k}')$ is the electron transition rate from the state $\mathbf{k}$ to $\mathbf{k}'$. BTE cannot be linearized in the case of the degenerate electron gas. Thus, in this case one

cannot use the methods based on the collision integral linearization, and the Monte-Carlo based methods become highly computational. It is worth noting that BTE is actually always nonlinear, because $W(\mathbf{k} \rightarrow \mathbf{k}')$ depends on the screening length λ , and λ depends on the distribution function.

Material parameters used in simulations [3-7] are presented in Table 1.

Table 1. Material parameters used in InN.

Quantity	Symbol	Unit	Value		
			Data 1 [7]	Data 2 [5, 6]	Data 3 [3, 4]
Mass density	ρ	g/cm^3	6.81		
Sound velocity	s	cm/s	3.78×10^5		
Static dielectric constant	χ_0		8.4	8.4	6.7
HF dielectric constant	χ_∞		15.3	15.3	9.3
Effective mass	m^*	m_0	0.07	0.11	0.04
Band gap	ε_g	eV	0.8	2.0	0.8
Deformation potential	Ξ	eV	7.1	7.1	3.6
Piezoelectric constant	β	C/m^2	0.375		
OP energy	$\hbar\omega_0$	eV	0.073		
$\Gamma_1 - \Gamma_3$ energy separation	$\Delta_{\Gamma_1 - \Gamma_3}$	eV	1.77		

The transition rates of the scattering mechanisms taken into account in the simulation are presented in Table 2. There $\bar{\chi} = (\chi_\infty^{-1} - \chi_0^{-1})^{-1}$, λ is the screening length, $\mathbf{q} = \pm(\mathbf{k} - \mathbf{k}')$, $\omega(\mathbf{q})$ is the phonon dispersion relation, $\omega(\mathbf{q}) = sq$ for DA and PA, $\omega(\mathbf{q}) = \omega_0$ for PO, $N_q = N_q(\omega(\mathbf{q}), T)$ is the number of phonons with the wave vector $\mathbf{q}$ at the lattice temperature T . The lattice temperature is assumed to be independent from the electron gas temperature T_e . For the phonon scattering mechanisms the upper and the lower signs refer to emission and absorption of a phonon, respectively.

Table 2. Transition rates.

Scattering mechanism	$W(\mathbf{k} \rightarrow \mathbf{k}')$	$ M(\mathbf{k} \rightarrow \mathbf{k}') ^2$	$B(q)$
Ionized impurity (i)	$NV \frac{2\pi}{\hbar} M(\mathbf{k} \rightarrow \mathbf{k}') ^2 \times \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}'))$	$\left(\frac{1}{V} \frac{4\pi e^2}{\chi_0} \frac{1}{q^2 + \lambda^{-2}} \right)^2$	
DA	$\frac{2\pi}{\hbar} M(\mathbf{k} \rightarrow \mathbf{k}') ^2 \left(N_q + \frac{1}{2} \pm \frac{1}{2} \right) \times \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}') \mp \hbar\omega(\mathbf{q}))$	$\frac{1}{V} B(q) \left(\frac{q^2}{q^2 + \lambda^{-2}} \right)^2$	$\frac{\hbar\Xi^2}{2\rho s} q$
PA			$\frac{\hbar(e\beta)^2}{2\rho s} q^{-1}$
PO			$\frac{2\pi e^2}{\chi} \hbar\omega_0 q^{-2}$

In the examined conditions AP-scattering can be treated as an elastic process. Thus, the DA- and PA-scattering mechanisms could be considered as one with the following transition rate

$$W_{\text{AP}}(\mathbf{k} \rightarrow \mathbf{k}') = \frac{1}{V} \frac{2\pi}{\hbar} (B_{\text{DA}}(q) + B_{\text{PA}}(q)) (2N_q + 1) \left(\frac{q^2}{q^2 + \lambda^{-2}} \right)^2 \delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}')). \quad (5)$$

Let us present the collision integral (4) in the following form

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = \left(\frac{\partial f}{\partial t} \right)_i + \left(\frac{\partial f}{\partial t} \right)_{\text{AP}} + \left(\frac{\partial f}{\partial t} \right)_{\text{PO}} \quad (6)$$

and consider each term taking axis symmetry of the distribution function $f(\mathbf{k}) = f(k_{\parallel}, k_{\perp})$ into account. The first term can be represented by the following expression

$$\left(\frac{\partial f}{\partial t} \right)_i = \frac{2\pi}{\hbar} \left(\frac{4\pi e^2}{\chi_0} \right)^2 ND(k) I_{\theta}^i(k_{\parallel}, k_{\perp}) I_{\varphi}^i(k_{\parallel}, k_{\perp}), \quad (7)$$

where the auxiliary functions are introduced

$$D(k) = \frac{1}{4\pi^3} \int dk' k'^2 (\varepsilon(k') - \varepsilon(k)) = \frac{m^* k}{4\pi^3 \hbar^2} \sqrt{1 + \frac{2\alpha \hbar^2 k^2}{m^*}}, \quad (8)$$

$$I_{\theta}^i(k_{\parallel}, k_{\perp}) = \int_{-1}^1 d \cos \theta (f(k \cos \theta, k \sin \theta) - f(k_{\parallel}, k_{\perp})), \quad (9)$$

$$\begin{aligned} I_{\varphi}^i(k_{\parallel}, k_{\perp}) &= \int_0^{2\pi} \frac{d\varphi}{(2k^2 - 2k_{\parallel}k \cos \theta - 2k_{\perp}k \sin \theta \cos \varphi + \lambda^{-2})^2} = \\ &= 2\pi \frac{2k^2 - 2k_{\parallel}k \cos \theta + \lambda^{-2}}{\left((2k^2 - 2k_{\parallel}k \cos \theta + \lambda^{-2})^2 - (2k_{\perp}k \sin \theta)^2 \right)^{3/2}}, \end{aligned} \quad (10)$$

where $k = \sqrt{k_{\parallel}^2 + k_{\perp}^2}$. Thus, the term $(\partial f / \partial t)_i$ contains only one integral.

In the elastic approximation

$$\left(\frac{\partial f}{\partial t} \right)_{\text{AP}} = \frac{2\pi}{\hbar} D(k') I_{\theta}^{\text{AP}}(k_{\parallel}, k_{\perp}) I_{\varphi}^{\text{AP}}(k_{\parallel}, k_{\perp}), \quad (11)$$

where

$$I_{\theta}^{\text{AP}}(k_{\parallel}, k_{\perp}) = \int_{-1}^1 d \cos \theta (f(k' \cos \theta, k' \sin \theta) - f(k_{\parallel}, k_{\perp})), \quad (12)$$

$$I_{\varphi}^{\text{AP}}(k_{\parallel}, k_{\perp}) = \int_0^{2\pi} d\varphi (B_{\text{DA}}(q) + B_{\text{PA}}(q)) (2N_q + 1) \left(\frac{q^2}{q^2 + \lambda^{-2}} \right)^2, \quad (13)$$

$$k' = k, \quad (14)$$

$$q = q(k, \theta, \varphi) = (2k^2 - 2k_{\parallel}k \cos \theta - 2k_{\perp}k \sin \theta \cos \varphi)^{1/2}. \quad (15)$$

The term $(\partial f / \partial t)_{\text{AP}}$ contains a double integral. Next,

$$\left(\frac{\partial f}{\partial t} \right)_{\text{PO}} = \frac{2\pi}{\hbar} \left(\left(\frac{\partial f}{\partial t} \right)_{\text{PO}}^{\text{absorption}} + \left(\frac{\partial f}{\partial t} \right)_{\text{PO}}^{\text{emission}} \right), \quad (16)$$

$$\left(\frac{\partial f}{\partial t} \right)_{\text{PO}}^{\text{absorption, emission}} = D(k_{\pm}') I_{\theta}^{\text{PO}\pm}(k_{\parallel}, k_{\perp}) I_{\varphi}^{\text{PO}}(k_{\parallel}, k_{\perp}), \quad (17)$$

$$I_{\theta}^{\text{PO}+}(k_{\parallel}, k_{\perp}) = \int_{-1}^1 d \cos \theta \left[f(k'_{+} \cos \theta, k'_{+} \sin \theta) (1 - f(k_{\parallel}, k_{\perp})) (N_0 + 1) - \right. \\ \left. - f(k_{\parallel}, k_{\perp}) (1 - f(k'_{+} \cos \theta, k'_{+} \sin \theta)) N_0 \right], \quad (18)$$

$$I_{\theta}^{\text{PO}-}(k_{\parallel}, k_{\perp}) = \int_{-1}^1 d \cos \theta \left[f(k'_{-} \cos \theta, k'_{-} \sin \theta) (1 - f(k_{\parallel}, k_{\perp})) N_0 - \right. \\ \left. - f(k_{\parallel}, k_{\perp}) (1 - f(k'_{-} \cos \theta, k'_{-} \sin \theta)) (N_0 + 1) \right], \quad (19)$$

$$I_{\varphi}^{\text{PO}}(k_{\parallel}, k_{\perp}) = \int_0^{2\pi} d\varphi B_{\text{PO}}(q) \left(\frac{q^2}{q^2 + \lambda^{-2}} \right)^2, \quad (20)$$

where $q_{\pm} = q_{\pm}(k, k'_{\pm}, \theta, \varphi) = (2k^2 - 2k_{\parallel}k'_{\pm} \cos \theta - 2k_{\perp}k'_{\pm} \sin \theta \cos \varphi)^{1/2}$, and $k'_{\pm}$ should be determined from the relation $\varepsilon(k'_{\pm}) = \varepsilon(k) \pm \hbar\omega_0$, N_0 is the number of PO in the crystal. The term $(\partial f / \partial t)_{\text{PO}}$ contains a double integral.

It is worth noting that if the AP-scattering is to be treated as an inelastic process then the AP-terms in the collision integral contain triple integrals and our problem becomes highly computational. But the following quasi-elastic approximation could be made. Taking $q = q(k, \theta, \varphi)$ in elastic approximation according to (15) and substituting the following expression for k'

$$k' \rightarrow k'_{\pm}(k, \theta, \varphi) = k \pm \left(\frac{\partial \varepsilon}{\partial k} \right)^{-1} \hbar s q(k, \theta, \varphi), \quad (21)$$

one can proceed in full analogy to the PO-scattering considered above and obtain double integral in the AP-term.

The screening length λ depends on the distribution function

$$\lambda(f(\mathbf{k})) = \left(\frac{4\pi e^2}{\chi_0} \left| \sum_{\mathbf{k}} \frac{\partial f(\mathbf{k})}{\partial \varepsilon(\mathbf{k})} \right| \right)^{-1/2} = \left(\frac{4\pi e^2}{\chi_0} 4\pi^3 \left| \sum_{\mathbf{k}} \frac{\partial f(\mathbf{k})}{\partial \mathbf{k}} \frac{D(k)}{k^2} \frac{\mathbf{k}}{k} \right| \right)^{-1/2}. \quad (22)$$

Note that (22) gives Debye and Thomas-Fermi screening length in the cases of nondegenerate and degenerate statistics, respectively.

The numerical method

We consider isotropic space-uniform case. The iterative method introduced assumes only smoothness of the distribution function. An iteration step is organized in the following way. We approximate the distribution function using a bicubic interpolation from a sparse grid $k_{\parallel}^i = -k_{\text{max}} + (i + 1/2)\Delta_0$, $k_{\perp}^j = j\Delta_0$, $i = 0, 1, \dots, 2k_{\text{max}}/\Delta_0 - 1$, $j = 0, 1, \dots, k_{\text{max}}/\Delta_0$ in $(k_{\parallel}, k_{\perp})$ -space. By substituting interpolated values of the distribution function $f^n(k_{\parallel}, k_{\perp})$ into the collision integral considered above (6)-(20) one calculates its values $(\partial f / \partial t)_{\text{coll}}^{ij}$ for the grid nodes only, but the integrating could be performed on a fine mesh. Then, giving the time a small increment Δt , we obtain the following approximation to the distribution function at the grid nodes directly from BTE

$$f_{ij}^{n+1} = f^n \left(k_{\parallel} - \frac{eE}{\hbar} \Delta t, k_{\perp} \right) + \Delta t \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}^{ij}. \quad (23)$$

According to (22), one calculates the screening length $\lambda^{n+1} = \lambda(f^n(\mathbf{k}))$ and put it in (23). Thus, the problem under consideration is self-contained and has no fitting parameters. The iterations are repeated until the steady state is approached.

As a first approximation $f_{ij}^0 = f^0(k_{\parallel}^i, k_{\perp}^j)$ we use the Fermi equilibrium distribution function with the lattice temperature.

For the considered electric fields E we used $k_{\max} \approx 10^7 \text{ cm}^{-1}$, so that the distribution function was localized in the simulation area (Fig. 1). The one-valley model is applicable, because $\varepsilon(k_{\max}) = 0.34 \text{ eV} \ll \Delta_{\Gamma_1-\Gamma_3}$.

The convergence of the method is verified in following numerical tests (Fig. 2). For fixed $E = 10 \text{ kV/cm}$, $T = 77 \text{ K}$ and the material parameters “data 2” (Table 1) different time increments Δt and grid sizes are examined. We assume $\Delta t = 10^{-15} \text{ s}$ and the grid size 15×30 to be optimal. In this case simulation time $t_{\text{sim}} = 10^{-12} \text{ s}$ corresponds to roughly 5 minutes of CPU time (Intel Core 2 Duo T72500, 2GHz, one core was used). By taking as the initial approximation the non-equilibrium (n/eq) distribution function

$$F_{\text{n/eq}}(\mathbf{k}) = \frac{1}{\exp\left(\frac{\varepsilon(\mathbf{k}) - \mu}{T}\right) + 1} + \cos(10^{-6} k) \quad (24)$$

one could see that the result is independent of the initial approximation (Fig. 2). Testing the AP-scattering in quasi-elastic approximation (q/el) described above one obtains the same result (Fig. 2). Thus, the elastic approximation can be used.

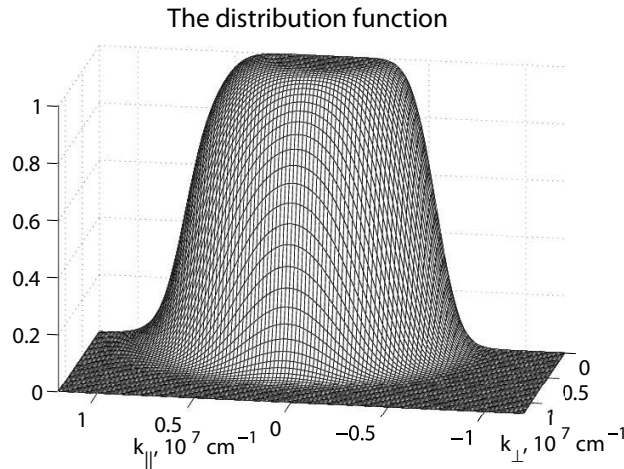


Fig. 1. The calculated distribution function, grid 15×30 , “data 2”, $t_{\text{sim}} = 5 \times 10^{-13} \text{ s}$, $\Delta t = 10^{-15} \text{ s}$, $T = 77 \text{ K}$, $E = 15 \text{ kV/cm}$.

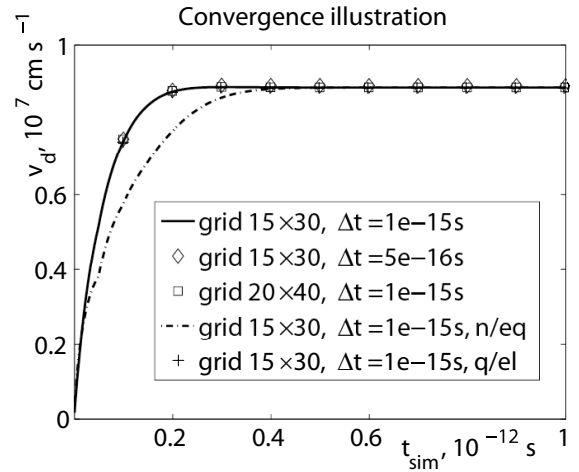


Fig. 2. The illustration of the convergence, “data 2”, $E = 10 \text{ kV/cm}$, $T = 77 \text{ K}$.

The main results

Different sets of material parameters (Table 1) are used in the simulation to obtain the field dependence of the drift velocity. The results are compared with the experimental data of [8]. In the considered conditions “data 2” set fits well the experimental curve (Fig. 3, left panel). One should remark that “data 2” set involves the “old” (before works [1] were published) band parameters obtained just for heavily doped samples with the electron concentration close to the value $N = 9 \times 10^{18} \text{ cm}^{-3}$ used in our calculations.

The right graph in Fig. 3 illustrates the calculated field dependence of the drift velocity for “data 2” and different lattice temperatures.

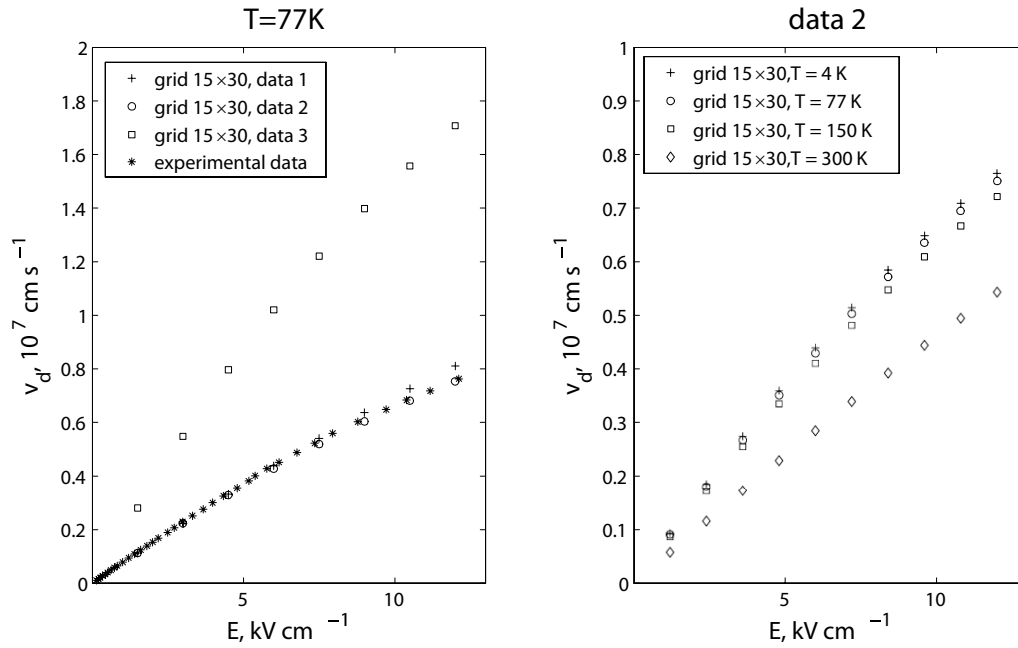


Fig. 3. Field dependence of the drift velocity, grid 15×30 , $t_{\text{sim}} = 5 \times 10^{-13} \text{ s}$, $\Delta t = 10^{-15} \text{ s}$. Left panel: Calculation results for different sets of material parameters are compared with the experimental data, $T = 77 \text{ K}$. Right panel: Field dependence of the drift velocity for different temperatures is obtained using material parameters “data 2”.

Conclusions

A new numerical method for solution of the Boltzmann transport equation in the isotropic space-uniform case is introduced. The method is self-contained, flexible and could be used in the wide range of conditions. Simultaneously it is quite computational effective. We regard it as a powerful tool for investigating the electron system of polar semiconductors.

The method is applied to InN. The optimal numerical method parameters are determined. Different sets of the material parameters are examined and the corresponding results are compared with the experimental data. Best agreement is obtained with the material parameters “data 2” set. The field dependence of the drift velocity is predicted for the different temperatures.

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