# Non-Linear Electron Mobility in n-Doped III-Nitrides

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A theoretical study of the mobility of n-doped III-Nitrides in wurtzite phase is reported. We have determined the nonequilibrium thermodynamic state of the bulk n-InN, n-GaN, and n-AlN systems - driven far away from equilibrium by a strong electric field - in the steady state, which follows after a very fast transient. For this we solve the set of coupled nonlinear integro-differential equations of evolution of the nonequilibrium thermodynamic variables, for the three materials, to obtain their steady state values. The dependence of the mobility (which depends on the nonequilibrium thermodynamic state of the sample) on the electric field strength and the concentration (of electrons and impurities) is derived, which decreases with the increase of the electric field strength and the concentration of carriers, evidencing the influence of the nonlinear transport involved.

Keywords: III-Nitrides; Mobility; Nonlinear transport

The so-called nitride materials, like GaN, InN, and AlN, are presently the object of intense research as a result of the large interest associated with application for blue/UV light emitting diodes and diode lasers [1-4]. We contribute here a theoretical study consisting in an analysis of the electron mobility in n-doped samples of III-Nitrides – which are large direct-gap strong-polar semiconductors – at moderate to high electric fields. Basically we study transport phenomena which develop in the nonequilibrium thermodynamic state of the resulting "hot plasma" consisting of mobile electrons moving in, and interacting with, the lattice and with impurities, and warmed up by the presence of the electric field.

We study transport phenomena which develop in n-doped samples of GaN, InN, and AlN, that is the change in the average energy of electrons and phonons, and the electronic current that ensues as a result of the presence of the electric field. This kind of studies are in general pursued with the help of Monte Carlo-like simulations; instead, we here resort to a powerful, concise, and soundly based kinetic theory for far-from equilibrium systems [5]. It is the one based on a nonequilibrium statistical ensemble formalism [6-8], the so-called NESEF for short, which provides an elegant, practical, and physically clear picture for describing irreversible processes, as for example in far-away-from-equilibrium semiconductors which is the case considered here. Moreover, we use the effective-mass approximation and therefore parabolic bands; this implies that in explicit applications it needs to be taken into account that there exists an upper limiting value for the electric field strength, corresponding to values below which intervalley scattering can be neglected. In this work we consider the contributions to the mobility arising out of the different channels of electron scattering, namely, the polar-optic, deformation, and piezoelectric interactions with the phonons, and the interaction with impurities. For numerical calculations we used the same characteristic parameters indicated in Ref. [9].

Proceeding with the calculations we obtain the corresponding set of equations of evolution, namely

$$\frac{d}{dt}E_e(t) = -\frac{e\mathbf{F}}{m_e^*}\cdot\mathbf{P}_e(t) + J_{E_e}(t)\ , \tag{1}$$

$$\frac{d}{dt}\mathbf{P}_e(t) = -nVe\mathbf{F} + \mathbf{J}_{\mathbf{P}_e,ph}(t) + \mathbf{J}_{\mathbf{P}_e,imp}(t)\ , \tag{2}$$

$$\frac{d}{dt}E_{LO}(t) = J_{E_{LO}}(t) + J_{LO,an}(t)\ , \tag{3}$$

$$\frac{d}{dt}E_{AC}(t) = J_{E_{AC}}(t) - J_{LO,an}(t) + J_{AC,dif}(t)\ , \tag{4}$$

where $E_e$ is the electrons' energy and $\mathbf{P}_e$ their linear momentum; $E_{LO}$ the energy of the LO phonons, which strongly interact with the carriers via Fröhlich potential in these strong-polar semiconductors; $E_{AC}$ is the energy of the acoustic phonons, which play a role of a thermal bath; and $\mathbf{F}$ stands for the constant electric field in the $x$-direction. We call the attention to the fact that the nonequilibrium macrostate of the system can be alternatively, and completely, characterized by a set of nonequilibrium equations of state [7,8], in the present case the quasitemperature $T^*$, the drift velocity $\mathbf{v}$, and the quasi-chemical potential $\mu^*$ of the electrons, and the quasitemperature of the optical and acoustic phonons, $T^*_{LO}$ and $T^*_{AC}$ [12].

Let us analyze these equations term by term. In Eq. (1) the first term on the right accounts for the rate of energy transferred from the electric field to the carriers, and the second term accounts for the transfer of the excess energy of the carriers – received in the first term – to the phonons. In the equation of evolution for the electron energy, Eq. (1), we have omitted the influence of scattering by impurities, which at room temperature is negligible as compared with the contribution arising out of the interaction with the phonons. In Eq. (2) the first term on the right is the driving force generated by the presence of the electric field. The second term is the rate of momentum transfer due to interaction with the phonons.

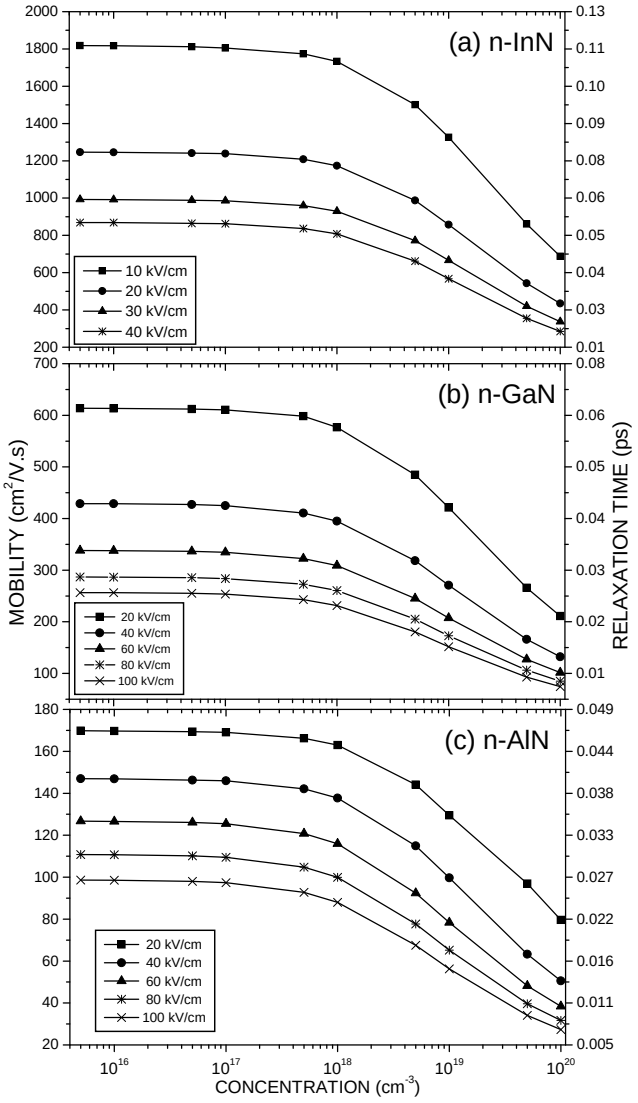


FIG. 1: Dependence of the carrier mobility in the steady state on the carrier concentration for several values of the electric field strength.

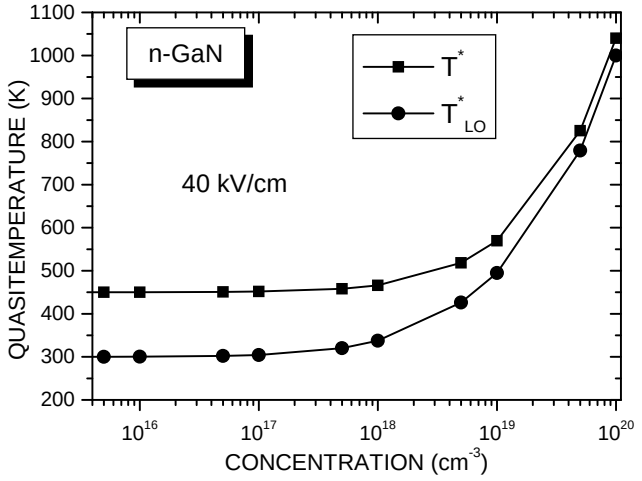


FIG. 2: The quasitemperatures (nonequilibrium temperatures) of electrons and LO phonons for the case of GaN and a field of 40 kV/cm.

The last contribution on the right of Eq. (2) is the collision integral accounting for scattering by impurities: we write it in a relaxation-time approximation using for the relaxation time the expression of Brooks and Herring as applied by Ridley [10], but adapted to the present case of nonequilibrium conditions, meaning that in it the temperature is substituted by the (nonequilibrium) quasitemperature $T^*$ (see Ref. [11]).

In Eq. (3) and Eq. (4) the first term on the right describes the rate of change of the energy of the phonons due to interaction with the electrons. More precisely they account for the gain of the energy transferred to then from the hot carriers and then the sum of contributions $J_{E_{LO}}$ and $J_{E_{AC}}$ is equal to the last in Eq. (1), with change of sign. The second term in Eq. (3) accounts for the rate of transfer of energy from the optical phonons to the acoustic ones via anharmonic interaction. The contribution $J_{LO,an}$ is the same but with different sign in Eq. (3) and (4). Finally, the diffusion of heat from the AC phonons to the reservoir is account for in the last term in Eq. (4). The detailed expressions for the collision operators are given in Ref. [12]. Proceeding to the solution of the coupled set of nonlinear integro-differential equations (it can be noticed that after a fast transient (ps scale) there follows a steady state) namely Eqs. (1) to (4), using the parameters of Table I of Ref. [9], and a reservoir temperature of 300 K, we can derive the mobility $\mathcal{M}$ of the carriers, as given by

$$\mathcal{M} = \frac{|\mathbf{v}_e|}{|\mathbf{F}|}, \tag{5}$$

with the drift velocity $\mathbf{v}_e$ related to linear momentum per electron by $\mathbf{P}_e = nm_e^*\mathbf{v}_e$. In the case of these semiconductors (GaN, InN, and AlN) the main contribution comes from the polar-optic interaction in these strongly polar semiconductors [13].

In Fig. 1(a-c) is shown the mobility in the steady state in terms of the concentration, with $n = \mathcal{N}_i$, for different values of the electric field strength. It can be noticed that the larger mobility corresponds to InN, which can be ascribed to the electrons having a smaller effective mass in InN than in GaN and AlN. The mobility is proportional to the relaxation time, which is composed of the contributions due to scattering by phonons and by impurities, but the latter is orders of magnitude smaller than the former, and then the mobility is very approximately proportional to the momentum relaxation time whose values are indicated on the right-ordinate in the figure. It depends on the macrostate of the system, that is, on the quasi-temperature $T^*$ and drift velocity, as well as the concentration of carriers, and the quasitemperature of LO phonons, $T^*_{LO}$.

Inspection of Fig. 1 tells us that at carrier concentrations smaller than roughly $5 \times 10^{17} cm^{-3}$ the mobility, and also the momentum relaxation time, are nearly concentration independent. For $n$ larger than this value mobility and relaxation time keep decreasing with increasing concentration (it can be no-

ticed that for $n \gtrsim 5 \times 10^{17} cm^{-3}$ there follows an approximate fractional power law, i.e. $\mathcal{M}$ (or $\tau_P$) depends one $n$ as $An^{\nu}$. This is the result of the influence of the variation of the quasitemperatures of electrons and of LO phonons, shown in Fig. 2 for GaN and a field of 40 kV/cm: for all other field intensities and the other two materials the behavior is quite analogous. For concentration larger than, roughly, $5 \times 10^{17} cm^{-3}$ these quasitemperatures – that are nearly constant for concentrations lower than this value – increase with concentration. This indicates that in fact one should expect a momentum relaxation time diminishing with the concentration as a result of the increase of the effectiveness of the collisional processes.

In conclusion, we have presented a study on the transport characteristics (focusing on the dependency of the electron mobility with the electric field and concentration of electrons and impurities) of wurtzite GaN, AlN, and InN using a nonlinear quantum transport theory derived from the nonequilibrium statistical ensemble formalism NESEF.


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