Hole mobility in zincblende c–GaN

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We consider the nonequilibrium thermodynamic state of carriers in III-nitrides, and calculate the mobility of holes in cubic GaN layers under electric fields of low intensity. The contribution of different scattering mechanisms to the mobility is analyzed, and the relevance of each one is characterized. Satisfactory agreement with recently published experimental data is obtained. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1690865]

I. INTRODUCTION

After the successful development of III-nitrides-based lasers, considerable effort is being centered on taking advantage of their thermal stability, high-breakdown voltage, and transport characteristics, for the implementation of high-power and high-temperature electronics, principally in the microwave power range of electronic applications.[1–3] Seeking device optimization, a key aspect is the search to increase the carriers' mobility, which can be pursued through the improvement of the growth techniques, with, e.g., reduction of dislocations and point defects, dimensional reduction (going from bulk to two-dimensional heterostructure-based devices), and choice of the crystalline phase, once III-nitrides in the zincblende (cubic) phase have better electronic transport properties than the hexagonal (wurtzite) phase, in either the steady state[4] or the transient regime.[5,6]

In the last few years, a marked increase in the electron mobility, $\mathcal{M}_c$, in bulk wurtzite GaN films was obtained, with presently recorded values of about 1200 cm^2/Vs at 300 K, and 7300 cm^2/Vs at 77 K in samples with carrier densities of the order of 10^{18} cm^{-3}.[7–9] On the other hand, due to difficulties in the growing processes, there exist scarce measurements of mobility in bulk zincblende films, but mobility values of about 530 cm^2/Vs at 300 K and 10000 cm^2/Vs at 77 K have been obtained in samples with carrier densities of the order of 10^{18} cm^{-3}.[10–12] A recent two-dimensional Monte Carlo simulation indicating that a 50% gain in performance can be obtained for a zincblende–GaN MESFET as compared with one based in wurtzite–GaN,[13] and the fact that good improvements have been attained on the growth techniques of zincblende GaN,[14] suggests that the zincblende family of these materials may provide technological advantages. In the theoretical analysis of the experimental results, generally based on the Boltzmann-equation formalism and with agreement varying from broad to very good,[15–18] one or more open parameters are usually considered to take into account effects like degenerate layers, carrier compensation, dislocations, etc.

In this work, we perform a parameter-free calculation of the hole mobility in zincblende GaN within the framework of the nonequilibrium statistical ensemble formalism.[19,20] The contribution of different scattering mechanisms to the hole mobility is analyzed, and the relevance of each one is characterized. The results we obtain compare well with recently published experimental data.[12]

II. MOBILITY OF HOLES IN CUBIC GAN

Let us analyze the experimental measurement reported by Fernandez *et al.*[12] Their sample consists of intrinsic cubic GaN (c–GaN) MBE-grown epitaxial layers 0.8 μm thick. Hall measurements at 0.5 T magnetic field were performed to obtain hole concentrations and mobilities in the temperature range 10–350 K. Due to the presence of an intrinsic acceptor level, the background hole concentration changed from $p = 3.7\times10^{13}$ cm^{-3} at 100 K to $p = 2.0\times10^{16}$ cm^{-3} at 350 K, and an acceptor concentration $N_A = 4\times10^{18}$ cm^{-3} was estimated for the nominally undoped sample. The electric field applied to the c–GaN MBE-grown epitaxial layers is weak, and the hole system is in the condition corresponding to the lower part of the ohmic region. Hence, under such weak excitation, in regards to the nonequilibruim thermodynamic state of the system, we can consider that $T_h^* \simeq T_{LO}^* \simeq T_{TO}^* \simeq T_{AC}^* \simeq T_0 \simeq 300$ K, which concerns the quasitemperatures of holes, optical longitudinal LO, optical transversal TO, and acoustic AC phonons, and bath temperature, respectively. In respect to the concentration n_h of holes, we recall that the impurity concentration N_A is roughly 4×10^{18} cm^{-3}, and therefore n_h is smaller than this value (i.e., it is the concentration of the carriers freed in thermal ioniza-

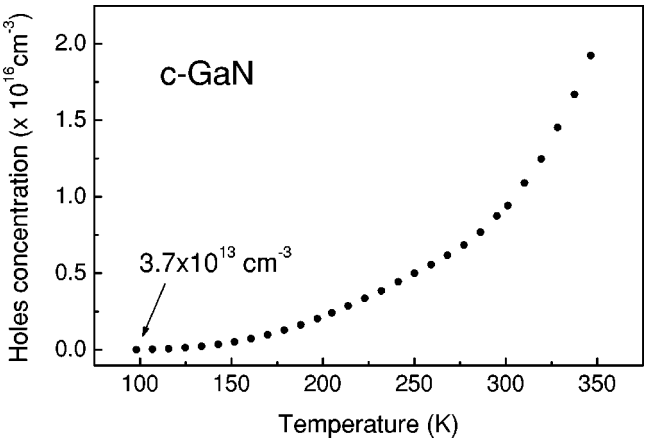

FIG. 1. The concentration of holes in terms of the lattice temperature in c–GaN in the experimental conditions of Ref. 12.

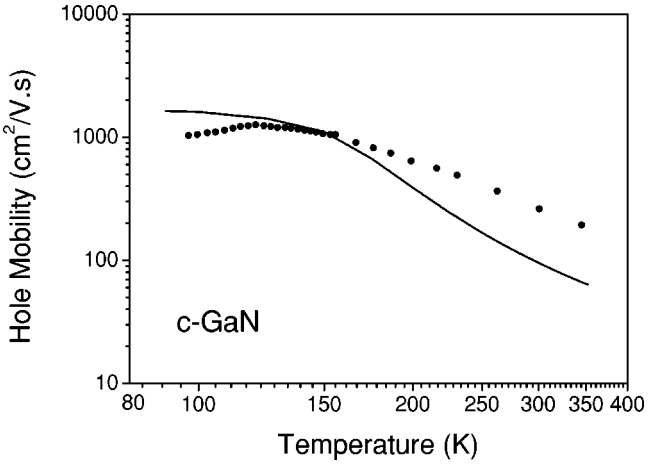

FIG. 2. Temperature dependence of the mobility in c–GaN in the conditions of the experiment of Ref. 12. Full line is the theoreticaly calculated mobility; dots are experimental data from Ref. 12.

tion of the impurity states), the whole ionization occurring at the Mott transition point, which corresponds approximately to a temperature of 1930 K.[21]

The density of mobile holes is determined from the experiment, and shown in Fig. 1. Notice the smooth increase at low temperatures, say, up to 260 K, followed by an exponential growth for temperatures above 260 K, satisfying an Arrehnius-type law characterized by an excitation energy, E_A, of approximately 166 meV. Solving nonlinear transport equations[22,23] for the range of temperatures in the interval 80–350 K, the above given concentration of impurities, the values of the holes' concentration as given by Fig. 1, and the c–GaN parameters as given in Table I, we obtain, in the limit of weak fields (lower part of the ohmic region of the conductivity), the mobility as shown by the full line in Fig. 2, without using any adjustment parameter.

In Fig. 2, a good qualitative and semiquantitative agreement between the theoretical and experimental results can be seen. The differences that can be noticed at the lower and the higher temperatures can be ascribed to indeterminacies in the theoretical calculation due to: (i) the inaccuracy existing so far concerning the value of the hole effective mass;[24,25] (ii) at low temperatures, the inaccuracy in the value of the density of impurities (the corresponding scattering operator is sensitive to it; it can be shown that if instead of the reported estimated value of $4\times10^{18}\,\mathrm{cm}^{-3}$ the value of $6\times10^{18}\,\mathrm{cm}^{-3}$ is used, the agreement becomes better); (iii) at high temperatures, there is a predominance of the scattering due to Fröhlich interaction, which in the calculations has been used in the form of a bare Fröhlich potential, but at the involved holes' concentrations, screening effects may become relevant, and then the resulting mobility would increase, leading to a better agreement with the experimental results (we have verified this in a rough modeling); (iv) finally, we have assumed the Hall scattering factor $r_H=1$ in the expression $\mu_H=r_H\mathcal{M}_c$, where μ_H is the experimental Hall data mobility, when comparing the theoretical result with the experimental data. If the weak temperature dependence of the Hall factor is considered (a variation of the order of 10%), a better agreement can be obtained since r_H can be considerably higher than 1 at low temperature, but very close to 1 at high temperature.[26]

A detailed analysis of the theoretical results (see Fig. 3) shows that at low temperatures, scattering by impurities is the leading mechanism determining the mobility (as expected, once this is the domain of the so-called residual resistivity[27]). For intermediate to high temperatures (roughly above 200 K in Fig. 3) the leading mechanism determining the mobility is the one due to scattering by phonons; but, out of all the possibilities, namely, deformation potential, piezoelectric, and polar interaction, the latter—i.e., Fröhlich potential involving the LO phonons—provides in large the main contribution (to be expected in these strong polar semicon-

TABLE I. Parameters of the c–GaN used in the numerical solution of the transport equations.

Hole effective mass (m_0)	0.86	c–GaN lattice constant (Å)	4.5
LO-phonon energy (meV)	92	Optical dielectric constant ϵ_∞	5.35
Density (g/cm^3)	6.09	Static dielectric constant ϵ_0	9.5
Sound velocity (cm/s)	4.4	Piezoelectric constant (C/m^2)	0.56
Band gap energy (eV)	3.4	Acoustic def. potential E_{1h} (eV)	4.02

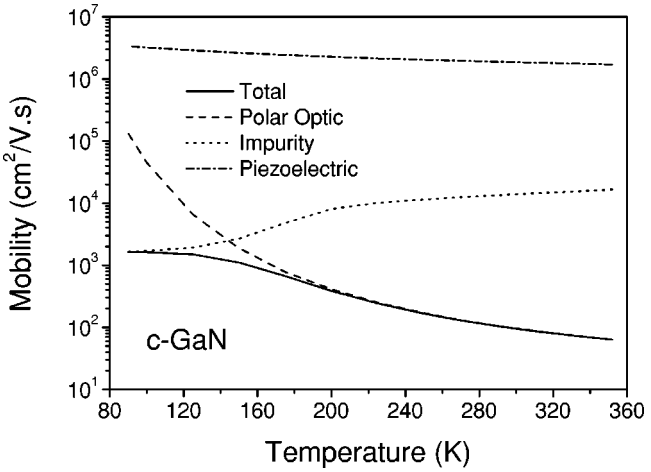

FIG. 3. Contribution to the mobility from the different scattering mechanisms [see Eq. (1)].

ductors). We call attention to the fact that the mobility follows a Mathiessen-type rule, i.e., the reciprocal of the total mobility is the sum of the reciprocals of the contributions associated with the different scattering mechanisms, namely

$$\frac{1}{\mathcal{M}_c} = \frac{1}{\mathcal{M}_{po}} + \frac{1}{\mathcal{M}_{imp}} + \frac{1}{\mathcal{M}_{pz}} + \frac{1}{\mathcal{M}_{dp}}, \tag{1}$$

where the indices po, imp, pz, and dp stand for the contributions from polar optical (Fröhlich), impurities, piezoelectric, and deformation potential contributions, respectively.

III. CONCLUDING REMARKS

Despite the continuing improvement on the growth techniques of III-nitrides during the last years, basic data resulting from optical and transport characterization remain highly dependent still on the sample used in the experiments. In general, an improved fitting of Hall mobility data, for example, is attained when fine details of the samples—like the existence of interfacial layers with a high density of dislocations, which give rise to an n-type charged region—are taken into account by theoretical models, as in the two-layer model sample description.[8,26] This explain why records on the carriers' Hall mobility are being reported frequently, while the basic mechanisms allowing a deep understanding are still a point of debate, in either doped[8,15–18,26] or undoped GaN samples.[28,29]

In this work, we have presented numerical solutions of transport equations based on the nonequilibrium statistical ensemble formalism for holes in c–GaN. We showed that the dependence of their mobility on the lattice temperature (at low fields) may change an order of magnitude when going from low temperatures (scattering by impurities predominates) to, say, room temperatures (when scattering by LO phonons via Fröhlich potential predominates). We have learned that the scattering by impurities is dependent on the density of impurities, and the scattering by polar LO phonons is sensitive to the density of mobile carriers and also to the temperature, in that they determine the screening parameter in Fröhlich potential. Evidently, going over conditions of not too low field intensities, the mobility—as already noticed in the first part of this work—becomes dependent on the whole characterization of the nonequilibrium thermodynamic state of the system.

It can be noticed that the theoretical results we have derived compare well with the experimental data of Fernandez *et al.*,[12] without using any adjustable parameter. This means that we have probably retained the most important features of the Hall mobility problem of holes in c–GaN under a low electric field, while indicating factors like the absence of a precise knowledge of the hole's effective mass, the inaccuracy in the determination of the impurities' density, influence of screening effects, and the temperature dependence of the Hall scattering, as necessary for an improved description. Our results are stimulating in the sense to encourage the search for new data on carriers' mobility in bulk III-nitrides to be explained within the framework of the nonequilibrium statistical thermodynamics, and the possibility in the near future to investigate the role of the scattering by dislocations on the mobility of III-nitrides within the scheme presented here.

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