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Electron mobilities, Hall factors, and scattering processes of *n*-type GaN epilayers studied by infrared reflection and Hall measurements

Y. Fu and M. Willander
Physical Electronics and Photonics, Microtechnology Centre at Chalmers, Department of Microelectronics and Nanoscience, Chalmers University of Technology, Fysikgränd 3, 412 96 Göteborg, Sweden

Z.-F. Li and W. Lu
National Laboratory for Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, 500 Yu-Tian Road, Shanghai 200083, China

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We have studied the drift and Hall mobilities of electrons in metal-organic chemical-vapor-deposited wurtzite GaN thin films on sapphire substrate by infrared (IR) reflection and Hall measurements. By analyzing the Hall factor (the ratio between the drift mobility obtained from IR reflection spectra and the Hall mobility from the Hall measurements), it has been concluded that the electron mobility in GaN epilayer is determined by the ionized impurity when the electron concentration is low. At a high carrier concentration of 3.2×10^{18} cm^{-3}, electronic states of more than 70 meV become populated taking into account the thermal excitation, so that the optical-phonon-scattering process becomes activated (the optical-phonon energy is 69.43 meV obtained from IR reflection measurements). Thus, in highly doped wurtzite GaN epilayers, ionized-impurity- and optical-phonon-scattering processes jointly determine the carrier transport properties.

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GaN-based III-V semiconductors have been under intensive investigation for their potential micro optoelectronics applications.[1] In this work, we report the theoretical analysis of the IR reflection spectrum and Hall measurements about electron concentrations and mobilities in epitaxial GaN thin films in wurtzite structure on sapphire substrates. The *c* axis of the wurtzite structure is along the sample growth direction. The four samples under investigation have different film thicknesses and doping levels (see Table I). IR reflection spectra were measured using Nicolet 200SXV and Bruker IFS-113v Fourier-transform infrared spectrometers. Results of IR reflection spectra are presented in Fig. 1.

To analyze the IR reflection spectra, we consider the wave propagation and reflection in and from a composite lossy medium consisting of the free space ($z\leqslant 0$), the GaN epilayer ($0<z\leqslant d$), and the sapphire substrate ($z>d$), where d is the thickness of the GaN epilayer. The GaN epilayer and the sapphire substrate are characterized by their conductivities, $\sigma_f(\omega)$ and $\sigma_s(\omega)$, and complex permittivities, $\epsilon_f(\omega)$ and $\epsilon_s(\omega)$, where subscript f and s stand for "film" and "substrate." ω is the IR radiation frequency. It is assumed that the material is nonmagnetic so that the permeability is μ_0.

Assuming $\gamma_f^2=\omega^2\mu_0\epsilon_f$, $\gamma_s^2=\omega^2\mu_0\epsilon_s$, and neglecting the reflection from the bottom of the thick substrate, the continuities of the tangential components of the electric and magnetic fields at interface $z=0$ and $z=d$ lead to the expression for the reflectivity R,

$$R=\left|\frac{e^{2\gamma_f d}(n_f+1)(n_f-n_s)-(n_f-1)(n_f+n_s)}{e^{2\gamma_f d}(n_f-1)(n_f-n_s)-(n_f+1)(n_f+n_s)}\right|^2, \tag{1}$$

where $n_i=\sqrt{\epsilon_i/\epsilon_0}$ $(i=f,s)$.

The dielectric constant variation due to damped lattice vibrations is described by

$$\epsilon_{i,\mathrm{TO}}(\omega)=\epsilon_{i,\infty}+\frac{S_i\omega_{i,\mathrm{TO}}^2}{(\omega-\omega_{i,\mathrm{TO}})^2+\gamma_i^2}, \tag{2}$$

where $\omega_{i,\mathrm{TO}}$, S_i, and γ_i are the frequency, oscillator strength, and damping parameter of the transverse optical (TO) phonon in layer i $(i=f,s)$.

In Eq. (1), n_i depends on σ_i and ϵ_i, while σ_i and ϵ_i are all frequency dependent,[2]

$$\sigma_i(\omega)=\frac{\sigma_{i,0}}{1\pm i\omega\tau_{i,\mathrm{d}}}\quad \sigma_{i,0}=\frac{N_ie^2\tau_{i,\mathrm{d}}}{m^*}. \tag{3}$$

$\tau_{i,\mathrm{d}}$ is related to the carrier's drift mobility $\mu_{i,\mathrm{d}}$ by $\tau_{i,\mathrm{d}}=\mu_{i,\mathrm{d}}m_i^*/e$, where m_i^* is the effective mass of carriers and N_i is the carrier concentration.

Now we model the modification of the dielectric constant by free carriers having a carrier density of N and a drift carrier mobility μ_d. Neglecting the effect of the free carriers on the electromagnetic (EM) wave (the carrier concentration in semiconductor is normally rather small to have a significant impact on the EM waves), the Maxwell's equations describing the EM wave are

$$\nabla\cdot\boldsymbol{E}=0,\quad \nabla\cdot\boldsymbol{H}=0,$$

$$\nabla\times\boldsymbol{E}=-\mu_0\frac{d\boldsymbol{H}}{dt},$$

TABLE I. Carrier concentrations (N_{H} and N_{d} in unit of cm^{-3}) and electron mobilities ($\mathrm{cm}^2/\mathrm{V\,s}$) of Si-doped GaN epilayers measured by IR reflection and Hall method.

Sample	Film thickness (μm)	N_{H}	μ_{H}	N_{d}	μ_{d}	γ
1	2.0	5.3×10^{17}	370	8.4×10^{17}	205	1.80
2	2.0	1.5×10^{18}	320	1.6×10^{18}	184	1.74
3	1.8	3.7×10^{18}	234	4.8×10^{18}	134	1.75
4	2.3	1.3×10^{19}	178	1.4×10^{19}	91	1.96

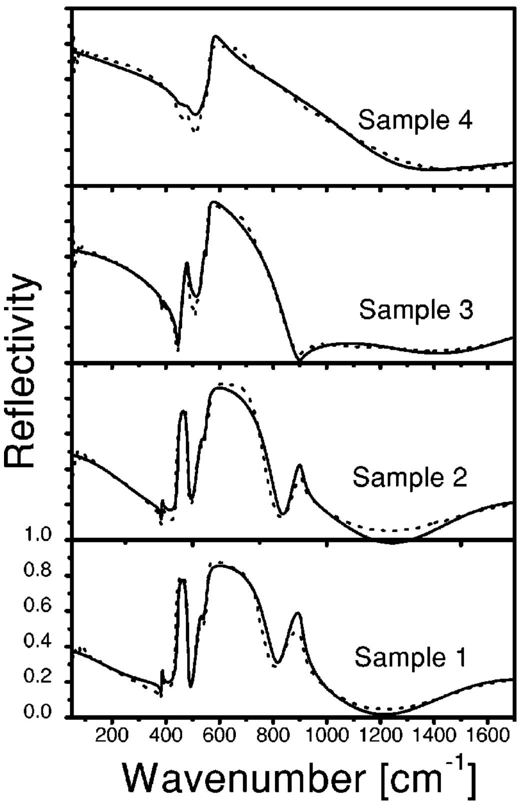

FIG. 1. IR reflection spectra of GaN epilayers on sapphire substrate. Dotted lines, experimental; solid lines, theoretical fitting spectra.

$$\nabla\times\boldsymbol{H}=\sigma_{i,\mathrm{d}}\boldsymbol{E}+\epsilon_{i,\mathrm{TO}}\frac{d\boldsymbol{E}}{dt},\tag{4}$$

where we consider the material as linear, homogeneous, and isotropic. Due to the temporal variation $e^{i\omega t}$ of the EM wave, we obtain the complex permittivity of the medium

$$\epsilon_i(\omega)=\epsilon_{i,\mathrm{TO}}(\omega)\mp\frac{i\sigma_i(\omega)}{\omega},\tag{5}$$

so that

$$-\nabla^2\boldsymbol{E}=\omega^2\mu_0\epsilon_i(\omega)\boldsymbol{E}.\tag{6}$$

Including the effects of TO phonon and free carriers, the total complex permittivity of each layer is

$$\epsilon_i(\omega)=\epsilon_{i,\infty}+\frac{S_i\omega_{i,\mathrm{TO}}^2}{(\omega+i\gamma_i)^2-\omega_{i,\mathrm{TO}}^2}-\frac{\omega_{i,p}^2}{\omega^2\pm i\omega/\tau_{i,\mathrm{d}}},\tag{7}$$

where $\omega_{i,p}^2=N_ie^2/m_i^*$ is known as the plasma frequency.

By taking the electron effective mass m^* to be $0.2m_0$ (Ref. 3) and the high-frequency dielectric constant ϵ_∞ to be 5.35 in GaN,[4] the fitted theoretical reflection spectra are plotted in Fig. 1 as dotted lines, while parameters are listed in Table I. The optical-phonon energy is $\hbar\omega_{\mathrm{TO}}=69.43$ meV in GaN. Also listed are the data from Hall measurements. It has been observed that the values of the free-carrier concentration derived from the two methods agree well with each other, while the mobility values differ.

The Hall and IR measurements measure different activities (thus different components of conductivity tensor) of the same group of electrons (thus the same carrier concentration), see discussions and equations below. And the difference in the mobilities is due to the dependence of the scattering processes in determining the mobilities and the detailed energy band structure of the material under investigation. The ratio between the Hall mobility and the drift mobility is defined as the Hall factor. We have discussed the Hall factor of strained p-type $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ alloy, where the valence-band structure is rather complicated.[5] For the present n-type GaN material, the conduction band is described by an electron effective mass m^*,[3,6] so that we concentrate on the scattering processes of acoustic phonon (ac), optical phonon (op), alloy and ionized-impurity-(I) scattering mechanisms. In general, the related relaxation times τ are[7]

$$\frac{1}{\tau_{\mathrm{ac,alloy}}}\propto\sqrt{E},$$

$$\frac{1}{\tau_{\mathrm{op}}}\propto n_{\mathrm{op}}\sqrt{(E+\hbar\omega_{\mathrm{TO}})}+(n_{\mathrm{op}}+1)\sqrt{(E-\hbar\omega_{\mathrm{TO}})},$$

$$\frac{1}{\tau_{\mathrm{I}}}\propto E^{-3/2}\tag{8}$$

in bulk material, where E is the energy of the electron measured from the conduction-band edge, and

$$n_{\mathrm{op}}=\frac{1}{\exp(\hbar\omega_{\mathrm{TO}}/k_BT)-1}\tag{9}$$

is the phonon occupancy. Here we concentrate on only the GaN layer so that subscript "f" is neglected.

Knowing the relaxation times, it is easy to calculate the drift mobility, Hall mobility, and finally the Hall factor. Assuming steady state, the current density induced by an external electromagnetic field ($\boldsymbol{E}$,$\boldsymbol{B}$) is given by

$$j_i=\sum_j \sigma_{ij}E_j+\sum_{jk}\sigma_{ijk}E_jB_k+\cdots, \tag{10}$$

where $i,j,k=x,y,z,$

$$\sigma_{xx}=-e^2\int \frac{d\boldsymbol{k}}{4\pi^3}\tau v_x^2\frac{\partial f_0}{\partial E},$$

$$\sigma_{xyz}=\frac{e^3}{\hbar}\int \frac{d\boldsymbol{k}}{4\pi^3}\tau^2 v_x\frac{\partial f_0}{\partial E}\left[v_x\frac{\partial v_y}{\partial k_y}-v_y\frac{\partial v_y}{\partial k_x}\right], \tag{11}$$

$$\boldsymbol{v}=\frac{1}{\hbar}\nabla_{\boldsymbol{k}}E(\boldsymbol{k}) \tag{12}$$

is the group velocity. $E=E(\boldsymbol{k})$ is the energy dispersion relation. f_0 is the distribution function when the system is at its equilibrium state.

The drift and Hall mobility are obtained as

$$\mu_{\mathrm{d},xx}=\frac{\sigma_{xx}}{Ne},\quad \mu_{\mathrm{H},xyz}=\frac{\sigma_{xyz}}{Ne\mu_{\mathrm{d},xx}} \tag{13}$$

and the Hall factor γ is defined as

$$\gamma=\frac{\mu_{\mathrm{H},xyz}}{\mu_{\mathrm{d},xx}}, \tag{14}$$

where N is the carrier concentration.

For the conduction band of $E=\hbar^2k^2/2m^*$, it is easy to obtain

$$\gamma=\frac{Nm^*}{\hbar^2}\frac{\displaystyle\int \frac{d\boldsymbol{k}}{4\pi^3}\tau^2k_x^2\frac{\partial f_0}{\partial E}}{\left[\displaystyle\int \frac{d\boldsymbol{k}}{4\pi^3}\tau k_x^2\frac{\partial f_0}{\partial E}\right]^2}, \tag{15}$$

which results in $\gamma=1$ only when the temperature is zero (at this moment, the Fermi distribution function is a step function), or when the doping level is so high that the Fermi distribution function can be well approximated by a step function.

Figure 2 shows the calculated Hall factors of individual scattering processes as functions of the carrier concentration together with measurement data. Assuming the dominance of the ionized-impurity-scattering process in determining the electron-transport properties, a perfect agreement between the theory and the measurement is observed when the carrier concentration is not too high ($<2.0\times10^{18}$ cm^{-3}). However, the dependence of the ionized-impurity-scattering relaxation time on electron energy is weaker than $E^{3/2}$ due to the screening effect.[7,9] By taking $\tau\propto E^{1.25}$, the calculated Hall factor is much reduced. As indicated by Blatt,[9] the power reduction is only significant at low temperature, while the sample temperature at which our measurements were performed is the room temperature. It is thus concluded that the ionized-impurity scattering dominates in our not too highly doped samples.

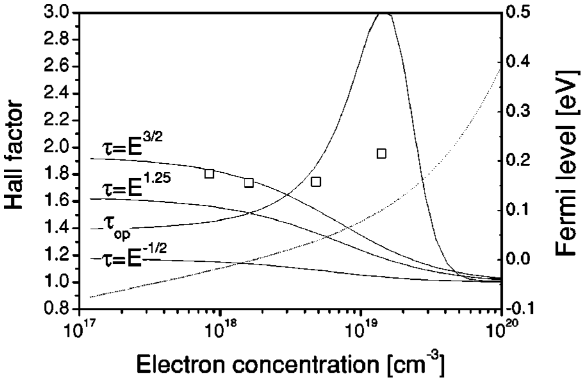

FIG. 2. Hall factors of individual scattering processes as functions of the carrier concentration in the GaN epilayer at room temperature. The dotted line is the Fermi level. □'s are measurement data.

At a high carrier concentration, the Fermi level is much increased. For example, when $n=3.2\times10^{18}$ cm^{-3}, $E_f=21.85$ meV measured from the conduction-band edge. Taking into account the thermal excitation energy of $k_BT=25.85$ meV at room temperature, we see that the electronic states of more than 70 meV above the conduction-band edge become occupied, which activates the optical-phonon-scattering process ($\hbar\omega_{\mathrm{TO}}=69.4$ meV). The physical process is clearly indicated by Fig. 2. It is also noticed that at high donor concentrations, the deionization of ionized donor impurities takes place, resulting in a weaker dependence of the relaxation time on electron energy.[7] By the curve of $\tau=E^{1.25}$ in Fig. 2 it is observed that the deionized impurity and optical-phonon-scattering processes jointly determine the total relaxation time at high carrier concentrations.

In a brief summary, we have measured the IR reflection spectra of GaN epitaxial thin films on sapphire substrates with various doping levels, from which we have extracted fundamental physical parameters of the GaN thin films. By comparing Hall measurements with theoretical calculations of Hall factors including important scattering processes, we have concluded that the electron mobility in the GaN epilayer is dominated by ionized-impurity-scattering process when the carrier concentration in the layer is low. At high carrier concentrations when the electron energy is large enough to activate the optical-phonon emission process, the ionized-impurity- and optical-phonon-scattering processes jointly determine the transport properties of electrons in the wurtzite GaN epilayer.

Moreover, it is known that IR reflection spectrum is not only one of the dominating techniques for studying phonons, but also a contactless and nondestructive method. It has been used very effectively for determining carrier concentration and mobility.[8] The effectiveness of the infrared reflection spectroscopy is further elucidated by the present work.

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