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Temperature dependence of Hall electron density of GaN-based heterostructures*

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The theoretic calculation and analysis of the temperature dependence of Hall electron density of a sample AlGaN/GaN heterostructure has been carried out in the temperature range from 77 to 300K. The densities of the two-dimensional electron gas and the bulk electrons are solved by self-consistent calculation of one-dimensional Schrödinger and Poisson equations at different temperatures, which allow for the variation of energy gap and structure strain, and are used for evaluation of the temperature dependence of Hall electron density. The calculated Hall electron density agrees with the measured one quite well with the appropriate bulk mobility data. Analysis revealed that for the temperature range considered, even in the heterostructures with a small bulk conductance the factors that determine the Hall mobility and electron density could be of different sources, and not just the two-dimensional electron gas as generally supposed.

Keywords: GaN-based heterostructures, Hall electron density, coupled Schrödinger-Poisson equations, temperature dependence

PACC: 7280, 7361, 8105

1. Introduction

The III-group nitrides have been one of the focuses of new semiconductor electronics research, and they are often grown in heterostructures for device applications. The basic properties of these structures are shown in one aspect by temperature-varying Hall data, analyses of which usually aimed at the mobility $\mu_{\rm Hall}$ but not the electron density $Ns_{\rm Hall}$. Hall data reflect the comprehensive effects of different kinds of conductance[1,2] in a heterostructure: say, the two-dimensional one at the heterointerface and the bulk ones elsewhere. This fact caused the difficulties of theoretic analysis of the temperature dependence of $Ns_{\rm Hall}$ along with some other reasons: namely, the origin of the huge density of electrons in nitride heterostructures, the still quite unknown surface conditions, and so on. Generally, the Hall data of a nitride heterosturcture are taken roughly as those of the two-dimensional electron gas (2DEG).

With now quite a few published Hall data [2,3] and the theoretic investigation of electron systems in nitride heterostructures by several one-dimensional Schrödinger–Poisson solvers,[4,5] we can give some preliminary analysis of the temperature dependence of $Ns_{\rm Hall}$ in typical AlGaN/GaN heterostructures.

2. Model

2.1. An insight into Hall data

Various conductance in heterostructures contributes to $\mu_{\rm Hall}$ and $Ns_{\rm Hall}$ as follows:[1]

$$\mu_{\rm Hall} = \frac{Ns_{\rm 2D}\mu_{\rm 2D}^2 + Ns_{\rm 3D}\mu_{\rm 3D}^2}{Ns_{\rm 2D}\mu_{\rm 2D} + Ns_{\rm 3D}\mu_{\rm 3D}}, \quad (1)$$

$$Ns_{\rm Hall} = \frac{(Ns_{\rm 2D}\mu_{\rm 2D} + Ns_{\rm 3D}\mu_{\rm 3D})^2}{Ns_{\rm 2D}\mu_{\rm 2D}^2 + Ns_{\rm 3D}\mu_{\rm 3D}^2}, \quad (2)$$

where the subscript 2D represents the two-dimensional contribution and 3D the bulk. We neglect the bulk electron transport in AlGaN, whose mobility information is scarce, and what we need is to calculate $Ns_{\rm 2D}$ and $Ns_{\rm 3D}$ first, and then to work out $\mu_{\rm 2D}$ and $Ns_{\rm Hall}$ with the measured $\mu_{\rm 3D}$ and $\mu_{\rm Hall}$.

2.2. Electron densities at temperature T

Along the longitudinal direction the quantum

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confinement of the conduction band for electrons can be described by Schrödinger equation,

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}\psi_i(z) + \frac{2m^*}{\hbar^2}(E_i - Ec(z))\psi_i(z) = 0, \quad (3)$$

where m^* is the effective electron mass, E_i and Ψ_i, i=1, 2, 3,..., are 2DEG energy levels and wavefunctions respectively. The conduction band edge satisfies $Ec(z) = -eV(z) + \Delta Ec(z)$, where $V(z)$ is static electric potential, and ΔEc is the conduction band offset at the heterointerface.

From Eq.(3) the 2DEG sheet density Ns_{2D} and spacial distribution $n_{2D}(z)$ are obtained,

$$Ns_{2D} = \sum_i N_i = \sum_i \frac{m^* k_B T}{\pi\hbar^2} \ln\left(1 + \exp\left(\frac{E_f - E_i}{k_B T}\right)\right), \quad (4)$$

$$n_{2D}(z) = \sum_i n_i \psi_i^*(z)\psi_i(z), \quad (5)$$

where k_B is the Boltzmann constant.

The conduction band edge is solved by the Poisson equation,

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}V(z) = -\frac{\rho(z)}{\varepsilon_0\varepsilon(z)},$$

$$\rho(z) = e(N_D^+(z) - n_{2D}(z) - n_{3D}(z)). \quad (6)$$

In Eq.(6) the ionized donor density is

$$N_D^+(z) = N_D/(1 + 2\exp((E_f - E_d)/(k_B T))), \quad (7)$$

and the bulk electron density obeys Fermi distribution,

$$n_{3D}(z) = NcF_{1/2}((E_f - Ec(z))/(k_B T)), \quad (8)$$

$$Ns_{3D} = \int n_{3D}(z)\mathrm{d}z, \quad (9)$$

where Nc is the effective state density, and $F_{1/2}$ is a half-order Fermi integral. The 2DEG and bulk electrons are differentiated by energy, and there is a natural criterion that if the difference between energy levels E_i and E_{i+1} is less than $k_B T$, E_i would be the upper limit of 2DEG subbands and E_{i+1} would be the lower energy limit of bulk electrons E_{lb}.

With the Fermi level E_f chosen as the energy reference, the boundary conditions for Poisson equation are $Ec|_{z=0} = e\phi_s$=1.2(eV) at the AlGaN surface and $F|_{z=z_{max}}$=0 at the bottom of GaN, where F is the electric field.

At the heterointerface there is electric displacement continuity,

$$\varepsilon_1\varepsilon_0 F_1 + \sigma_{pol} = \varepsilon_2\varepsilon_0 F_2, \quad (10)$$

$$\sigma_{pol} = P_{PE1} - P_{PE2} + P_{SP1} - P_{SP2}, \quad (11)$$

where ε is dielectric constant and σ_{pol} is polar sheet charge. The number 1 is for AlGaN and 2 for GaN. P_{PE} is piezoelectric polarization and P_{SP} is spontaneous polarization.

Ns_{2D} and Ns_{3D} at a given temperature can be solved by the self-consistent solution of the above equations. It seems that just the effective state densities of and the energy separation between 2DEG and bulk electrons change with temperature. But that is far from truth.

2.3. Temperature-dependent factors

An evaluation of the possible temperature-dependent factors involved is necessary. For the 2DEG in modulation-doped nitride heterosturctures, there is a representative approximation of its sheet density,

$$Ns_{2D} = \sigma_{pol}/e - (\varepsilon_0\varepsilon_1/de^2)(e\phi_s + e\phi_{ch} - \Delta Ec) + N_D(d - d_i)^2/2d, \quad (12)$$

where $e\phi_s$ and $e\phi_{ch}$ are the surface and channel potential energies respectively. The barrier layer with a thickness d is composed of a doped layer of doping density N_D and a spacer of a thickness d_i. Taking into account the prerequisite of the approximation, i.e. completely ionized donors and omitted background carriers, the factors that can affect the temperature dependence of the electron densities include the variation of conduction band offset caused by the temperature-dependent band gap, polarization, donor ionization, surface potential, and so on. While lack of experimental data allows one to consider only the former two factors.

The nitride band gap varies with temperature as follows:[6]

$$Eg = Eg_0 - AT^2/(T + B) \ \text{(eV)}. \quad (13)$$

And the strain variation caused by thermal expansion of the lattice is reflected by piezoelectric polarization,

$$P_{PE}(Al_xGa_{1-x}N) \propto \zeta = (a_{GaN} - a(x))/a(x), \quad (14)$$

$$a(T) = a_0(1 + \beta(T - T_0)), \quad (15)$$

where $a(x)$ in Eq.(14) is the lattice constant of $Al_xGa_{1-x}N$, and β in Eq.(15) is the thermal expansion coefficient of a. T_0=300K, and a_0 is the lattice constant at 300K.

In Table 1, parameters needed for Eqs.(13)–(15) are presented.[6]

Table 1. Some basic parameters.

	a_0/nm	$\beta/10^{-6}{}^{\circ}\mathrm{C}^{-1}$	Eg_0/eV	$A/10^{-4}$	B
AlN	0.3112	4.20	6.13	17.99	1462
GaN	0.3189	5.59	3.47	7.7	600

3. Sample analysis

Figure 1 presents the sample structure labelled XD060, a metal-oxide chemical vapour deposition (MOCVD) grown one on SiC substrate. The unintentional doping (UID) density is less than $4\times10^{16}\mathrm{cm}^{-3}$. In Figs. 2 and 3 we present the calculated and experimental curves for Hall mobility and electron density.

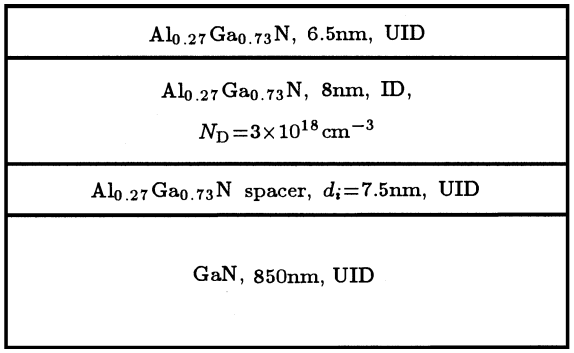


Fig.1. The sample structure.

3.1. Temperature-dependent Ns_{2D} and Ns_{3D}

In Fig.2, Ns_{2D} rises slightly as temperature falls. When the temperature is lower, ΔEc is larger and the potential well at the heterointerface is deeper. So the 2DEG energy levels move downward; this influence is counteracted partly by the decrease of σ_{pol} from variation of strain, which reduces the electric field in the potential well and weakens the two-dimensional confinement of electrons. So the 2DEG energy levels rise a little and the differences between them are lessened. With these effects clearly shown in Table 2, the change of Ns_{2D} is easily estimated from Eq.(4). Notice that by the energy criterion for differentiating 2DEG and bulk electrons, there are three energy levels of 2DEG in all for the temperature range considered. But the ratios of 2DEG subband sheet density N_i to Ns_{2D}, which change almost linearly with temperature, imply that the electrons mostly populate in the lowest subband and there should be fewer 2DEG energy levels towards low temperature. In the case of varying strain, the ratio N_1/Ns_{2D} increases from 89.57% to 93.23%, while N_2/Ns_{2D} decreases from 8.47% to 6.34%, and N_3/Ns_{2D} decreases from 1.96% to 0.43% from 300 to 77K.

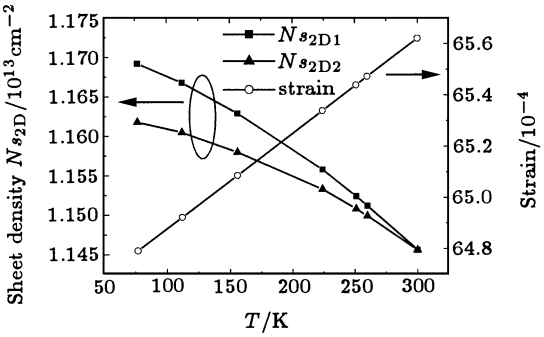


Fig.2. The calculated temperature dependence of Ns_{2D}. Ns_{2D1} corresponds to the strain of a constant value at 300K. Ns_{2D2}, also shown in Fig.3(b) as Ns_{2D}, corresponds to the strain curve here.

Table 2. The two lowest energy levels of 2DEG at different temperatures. The subscripts vs and cs represent varying and constant strain respectively, and $\Delta E_{12} = E_2 - E_1$.

T/K	$E_{1\mathrm{vs}}$/meV	$E_{1\mathrm{cs}}$/meV	$E_{2\mathrm{vs}}$/meV	$E_{2\mathrm{cs}}$/meV	$\Delta E_{12\mathrm{vs}}$/meV	$\Delta E_{12\mathrm{cs}}$/meV
300	–111.2	–111.2	17.7	17.7	128.9	128.9
224	–114	–114.3	8.9	8.8	122.9	123.1
77	–117.8	–118.5	–5.7	–5.8	112.1	112.7

Though it is lowered thereby, E_{lb} of bulk electrons is above the Fermi level. From the Boltzmann distribution we can see more clearly that Ns_{3D} changes more with temperature than with E_{lb},

$$n_{3D}(z) = Nc\exp(-(Ec - E_{\mathrm{f}})/(k_{\mathrm{B}}T)), \qquad (16)$$

$$Nc \propto T^{3/2}.$$

So Ns_{3D} decreases with decreasing temperature, as shown in Fig.3(b). The reduced strain modifies mainly the conduction band edge and electron densities in the potential well but influences Ns_{3D} little.

3.2. Calculation of Ns_{Hall}

From Eqs.(1) and (2), we can see that the temper-

ature dependence of μ_{2D} and μ_{3D} will affect the results of Ns_{Hall}. Various scattering mechanisms and different electron densities cause the difference of μ_{2D} and μ_{3D}, as shown in Fig.3(a). Relative to the bulk electrons, the high electron density of 2DEG effectively screens some scattering mechanisms such as ionized impurity scattering.[7] But as for alloy scattering and interface roughness scattering, both independent of temperature, higher density of 2DEG is helpful, for it means deeper penetration of the wavefunctions into the alloy barrier layer and closer average distance of 2DEG to the heterointerface. Meanwhile, higher electron density means occupation of more subbands, so inter-subband scattering is enhanced. Consequently, μ_{2D} increases towards low temperature and saturates between about 10–100K. And μ_{2D} is much higher than μ_{3D}, especially at low temperatures.

Since our sample XD060 lacks Hall mobility data of GaN, those of low-doped sample from Dziuba *et al*[2] and Look and Molnar[3] (μ_{3D1} and μ_{3D2} in Fig.3(a) respectively) are adopted to solve $\mu_{2D1,2}$ and $Ns_{Hall1,2}$. This makes the calculation and results of Ns_{Hall} an interesting subject.

In Fig.3(a), the almost overlapped μ_{2D1} and μ_{2D2} are very close to μ_{XD060} though there are considerable difference between μ_{3D1} and μ_{3D2}, while in Fig.3(b), the calculated temperature dependence of Ns_{Hall1} is quite different from that of Ns_{Hall2}. Both increase as Ns_{XD060} does, but Ns_{Hall1} is closer to the measured data and Ns_{Hall2} is very similar to Ns_{3D} in shape.

From Eqs.(1) and (2) a relation is inferred as follows:

$$Ns_{Hall}\mu_{Hall} = Ns_{2D}\mu_{2D} + Ns_{3D}\mu_{3D}, \quad (17)$$

$$= Ns_{2D}(\mu_{2D} + \mu_{3D}Ns_{3D}/Ns_{2D}), \quad (17a)$$

$$= \mu_{2D}(Ns_{2D} + Ns_{3D}\mu_{3D}/\mu_{2D}), \quad (17b)$$

and the relations among the calculated curves can be explained. In the sample, Ns_{3D} is far less than Ns_{2D}, so $\mu_{2D} \approx \mu_{XD060}$ results from Eq.(17a). In Eq.(17b), the greater change of Ns_{3D} than Ns_{2D} with temperature results in the change of Ns_{Hall1} and Ns_{Hall2} being more like Ns_{3D}. Since μ_{3D2} is much higher than μ_{3D1}, the similarity is greater for Ns_{Hall2}. But for a given heterostructure, μ_{3D} for its bulk conductance is unique. The fact that Ns_{Hall1} is closer to Ns_{XD060} implies that μ_{3D1} is more suitable for XD060.

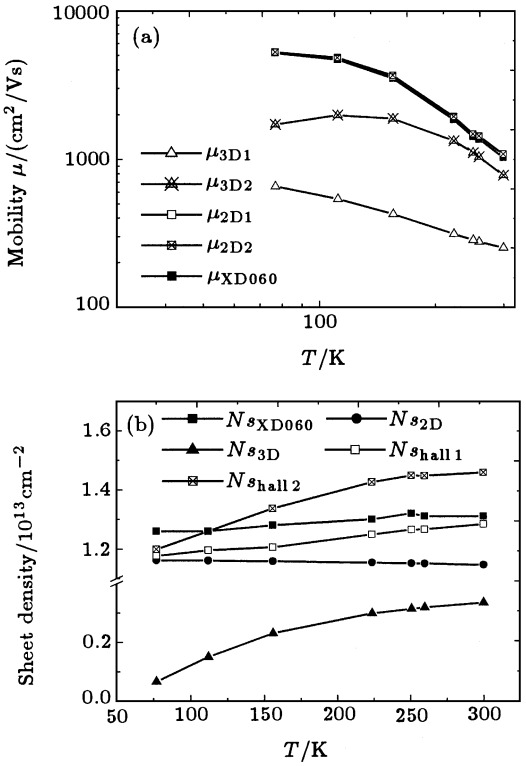


Fig.3. The calculated and measured Hall data. μ_{XD060} and Ns_{XD060} are the experimental curves for our sample. (a) The temperature dependence of Hall mobility. μ_{3D1} is from Dziuba *et al*[2] and μ_{3D2} is from Look and Molnar.[3] μ_{2D1} and μ_{2D2} are calculated curves. (b) The temperature dependence of Hall electron density. Ns_{Hall1} and Ns_{Hall2} correspond to μ_{2D1} and μ_{2D2} respectively.

The conductivity ratios are also worth mentioning. Given that the hall conductivity is $\sigma_{Hall} = Ns_{Hall1}\mu_{XD060}$, from 300 to 77K the ratio $\sigma_{2D}/\sigma_{Hall} = \mu_{2D1}Ns_{2D}/\sigma_{Hall}$ increases from 93.63% to 99.28%, and corresponding $\sigma_{3D}/\ \sigma_{Hall}$ decreases from 6.37% to 0.72%, both of which change in a nearly linear way. So the bulk conductance is small and we can expect that it will disappear at a certain temperature lower than 77K, below which the Hall data are an exact characteristic of 2DEG.

When calculating $Ns_{2,3D}$, only the effects of strain and ΔEc are considered, and the other factors unaccounted for may change the temperature dependence of the electron densities in trend and magnitude. From the above, however, we can find that from 77 to 300K, if the 2DEG sheet density varies little with temperature, even in samples with small bulk conductance, i.e. with low background carrier density or thin GaN layer, the temperature dependence of Hall mobility is determined by the 2DEG mobility, but Hall electron density tends to vary with temperature as the bulk electron density does.

4. Conclusions

The temperature dependence of 2DEG and bulk electron densities for nitride heterosturctures is calculated in a sample from 77 to 300K. The effects of variation of energy gap and strain with temperature are shown to be opposite to each other, and the former is stronger. The resulting 2DEG sheet density rises slightly towards low temperature.

With the experimental data of Hall mobility the temperature dependence of Hall electron density is obtained further. The agreement between the calculated and measured Hall electron densities could be quite well with the appropriate bulk mobility data for this temperature range. The investigation shows that in the heterostructures with small bulk conductance, the measured Hall mobility is a good approximation of 2DEG mobility, but the Hall electron density reflects more the temperature dependence of bulk electron density than that of 2DEG density. The exact behaviour of 2DEG should be observed by the Hall data at lower temperature.

References

[1] Petritz R L 1958 *Phys. Rev.* **110** 1254
[2] Dziuba Z *et al* 1997 *J. Appl. Phys.* **82** 2996
[3] Look D C and Molnar R J 1997 *Appl. Phys. Lett.* **70** 3377
[4] Jogai B 2002 *J. Appl. Phys.* **91** 3721
[5] Zhang Y F and Singh J 1999 *J. Appl. Phys.* **85** 587
[6] Levinshtein M E, Rumyantsev S L and Shur M S 2001 *Properties of advanced semiconductor materials* GaN, AlN, InN, BN,SiC, SiGe (New York: Wiley)
[7] Shur M, Gelmont B and Khan M A 1996 *J. Electron. Mater.* **25** 777