Mobility in epitaxial GaN: Limitation of electron transport due to dislocation walls

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Abstract. A theoretical model to explain the sharp transition to low-mobility regime in n-type GaN layers is proposed. We show that this peculiarity of the mobility versus free carrier concentration can be interpreted with the well-known Read model when the scattering due to charged dislocation walls is included in consideration. An agreement with experiments is found above the critical value of carrier density.

1. Introduction
It is well known that the extended defects of different types (mainly dislocations and dislocation substructures) frequently occur in thin semiconducting films and layers. In this context, the problem of their effect on carriers transport is of considerable present interest, both for theoretical and practical reasons [1].

Recently, these investigations have been stimulated additionally by the reason of new promising applications of GaN epitaxial films in optoelectronics [2, 3]. However, the performance of the devices based on GaN is limited by threading dislocations (exclusive of recently synthesized materials [4, 5]) with large densities $10^8 - 10^{11}$ cm$^{-2}$, which are result from the large lattice mismatch between epilayer and substrate [6, 7, 8]. To improve the device characteristics, the effect of dislocations on the mobility should be studied.

In this paper we show that some peculiarities in electron mobility at room temperature in application to GaN epitaxial films can be explained in the framework of the well-known Read approach [9, 10]. Namely, it is explained the sharp mobility drop at some critical carrier density which, in turn, depends on the dislocation substructure [11, 12]. The total transverse mobility $\mu$ versus carrier density $n$ is calculated when additional scattering due to electrostatic potential of row of dislocations or dislocation wall exists along with other mechanisms. The reason to consider dislocation walls is the fact found in most experiments that threading dislocations concentrate at subgrain boundaries lining up in row [11, 13]. In this picture, at some conditions (See discussion below) the mobility can be thermally activated because of the charged dislocation barriers present. The equation for the potential barriers is obtained here based on the model proposed in [14].

2. Electrostatic potential of dislocation wall
Let the wall of negatively charged dislocations be oriented along the $y$ axis with the distance between them equal to $D$, and the lines of each dislocation are directed along $z$ axis. The
negative charge in the dislocation line is compensated by a cylindrical positive space-charge
region, with radius $R$ around any dislocation. Thus, we have the periodically ordered cylinders
with radius $R$. The Poisson’s equation in this case in the Schottky approximation can be written
as

$$\frac{\partial^2 \phi(x, y)}{\partial x^2} + \frac{\partial^2 \phi(x, y)}{\partial y^2} = \frac{e}{\varepsilon_0} \left[ \left( N_d^+ - N_a^- \right) \theta(L(y) - |x|) \right] - \frac{\delta(x)}{c} \sum_{n=-\infty}^{\infty} \delta(y - nD),$$

where $N_d^+$, $N_a^-$ are the volume doping and unintentional acceptor densities, respectively.

$D = b/2 \sin \alpha/2$, $b$ is the absolute value of the Burgers vector, $f$ is the fraction of sites of dislocation
that are occupied, $\varepsilon$ is the dielectric constant, $L(y) = \sqrt{R^2 - y^2}$ is a periodic function along the
$y$ axis which is the screening length where potential $\phi(x, y)$ is not equal to zero (by definition, $\phi(x, y) = 0$ when $|x| \geq L(y)$). Notice that $\phi(x, y)$ is even function on $y$ with the period $D$, and
can be represented as a Fourier series

$$\phi(x, y) = \phi_0(x) + \sum_{n=1}^{\infty} \phi_n(x) \cos \left( \frac{2\pi ny}{D} \right),$$

where the expansion coefficients by Eq.(1) satisfy the equations

$$\frac{d^2 \phi_0(x)}{dx^2} = -\left( \frac{e(N_d^+ - N_a^-)}{\varepsilon_0} a_0(x) - \frac{2ef\delta(x)}{cD\varepsilon_0} \right),$$

$$\frac{d^2 \phi_n(x)}{dx^2} - A_n^2 \phi_n(x) = -\left( \frac{e(N_d^+ - N_a^-)}{\varepsilon_0} a_n(x) - \frac{2ef\delta(x)}{cD\varepsilon_0} \right),$$

$$A_n = \left( \frac{2\pi n}{D} \right) \left( \frac{2R}{D} + \frac{\sin \left( \frac{4\pi n R}{D} \right)}{2\pi n} \right)^{1/2},$$

$$a_n(x) = \frac{2}{D} \int_{-R}^{R} d\xi \theta(L(\xi) - |x|) \cos \left( \frac{2\pi n\xi}{D} \right).$$

The solutions for $\phi_0(x)$ and $\phi_n(x)$ can be found using Green functions for Eqs.(3),(4) when
$R = \sqrt{f/\pi c(N_d^+ - N_a^-)}$ (this equation can be obtained from $\phi(x, y) = 0$ when $|x| \geq L(y)$).

$$\phi_0(x) = -\frac{e(N_d^+ - N_a^-)}{D\varepsilon_0 \varepsilon} \left( 2Rx^2 + \frac{4R^2}{3} \right) + \frac{ef}{cD\varepsilon_0 \varepsilon} |x|,$$

$$\phi_n(x) = \frac{2e(N_d^+ - N_a^-)}{A_n^2 \varepsilon_0 \varepsilon \pi n} \sin \left( \frac{2\pi n R}{D} \right) - \frac{e(N_d^+ - N_a^-)\alpha_n}{A_n\varepsilon_0 \varepsilon D} \cosh(A_n x) - \frac{ef}{cDA_n\varepsilon_0 \varepsilon} \exp(-A_n|x|),$$

$$\alpha_n = \int_{-R}^{R} d\xi \cos \left( \frac{2\pi n\xi}{D} \right) \exp(-A_nL(\xi)).$$
3. Mobility

The barrier-limited mobility, generally, takes the form [15]

$$\mu_{GB} = \left(\frac{eL}{\sqrt{8kT\pi m^*}}\right) \exp(-V(0, y = R)/kT), \quad (7)$$

where $e$ is absolute value of the electron charge, $m^*$ its effective mass, $k$ is the Boltzmann constant, $T$ is the temperature, $L$ is the average grain size, $V(0, y = R) = -e\phi(0, y = R)$ is the value of the two-dimensional potential barrier caused by charged dislocations at $x = 0$. The explicit form of this potential can be derived from Eqs.(2),(5),(6). Notice that the potential $V(0, y = R)$ has quite simple form when $2R \approx D$ [14]

$$V(0, y = D/2) = -e\phi(0, y = D/2) = \frac{4e^2(N_d^+ - N_a^-)R^3}{3\epsilon_0\epsilon D} - \frac{e^2f^2}{2c\pi\epsilon_0\epsilon} \ln 2. \quad (8)$$

Thus, the total effective mobility takes the form [16, 15]

$$\frac{1}{\mu^*} = \frac{1}{\mu_1} + \frac{1}{\mu_{GB}}, \quad (9)$$

where $\mu_1$ is the mobility caused by different mechanisms of scattering in GaN films except charged dislocation walls. We have used the explicit form for $\mu_1$ and the main parameters for GaN from paper [17]. The total mobility $\mu^*$ vs free carrier density $n$ is defined by the Eqs.(7)-(9) with $V(0, y = R)$ from Eqs.(5),(6). The charge balance equation should be included in calculations $n = N_d^+ - N_a^- - n_t$, where $n_t$ is the density of electrons trapped at the dislocation line [12].

4. Results and discussion

Using the proposed here model, we are able quantitatively to reproduce the drop of the mobility $\mu^*$ at some critical meanings of carrier density as one can see from Figure 1. The sharp transition to the low mobility regime caused by domination of $\mu_{GB}$ as $n$ falls.

The nature of this domination is the rise of the potential barrier as the dopant density decreases, since $V(0, y = R)$ is a function of the ratio $2R/D$, while $R \sim 1/\sqrt{N_d^+ - N_a^-}$. As the result, $\mu_{GB}$ decreases as $n = N_d^+ - N_a^- - n_t$ decreases ($\mu_1 \gg \mu_{GB}$), and from Eq.(9) we have $\mu^* \approx \mu_{GB}$. Since the increase of the doping level, the bulk single-crystal mobility starts to dominate. Also, at fixed $2R$, $V(0, y = R)$ will be greater for smaller $D$ (increase of the local dislocation density in the dislocation wall). This explains the correlation between the position of the minimum of $n$ and the dislocation density. However, the model does not allow to reproduce the rise of the mobility below the minimum ($2R/D > 1$). Most likely, this increase can be explained in the framework of the percolation theory [15, 18].
Figure 1. Room temperature mobility vs free carrier concentration for two samples with $N_{\text{dis}} = 5 \times 10^9 \text{cm}^{-2}$ (open circles), $N_{\text{dis}} = 2 \times 10^{10} \text{cm}^{-2}$ (closed circles) from Ref.[12]. Solids lines are theoretical curves. A set of the model parameters used in calculations: (open circles) $f = 0.05$, $D = 1000 \AA$, compensation ratio equal to 0.3, $L = 30000 \AA$; (closed circles) $f = 0.05$, $D = 900 \AA$, compensation ratio equal to 0.4, $L = 30000 \AA$ Other parameters are taken from Ref. [17]

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