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On the Screening of a Negatively Charged Dislocation Line in Degenerate GaN

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Group-III-nitride semiconductors (GaN, AlN, AlGaN/GaN heterostructures) display a number of outstanding physico-chemical properties for applications in high-power, high-frequency electronics and short-wavelength optoelectronics [1,2]. Gallium nitride (GaN), the most thoroughly studied member of the nitride family, has a large direct bandgap of ~3.4 eV and is commonly grown heteroepitaxially on foreign lattice-mismatched substrates, such as *c*-plane sapphire or SiC [1,2]. Transmission electron microscopy observations show that device quality GaN epilayers usually contain high densities ($\sim 10^{8} \div 10^{11}$ cm^{-2}) of vertically aligned threading edge dislocations (TEDs) [1,2]. Density-functional-theory based electronic structure calculations [3] have suggested that the cores of TEDs in *n*-type GaN can behave as lines of acceptors and become highly negatively charged. Electron holography measurements [4] have yielded the result that a negative charge accumulation at a TED in *n*-GaN indeed takes place, and that the filling factor, f [5-11], of dislocation-related acceptor states in the bandgap assumes high values like $f \sim 1$. Optical absorption experiments [12,13] found that edge-dislocation core charges in plastically deformed *n*-GaN are also very high, $f \cong 3$. For comparison, in plastically deformed *n*-Ge crystals the experimentally determined typical values of the filling factor are much smaller, $f_{Ge} \sim 10^{-2} \div 10^{-1}$ (Refs. [6,7]).

It has been proposed in previous theoretical studies [8-11] that in degenerately doped *n*-GaN and related nitride epilayers the dielectric screening of a highly negatively charged ($f \sim 1$) TED can be accurately described by the conventional Thomas-Fermi (TF) shielding scenario. In this scenario, the selfconsistently screened electrostatic potential $\varphi_{TF}(r)$ around a uniformly charged dislocation line assumes the form [8-10]

$$\varphi_{TF}(\rho) = \varphi_0 K_0\left(\frac{\rho}{\lambda_{TF}}\right), \qquad (1)$$

$$\varphi_0 = 2fe/\varepsilon c\,, \qquad (2)$$

$$\lambda_{TF} = \left[(a_B/4)(\pi/3n)^{1/3}\right]^{1/2}, \qquad (3)$$

and the axially-symmetric distribution of the corresponding electric field is given by [12,13]

$$E_{TF}(\rho) = -\frac{\partial \varphi_{TF}}{\partial \rho} = \frac{\varphi_0}{\lambda_{TF}} K_1\left(\frac{\rho}{\lambda_{TF}}\right) = \frac{\varphi_0}{\rho}\begin{cases} 1, & \rho/\lambda_{TF} << 1, \\ (\pi\rho/2\lambda_{TF})^{1/2}\exp(-\rho/\lambda_{TF}), & \rho/\lambda_{TF} >> 1. \end{cases} \qquad (4)$$

Above, ρ is the radial distance from the dislocation axis, λ_{TF} is the TF screening length expressed in terms of the Bohr radius $a_B = \varepsilon\hbar^2/me^2$ and the carrier concentration *n*, *e* is the charge of the electron with effective mass *m*, the dielectric constant of the medium is denoted by ε, and *c* is the atomic-scale distance between the acceptor centres along the dislocation line; $K_0(x)$ and $K_1(x)$ are, respectively, the zero- and first-order modified Bessel functions of the second kind.

As can be noticed from the fundamental structure of Eq. (3), the quantum length scale originating in the TF screening picture has no information about the charged state of the line defect, $\partial\lambda_{TF}/\partial f = 0$. What this circumstance physically means, is that the actual screening mechanism operating around an electrically active dislocation in degenerate nitride layers can be conceptually different from the one suggested by the school of thought [8-13]. In this communication, our objective is to present physically transparent considerations for showing explicitly how a highly negatively charged dislocation line piercing through a quantum gas of electrons can be effectively screened via classical mechanism. In the course of this development, we introduce the notion of the critical carrier concentration, at which a hitherto undescribed crossover is occurring between the quantum and classical screening mechanisms.

Let us start our analysis by introducing the coulombic energy of the repulsive electron-dislocation interaction via relation

$$e\varphi_{TF}(\rho \sim \lambda_{TF}) \sim e\varphi_0 = U_0/3\,,$$

where U_0 characterizes the magnitude of the upward band bending in the vicinity of the line defect. As long as the band bending in a quasiclassical [14] electron gas with the Fermi energy $E_F = \hbar^2(3\pi^2 n)^{2/3}/2m$ (Refs. [8-11]) remains weak,

$$U_0 << E_0 << E_F\,,$$

$$E_0 \sim \frac{\hbar^2}{m\lambda_{TF}^2} \sim \frac{e^2}{\varepsilon} n^{1/3}\,,$$

or even becomes moderately strong,

$$E_0 << U_0 << E_F\,, \qquad (5)$$

a transition to the ultra-quantum limit $\hbar \to \infty$ is always possible, and the screening length (3) can be obtained, e. g., by linearizing [15] the cylindrically-symmetric Poisson equation for the dislocation line [5,15]. The situation becomes qualitatively different, however, in the opposite extreme,

$$E_0 << E_F << U_0 \,,$$

since now the passage to the limit $\hbar \to \infty$ is clearly prohibited. In order to obtain an asymptotically correct screening picture in this strong-coupling [16] case, one may rewrite the expression (3) in an alternative form,

$$\lambda_{TF} = \lambda_{TF}(E_F) = \left(\frac{\varepsilon E_F}{6\pi e^2 n} \right)^{1/2}, \qquad (6)$$

and perform in (5) a passage to the limit $E_0 << U_0 \to E_F$. Under this limiting transition, the $\hbar$-dependent Eq. (6) reorganizes it's structure in an essential way and delivers the result

$$\lambda_{TF}(E_F \to U_0) \to \left(\frac{\varepsilon U_0}{6\pi e^2 n} \right)^{1/2} = \left(\frac{\varepsilon \varphi_0}{2\pi e n} \right)^{1/2} \equiv R \,,$$

where the f-sensitive length scale,

$$R = \left(\frac{f}{\pi c n} \right)^{1/2}, \qquad (7)$$

shows no explicit dependence on $\hbar$.

It is apparent that R of (7) has the same physical meaning as the radius of the screening cylinder constructed by Read [5,6] around an acceptor-type dislocation line in a non-degenerate electronic semiconductor with shallow (completely ionized) donors. The reason for the appearance of R in our study is obviously connected with the fact that the mechanism of the negative line charge screening by the space charge [5,6,16] of positively charged donors is clearly insensitive to the type of the electron gas statistics. It is therefore clear that under degenerate doping conditions the screened electric field [12,13] of the dislocation line can be described not only by the TF formula (4), but also by Read's essentially different expression,

$$E_R(\rho) = -\frac{\partial \varphi_R}{\partial \rho} = \frac{\varphi_0}{\rho} \left[1 - \left(\frac{\rho}{R} \right)^2 \right], \; \rho \le R \ne \lambda_{TF} \,.$$

We now proceed further by noting that in accordance with Eqs. (3) and (7) the ratio of $\lambda_{TF}(n) \propto n^{-1/6}$ to $R(n) \propto n^{-1/2}$ can be represented as

$$\frac{\lambda_{TF}(n)}{R(n)} = \left(\frac{E_F}{U_0} \right)^{1/2} = \left(\frac{n}{n_0} \right)^{1/3},$$

where the critical Fermi gas concentration,

$$n_0 = \frac{8}{\pi^2} \sqrt{3} \left(\frac{f}{c a_B} \right)^{3/2} \propto \hbar^{-3} \,,$$

establishes a crossover point between the quantum ($n/n_0 >> 1,\; R << \lambda_{TF} \propto \hbar$) and classical ($n/n_0 << 1,\; \lambda_{TF} << R$) screening regimes. If the filling factor of the dislocation acceptor levels is sufficiently large ($f >> f_0 \sim c/a_B ,\; c < a_B$), then this point of crossover automatically finds it's residence in the quasiclassical [14] range of carrier densities,

$$n_0^{1/3} a_B \sim (f / f_0)^{1/2} >> 1 .$$

Furthermore, as can be seen from the scaling relation $n_0(f) \propto f^{3/2}$, the conditions for the realization of the classical mechanism of screening become more (less) favorable in heteroepitaxial systems hosting highly (weakly) charged dislocations.

In wide-gap GaN the conduction band electrons are rather "heavy", $m \sim 0.2 m_0$ (Refs. [8,10,11]), whereas the dielectric constant is not large, $\varepsilon \sim 10$ (Refs. [3,8]). Using for rough calculations these numerical values together with $f \sim 1$ (Refs. [4, 8-11]) and $c \sim 5 \times 10^{-8}$ cm [1-4], we obtain for the characteristic parameters the following estimates: $f_0 \approx 0.2$, $n_0 \approx 10^{21}\,\text{cm}^{-3}$. The relevant point here is that in GaN the Mott concentration is located around $n_M \approx 10^{18}\,\text{cm}^{-3}$ [17]. One thus has a good reason to expect that in this material the TF regime of dislocation line charge screening [8-13] can manifest itself only at extremely high doping levels, $n_M << n_0 < n$.

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On the Screening of a Negatively Charged Dislocation Line in Degenerate GaN

Theoretical studies have suggested in the past that in degenerately doped *n*-GaN and related III-nitride epilayers the dielectric screening of highly negatively charged dislocations is governed by the $\hbar$-dependent Thomas-Fermi mechanism. Here we show how in this super-wide-gap material system the screening of the dislocation line charge can occur in a $\hbar$-independent way. We also describe the salient features of the critical carrier concentration, at which a crossover takes place between the quantum and classical screening regimes.

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ՀՀ ԳԱԱ թղթակից անդամ Հ. Հ. Մաթևոսյան, Հ. Բ. Ներսիսյան

Այլասերված GaN-ում բացասական լիցք կրող դիսլոկացիայի էկրանավորման մասին

Տեսական հետազոտությունների ներկա փուլում ընդունված է համարել, որ *n*-GaN էպիտաքսիալ թաղանթներում բացասական լիցք կրող դիսլոկացիաների էկրանավորումն իրագործվում է Թոմաս-Ֆերմիի քվանտային մեխանիզմի միջոցով: Այս ուսումնասիրության նպատակն էր՝ ցույց տալ, որ լայն արգելված գոտիով օժտված նիտրիդային համակարգերում դիսլոկացիոն լիցքի էկրանավորման մեխանիզմը կա-

րող է ունենալ էականորեն այլ՝ դասական ծագում: Բնութագրված է Ֆերմի-գազի խտության այն տիրույթը, որտեղ դիսլոկացիաների էկրանավորման քվանտային մեխանիզմը փոխակերպվում է դասականի:

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Об экранировании отрицательно заряженной дислокации в вырожденном GaN

На современном этапе теоретических исследований принято считать, что в вырожденном *n*-GaN экранирование отрицательно заряженных краевых дислокаций осуществляется посредством квантового механизма Томаса – Ферми. В настоящей работе показано, что в вырожденных широкозонных нитридных полупроводниках закон экранирования дислокационного заряда может иметь существенно иное – классическое происхождение. Изучены основные характеристики той критической концентрации Ферми-газа, ниже которой квантовый механизм экранирования заряженной дислокации заменяется классическим.

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