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Analysis of the decrease of two-dimensional electron gas concentration in GaN-based HEMT caused by proton irradiation*

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Gallium nitride (GaN)-based high electron mobility transistors (HEMTs) that work in aerospace are exposed to particles radiation, which can cause the degradation in electrical performance. We investigate the effect of proton irradiation on the concentration of two-dimensional electron gas (2DEG) in GaN-based HEMTs. Coupled Schrödinger's and Poisson's equations are solved to calculate the band structure and the concentration of 2DEG by the self-consistency method, in which the vacancies caused by proton irradiation are taken into account. Proton irradiation simulation for GaN-based HEMT is carried out using the stopping and range of ions in matter (SRIM) simulation software, after which a theoretical model is established to analyze how proton irradiation affects the concentration of 2DEG. Irradiated by protons with high fluence and low energy, a large number of Ga vacancies appear inside the device. The results indicate that the ionized Ga vacancies in the GaN cap layer and the AlGaN layer will affect the Fermi level, while the Ga vacancies in the GaN layer will trap the two-dimensional electrons in the potential well. Proton irradiation significantly reduced the concentration of 2DEG by the combined effect of these two mechanisms.

Keywords: proton irradiation, GaN-based HEMT, two-dimensional electron concentration

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1. Introduction

Due to the superior material properties such as wide bandgap energy, high thermal and chemical stability, and high displacement threshold energy, GaN-based high electron mobility transistors (HEMTs) exhibit outstanding performance in high power and high frequency applications required in aerospace and military fields. Owing to the spontaneous and piezoelectric polarization in GaN-based HEMT, there is a large interface charge density in this system, which is associated with the formation of the two-dimensional electron gas (2DEG) channel near the AlN/GaN heterointerface. Even in the absence of intentional doping, 2DEG concentration can reach about 1×10^{13} cm^{-2}. In addition, the high mobility of 2DEG gives the GaN-based HEMTs a low on-resistance and perfect high-frequency performance. Inside the earth magnetosphere, there are two Van Allen regions of trapped fast particles, mostly electrons and protons.[1–3] Subjected to the high fluence proton irradiation, the performance of GaN-based HEMTs will degenerate despite its high irradiation tolerance, which has been investigated by many researchers. It has been found that defects produced by proton irradiation can reduce the concentration of 2DEG,[4,5] which in turn causes a shift in threshold voltage and an increase in on-resistance. However, the specific mechanism by which proton irradiation decreases the concentration of 2DEG and affects the band structure of GaN-based HEMTs remains unclear.

Proton irradiation can cause displacement damage and total ionizing dose (TID) radiation effects.[6–8] TID is typically caused by lattice displacement damage caused by ionizing radiation over the integrated exposure time. When GaN-based HEMTs are in operation, electrons and holes introduced by ionization effects can significantly affect the electrical properties of GaN-based HEMT. However, under the equilibrium condition, electrons and holes caused by ionization effects recombine rapidly and have no significant impact on the concentration of 2DEG, which can be ignored. Moreover, previous studies have demonstrated that the ionization effect have no significant contribution to radiation-induced damage in GaN-based devices.[3,6] The other extremely important effect is the displacement damage, which results from nuclear interactions and can lead to lattice defects, i.e., vacancies. Earlier, researchers concentrated on the role of N vacancies on the degeneration of GaN-based HEMTs,[9] and gradually shifted the focus of their researches to Ga vacancies. Lv *et al.*[5] conducted 3-MeV proton irradiation on AlGaN/GaN HEMTs at fluences of 4×10^{13} cm^{-2}, 6×10^{13} cm^{-2}, and 1×10^{15} cm^{-2}, the results suggest that Ga vacancies introduced by proton ir-

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radiation may be the main reason for the degradation of GaN-based HEMTs. Further, the energy of proton irradiation was found to be one of the key factors leading to the degradation of the device. Hu *et al.*[10] reported the effects of proton irradiation on AlGaN/GaN HEMTs at different energies and found that the degradation of GaN-based HEMTs is very small when the energy of proton is greater than 15 MeV. Most of the studies on the degradation of GaN-based HEMTs by proton irradiation have focused on the link between electrical performance degradation and proton irradiation, in contrast to the few studies on the underlying physical mechanisms.

In order to elucidate the physical mechanism by which proton irradiation reduces the 2DEG concentration in GaN-based HEMTs, we develop a model to obtain the simulation results of 2DEG concentration for 100 keV, 500 keV, 1 MeV, 1.8 MeV and 3 MeV proton irradiation on devices with fluences ranging from 1×10^{11} cm^{-2} to 1×10^{15} cm^{-2}. The coupled Schröodinger's and Poisson's equations are solved to calculate the band structure and 2DEG concentration by self-consistency method,[11] in which the vacancy data acquired by SRIM are taken into account. We find that 2DEG concentration decreases significantly after irradiation with 100 keV protons at a fluence of 1×10^{15} cm^{-2}.

2. Modeling

2.1. Proton irradiation simulation with SRIM software

SRIM is a software that simulates the stopping and range of the ions in matter by the Monte Carlo method.[12] As protons pass through the device, they will lose part of their energy, and the lost energy will be transferred to the lattice atoms in the form of non-ionizing energy loss (NIEL), which will displace the atoms from their lattice sites and create charged defect centers, i.e., Ga vacancies (V_{Ga}) and N vacancies (V_N). V_{Ga} is an acceptor-like defect, which acts as a compensation center and may be responsible for the carrier removal. For the N vacancies, there have been some research demonstrated that N vacancies as donor-like defects have little effect on the electrical properties of GaN-based HEMTs.[5] Therefore, we only consider V_{Ga} as the main factor for the decrease of 2DEG concentration and analyze the physical mechanism behind it.

The structure of the GaN-based HEMT we studied is shown in Fig. 1, which consists of four layers: GaN cap layer, AlGaN layer, AlN layer, GaN layer. Vacancy data will be given after the simulation completed, and Ga vacancies density changes with depth as shown in Fig. 2. Since the 2DEG is mainly concentrated in the GaN layer about 5 nm near the AlN/GaN interface (as shown in Fig. 3), we only consider the vacancies distribution in the 6 nm range in the GaN layer. The energy and fluences of proton irradiation are set to 100 keV, 500 keV, 1 MeV, 1.8 MeV, 3 MeV and 1×10^{11} cm^{-2}, 1×10^{12} cm^{-2}, 1×10^{13} cm^{-2}, 1×10^{14} cm^{-2}, 1×10^{15} cm^{-2}, respectively.

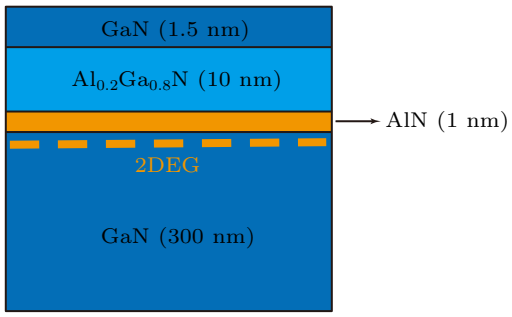


Fig. 1. Schematic device structures of GaN-based HEMT.

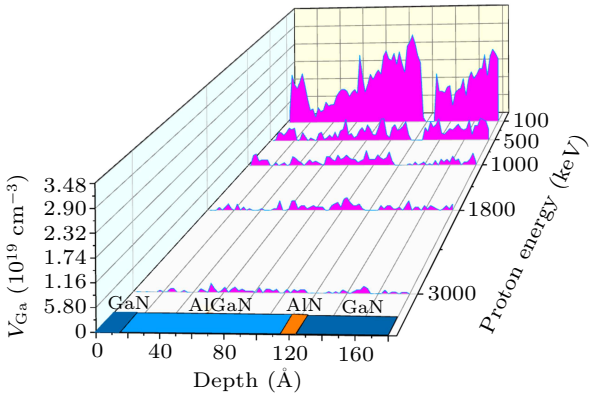


Fig. 2. Vacancy density vs. proton energy and depth in GaN-based HEMT. The proton fluence is 1×10^{15} cm^{-2}.

2.2. Calculation of 2DEG concentration

To calculate the concentration of 2DEG, we must solve the coupled Schrödinger's and Poisson's equations. The parameters we used in this work are shown in Table 1. The electrostatic potential in the GaN-based HEMT is related to charge distribution by Poisson's equation,

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon\frac{\mathrm{d}}{\mathrm{d}z}V(z)\right)=-q\left(N_{\mathrm{A}}^{-}+N_{\mathrm{el}}\right), \tag{1}$$

where N_{A}^{-} is the ionized acceptor density, and N_{el} is the density of conduction electrons. $V(z)$ is the total potential. Since the energy level of Ga vacancy is located at 0.86 eV above the valence band top (based on our calculation, the Fermi level is located 0.359–0.45 eV above the conduction band bottom, therefore $(E_{\mathrm{A}}-E_{\mathrm{F}})/KT\ll0$ for $T=300$ K),[5] it can be approximated that Ga vacancies as acceptor-like defects are almost completely ionized according to the following formula:

$$N_{\mathrm{A}}^{-}=N_{\mathrm{Ga}}\left[\frac{1}{1+g_{\mathrm{A}}\exp\left(\dfrac{E_{\mathrm{A}}-E_{\mathrm{F}}}{KT}\right)}\right]\approx N_{\mathrm{Ga}}, \tag{2}$$

where E_{F} and E_{A} are the Fermi level and acceptor level, respectively; N_{Ga} is the density of Ga vacancies, and g_{A} is the ground-state degeneracy factor.

Table 1. Material parameters used for the calculations.[15]

Parameter	Symbol	AlN	GaN
Bandgap	E_g (eV)	6.2	3.4
Lattice constant	a (Å)	3.112	3.189
Static dielectric constants	ε (F/m)	$8.5\varepsilon_0$	$10\varepsilon_0$
Spontaneous polarization	P_{sp} (C/m^2)	–0.081	–0.029
Piezoelectric constant	e_{31} (C/m^2)	–0.6	–0.49
Piezoelectric constant	e_{33} (C/m^2)	1.46	0.73
Elastic module	c_{31} (GPa)	108	106
Elastic module	c_{33} (GPa)	373	405
Effective electron mass	m^* (kg)	$0.3m_0$	$0.22m_0$

For free electrons, the enveloped electron wave function of the i-th subband $\psi(i)$ is determined by the Schrödinger equation:

$$\frac{\hbar^2}{2}\left[\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{m^*}\frac{\mathrm{d}\psi_i}{\mathrm{d}z}\right)\right]+(E_i-V(z))\,\psi_i=0, \tag{3}$$

with

$$V(z)=V_{\mathrm{B}}(z)+V_{\mathrm{P}}(z)+V_{\mathrm{A}}(z)+V_{\mathrm{el}}(z), \tag{4}$$

where m^* is the effective mass of the electron, and E_i is the eigenenergy of the i-th subband. Among the total potential $V(z)$ are the following terms: a barrier potential $V_{\mathrm{B}}(z)$ due to the conduction band offset at the interface; a potential $V_{\mathrm{P}}(z)$ resulting from the polarization charge at the interface; a potential $V_{\mathrm{A}}(z)$ related to the ionized acceptors; $V_{\mathrm{el}}(z)$ refers to the potential from electrons. Using dichotomy to solve coupled Schrödinger's and Poisson's equations self-consistently, the conduction band profile, free electron distribution, and the electron eigenstates are obtained. The total concentration of 2DEG is taken in the following form:

$$n(z)=\sum_i n_i|\psi_i(z)|^2, \tag{5}$$

$$n_i=\frac{m^*k_{\mathrm{B}}T}{\pi\hbar^2}\ln\left[1+\exp\left(\frac{E_{\mathrm{F}}-E_i}{k_{\mathrm{B}}T}\right)\right], \tag{6}$$

where the Fermi level E_{F} satisfies the following equation under equilibrium condition:[13]

$$\begin{aligned} n_s = {} & \frac{1}{(d_{\mathrm{GaN}}+d_{\mathrm{AlGaN}}+d_{\mathrm{AlN}})} \\ & \times\left\{\frac{\sigma_{\mathrm{GaN}}\cdot d_{\mathrm{GaN}}}{e}+\frac{\sigma_{\mathrm{AlGaN}}\cdot d_{\mathrm{AlGaN}}}{e}+\frac{\sigma_{\mathrm{AlN}}\cdot d_{\mathrm{AlN}}}{e}\right. \\ & -\frac{\varepsilon_0\varepsilon(x)}{e^2}\times\{e\Phi_{\mathrm{b}}(x)+E_{\mathrm{F}}-\Delta E_{\mathrm{C,AlN/GaN}} \\ & \left.+\Delta E_{\mathrm{C,AlGaN/AlN}}(x)+\Delta E_{\mathrm{C,GaN/AlGaN}}(x)\}\right\} \\ & +\sum_z N^-_{\mathrm{A,barrier}}(z)\,\mathrm{d}z, \end{aligned} \tag{7}$$

where σ_{GaN}, σ_{AlGaN} and σ_{AlN} are the total polarization charge induced by spontaneous and piezoelectric polarization across the GaN/AlGaN, AlGaN/AlN and AlN/GaN interface, respectively; x represents the composition of Al. $\Delta E_{\mathrm{C,GaN/AlGaN}}(x)$ is the band offset at GaN/AlGaN heterointerface. $\Delta E_{\mathrm{C,AlGaN/AlN}}(x)$ is the band offset at AlGaN/AlN heterointerface. $\Delta E_{\mathrm{C,AlN/GaN}}(x)$ is the band offset at AlN/GaN heterointerface.[14] $N_{\mathrm{A,barrier}}(z)$ is approximately equal to the distribution of V_{Ga} in the GaN cap layer, AlGaN layer, and AlN layer. The direction of z is perpendicular to the interface and extends inward. Here $e\Phi_{\mathrm{b}}(x)$ is Schottky barrier height, which is given by[15]

$$e\Phi_{\mathrm{b}}(x)=(1.3x+0.84)\ \mathrm{eV}. \tag{8}$$

So far, we have not considered the distribution of Ga vacancies in the GaN layer. According to the neutrality condition, the ionized Ga vacancies in the quantum well region have little effect on the energy band in the process of self-consistent calculation. Since the Ga vacancy trap electrons in the quantum well, the ionization of the Ga vacancies must lead to a decrease in the 2DEG concentration. The actual 2DEG concentration should be the calculated 2DEG concentration minus the concentration of ionized Ga vacancies, thus n_{s} is denoted as

$$n_{\mathrm{s}}=n_{\mathrm{s,cal}}-\sum_z N^-_{\mathrm{A,GaN}}(z)\,\mathrm{d}z, \tag{9}$$

where $n_{\mathrm{s,cal}}$ is the concentration of 2DEG by self-consistence calculation. $N^-_{\mathrm{A,GaN}}$ is the distribution of ionized Ga vacancies in GaN layer. In our calculation, we find that the concentration of 2DEG can be significantly reduced by Ga vacancies in the GaN layer only when the energy and fluence of proton irradiation are 100 keV and 1×10^{15} cm^{-2}, respectively. The reason is that irradiated by protons with high energy and low fluence, the concentration of Ga vacancies in the GaN layer is so small that the electrons trapped by Ga vacancies are negligible compared to the concentration of 2DEG. The conduction band profile before irradiation obtained by solving Schrödinger's and Poisson's equations self-consistently is shown in Fig. 3. The Fermi level is 0.45 eV above the conduction band bottom and the concentration of 2DEG is up to 2.48×10^{13} cm^{-2}.

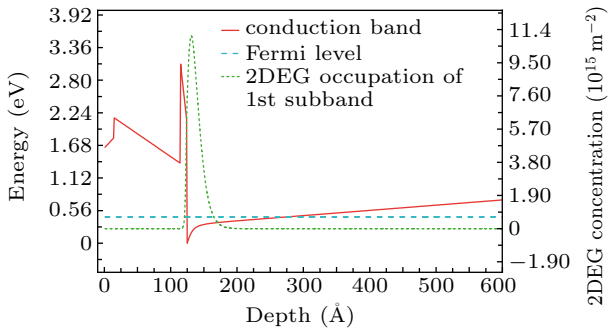


Fig. 3. The conduction band profile of GaN-based HEMT before irradiation, i.e., energy and 2DEG sheet charge concentration versus depth.

3. Results and discussion

The conduction band profiles and the concentrations of 2DEG near the AlN/GaN interface in GaN-based HEMT irradiated by protons with different fluences and energy are shown

in Figs. 4 and 5, respectively. As shown in Fig. 5, no significant decrease of 2DEG concentration is observed after proton irradiation at fluence below 1×10^{13} cm^{-2}. When proton fluence rises to 1×10^{15} cm^{-2}, 2DEG concentration decreases significantly at each irradiation energy. For 100 keV proton irradiation, the 2DEG concentration decreases dramatically when the fluence rises to 1×10^{14} cm^{-2}. As shown in Fig. 2, 100 keV proton irradiation introduces much more Ga vacancies than the higher energy proton irradiations. The reason is that the proton with low energy will decelerate rapidly when they collide with the lattice atoms, transferring more energy to lattice atoms in the form of NIEL. Apparently, that will create more Ga vacancies, which may be responsible for the decrease of 2DEG concentration.

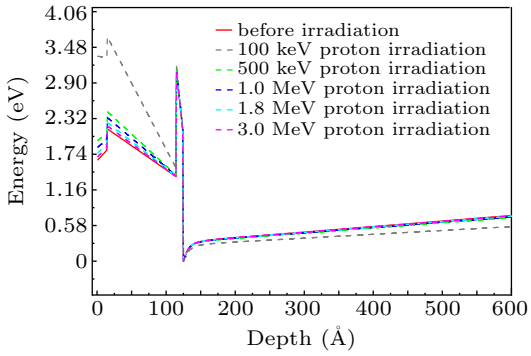


Fig. 4. The conduction band profiles of GaN-based HEMT before irradiation and after proton irradiation with different energy at fluence of 1×10^{15} cm^{-2}.

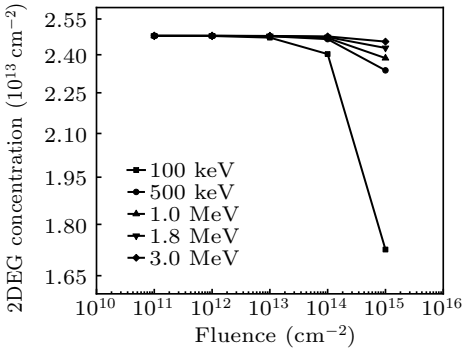


Fig. 5. The 2DEG concentration vs proton irradiation fluence and energy.

When Ga vacancies ionize as acceptor-like defects, it will capture the electron and become a negative center after ionization. In the GaN cap layer and AlGaN layer, a great number of Ga vacancies ionize, and electrons are trapped in the energy level introduced by Ga vacancies. Meanwhile, as shown in Fig. 4, the formation of negative centers in the barrier will also affect the conduction band structure for the reason that ionized Ga vacancy increases the electric field intensity in the AlGaN layer significantly.

When the fluences of proton radiation are increased from 1×10^{11} cm^{-2} to 1×10^{15} cm^{-2}, the 2DEG concentration decreases more sharply at 100 keV proton irradiation compared to the higher energy proton irradiation. There are two reasons: (1) Under 100 keV proton irradiation, there will be much more Ga vacancies introduced by proton irradiation in the quantum well area where the 2DEG is located. (2) The Ga vacancies in the barrier increase significantly, affecting the band structure and the relative position of Fermi level (E_F) to the ground-state energy level (E_0).

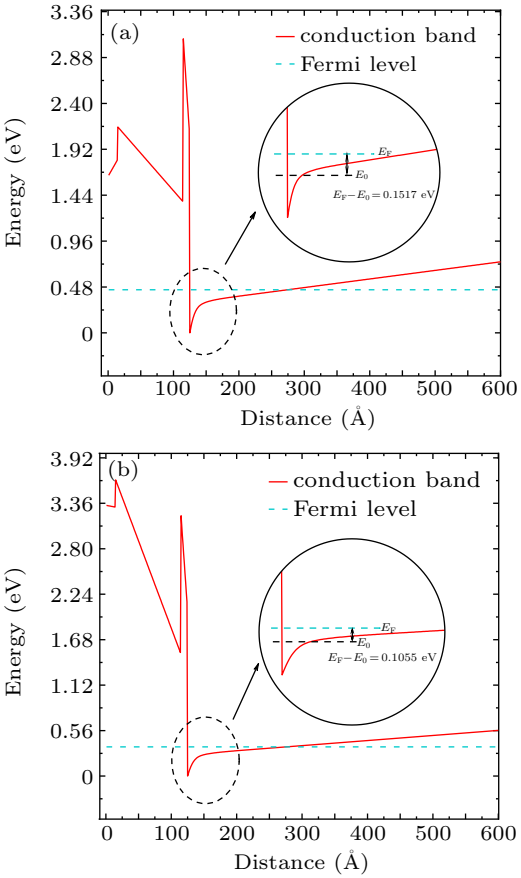


Fig. 6. The relative position of the ground-state energy level and the Fermi level (a) before irradiation and (b) after 100 keV proton irradiation at fluence of 1×10^{15} cm^{-2}.

Clearly, if more Ga vacancies are in the area where the 2DEG is located, the 2DEG concentration will decrease more dramatically due to the ionization of Ga vacancies. Based on Eq. (6), the change of relative position of E_F to E_0 will be a crucial factor in the reduction of the 2DEG concentration. As shown in Fig. 6, the value of $(E_F - E_0)$ decreases from 0.1517 eV to 0.1055 eV after 100 keV proton irradiation, which will reduce the 2DEG concentration by about 30% even if we do not consider the Ga vacancies in the GaN layer, based on our calculation. Under the combined effect of the two mechanisms discussed above, ionized Ga vacancies introduced by proton irradiation are the key factor for the reduction of 2DEG concentration. For the same irradiation fluence, a relatively lower proton irradiation energy will introduce more Ga vacancies and thus reduce the 2DEG concentration more significantly. Therefore, when designing irradiation-resistant devices, special attention should be paid to the effect of low en-

ergy protons on the device and the protective structure should be designed.

4. Conclusions

We have investigated the impact of proton irradiation on the 2DEG concentration in GaN-based HEMTs. Considering the defects introduced by proton irradiation, a model has been developed to calculate the 2DEG concentration. The results reveal that Ga vacancies in the GaN layer can trap two-dimensional electrons in the quantum well, while Ga vacancies in the AlGaN layer and the GaN cap layer reduce the 2DEG concentration by affecting the energy band structure and the Fermi level. The Ga vacancies in the AlGaN layer and the GaN cap layer take the dominant contribution to the reduction of 2DEG concentration by affecting the Fermi level and ground-state energy level, which is the key mechanism for the reduction of the 2DEG concentration when the fluence of proton irradiation is relatively low. Our calculations show that low-energy proton irradiation will introduce relatively more Ga vacancies inside the device and the concentration of 2DEG will be significantly reduced through the two mechanisms described above.

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