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# Mechanism of Normally-Off Operation in GaN-Based Transistors by Interstitial Fluorine Incorporation

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### 1. Introduction

AlGaN/GaN heterojunction field-effect transistors (HFETs) are very attractive for high-power switching applications taking advantages of the high breakdown strength and the high saturation electron velocity. Aiming at practical switching applications, the normally-off operation is strongly desired for fail-safe systems. Recently normally-off HFETs with fluorine (F) ion surface treatment have been reported[1]. The F reduces the carrier concentration in the two-dimensional electron gas (2DEG) at AlGaN/GaN. Secondary ion mass spectroscopy study reveals that F atoms are incorporated in the AlGaN layer of the as-treated samples and are then accumulated at the AlGaN/GaN interface after rapid thermal annealing (RTA) process[1,2].

So far, passivation of donors originated from F incorporation into GaAs- and InP-based HFETs were investigated[3,4]. Here, F atoms accumulate significantly at Si- $\delta$ -doped InAlAs layer after annealing. First-principles calculation reveals that the donor passivation is induced by interstitial F, which holds electrons in the conduction band and is then stabilized in -1 charge state[5]. Interstitial F also tends to form F-Si defect complex, resulting in the accumulation at Si- $\delta$ -doped layer[5]. Similar mechanism can be attributed to the F incorporation in the AlGaN, however, the details have never been investigated.

In this study, we estimate the formation energy of various atomic configurations containing F in GaN using first-principles calculation technique. The results indicate that interstitial F is the dominant reason for the normally-off operations.

#### 2. Calculation models and method

A  $3a \times 3a \times 2c$  (Ga<sub>36</sub>N<sub>36</sub>) supercell is used for the calculation models which contain either interstitial or substitutional F. The N vacancy (V<sub>N</sub>) model is also calculated. In the wurtzite structure, there are two types of interstitial positions with C<sub>3v</sub> point symmetry, labeled as *T* and *O* shown in Fig. 1. The *T* site is located in the middle of nonbonded Ga and N atoms. The *O* site locates at the center of the largest empty space in the wurtzite crystal.

The Vienna Ab-initio Simulation Package[6,7] based on the Kohn-Sham density-functional theory using a projected augmented planewave method is used for the calculation. The generic gradient approximation are applied to the exchange-correlation functional[8]. The cutoff energy of the basis set is set at 30 Ry. The 3*d* electrons of Ga are also considered in the calculation.

After completing the structural relaxation for each model while the lattice-constants are fixed at those of the ideal GaN crystal, the total energy  $E_{\text{total}}$  is estimated.

The formation energy  $E_{\text{form}}$  in a charge state q is given as a function of the atomic chemical potentials  $\mu_x$  (x=Ga, N or F) and the Fermi energy  $E_{\text{F}}$ , i.e.,

$$E_{\rm form}(q) = E_{\rm total}(q) - n_{\rm Ga}\mu_{\rm Ga} - n_{\rm N}\mu_{\rm N} - n_{\rm F}\mu_{\rm F} + qE_{\rm F}, \qquad (1)$$

where  $n_x$  is the number of atoms[5,9].  $\mu_{Ga}$  and  $\mu_N$  are variables correlated as

$$\mu_{\rm Ga} + \mu_{\rm N} = \mu_{\rm GaN(bulk)},\tag{2}$$

where  $\mu_{GaN(bulk)}$  is the chemical potential of the bulk GaN. The chemical potentials should vary within the range where the elements are not precipitated in GaN crystal.

#### **3.** Calculation Results

Fig. 2 shows the formation energies of various models for F incorporation as a function of N chemical potential.  $\Delta \mu_N$  is defined as the difference from the chemical potential of N<sub>2</sub> molecule. The charge state for each model is neutral (q=0), in which the formation energy is independent from the Fermi energy. The F chemical potential  $\mu_F$  is set at F-rich limit, which is the most favorable condition to incorporate F into GaN.

As shown in Fig. 2, F at the *O* site,  $F_O$ , is quite stable by 2.5 eV or more compared with that at the *T* site ( $F_T$ ). However, the perfect crystal model, denoted as "p.c." in Fig. 2, is most stable in all models in the wide range of  $\Delta\mu_N$  in spite of the F-rich condition. The substitutional F at Ga site ( $F_{Ga}$ ) is not realistic because of the high formation energy. In contrast to this, the substitutional F at N site ( $F_N$ ) is the most favorable case in all F-containing models; however, it works as a double donor. If there is  $V_N$  near the interstitial F, F will be trapped at  $V_N$  and become  $F_N$  because  $V_N$  is unstable as shown in Fig. 2. However, this transition should hardly occur since there are few vacancies in GaN of which crystal quality is good enough for device fabrication. From the above considerations, most of F atoms incorporated by the plasma treatment should be located at the interstitial *O* site.

The formation energies of  $F_O$  model for various charge states are calculated as shown in Fig. 3.  $E_F$  can move within the GaN bandgap. As shown in Fig. 3, if  $E_F$  is near the valence band maximum ( $E_{VBM}$ ), interstitial F prefers the neutral charge state (q=0). In contrast to this, the -1 charge state becomes the most stable as  $E_F$  increases from  $E_{VBM}$ , and then gains the formation energy of 0.4 eV from the neutral charge state at the conduction band minimum ( $E_{CBM}$ ). One F atom can capture one electron in excess electron conditions. This result can be explained by the fact that F has the largest electronegativity among the elements.

#### 4. Discussions

The band diagram of a typical AlGaN/GaN HFET without any F incorporation is shown in Fig. 4 (a). 2DEG is induced by strong polarization effects and is fixed close to the interface. According to the reported experimental results[1,2], F atoms are incorporated into the AlGaN layer after CF<sub>4</sub> plasma treatment as shown by the dashed line in Fig. 4 (c). F atoms should be at the interstitial O site as

mentioned above.

During the RTA process, most of F atoms still remain in the AlGaN layer, however, a certain part of the F atoms move toward the AlGaN/GaN interface. F atoms near the interface capture electrons in 2DEG, and then stay there as the -1 charge state which is the most stable. The solid line in Fig. 4 (c) shows the depth profile of F atoms after the RTA process. F atoms are accumulated near the AlGaN/GaN interface.

Fig. 4 (b) shows the corresponding band diagram after the RTA process. As shown in Fig. 4 (b), F atoms near the interface capture electrons and are at the -1 charge state, resulting in reduction of sheet carrier density. In contrast to this, F atoms in the AlGaN layer are still electrically neutral, which will lift the conduction band up from the Fermi level, leading to increase of the threshold voltage of the HFETs.

From the above considerations, the interstitial F atoms are the most possible origin of the normally-off operation.

#### 5. Conclusion

We calculate the formation energies of various F-containing atomic models to estimate the stability using first-principles calculation technique. F atoms at the *O* site become more stable by capturing electrons under excess electron conditions, while those are electrically neutral for  $E_{\rm F} \sim E_{\rm VBM}$ . These calculation results can well explain the mechanism of the normally-off operation in AlGaN/GaN HFET by F incorporation.

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**Fig. 1.** Calculation model of interstitial F in GaN crystal. There are two types of interstitial positions as labeled *T* and *O*.



**Fig. 2.** Formation energies at the neutral charge state (q=0) as a function of N chemical potential  $\Delta \mu_{\rm N}$ . The chemical potential of F is set at the upper limit (F-rich condition).



**Fig. 3.** Formation energies of interstitial F model for various charge states as a function of Fermi energy  $E_{\rm F}$ .



**Fig. 4.** Band diagrams AlGaN/GaN HFETs (a) without and (b) with interstitial F atoms. (c) The corresponding distributions of F atoms are schematically illustrated[1].