Modification of Amorphous-SiN_x/GaN Interface Trap Density by Nitridation: A First-Principles Calculation Study

Zhaofu Zhang, Mengyuan Hua, Jiabei He, Qingkai Qian, and Kevin J. Chen

Department of Electronic and Computer Engineering, The Hong Kong University of Science and Technology, Hong Kong
Email: zzhangbc@connect.ust.hk, eekjchen@ust.hk, Phone: +852-23588530

Keywords: SiN_x/GaN interface, nitridation treatment, first-principles calculation, threshold voltage stability

Abstract

The amorphous-SiN_x/GaN interface is studied by first-principles calculation to understand the underlying mechanism of enhanced interface quality by nitridation treatment. The calculation results reveal that both shallow and deep traps exist in a wide energy range within the GaN bandgap for SiN_x/GaN interface without nitridation treatment. Meanwhile, with proper surface nitridation prior to SiN_x deposition, a much cleaner interface bandgap structure with significantly suppressed interface state density (D_{it}) can be obtained. The low D_{it} would eventually lead to enhanced V_{th} stability in GaN MIS-gate power and RF devices. The nitridation effects on D_{it} is further verified by *C-V* measurement in GaN MIS diode with and without interface nitridation.

INTRODUCTION

Wide bandgap semiconductor GaN based power devices are attractive candidates for next generation high-efficiency power converters with high power density [1, 2]. Compared with the commercially-available *p*-GaN gate device, GaN power devices with metal-insulator-semiconductor (MIS) gate structures exhibit desirable characteristics such as lower gate leakage and larger safe operating range for gate voltage. The interface between the gate dielectric (e.g., SiN_x [3, 4]) and GaN channel is of particular importance since this interface is in the close vicinity of the channel (only a few tens of nanometers), thus the density of interface states (D_{it}) is of particular significance to performance stability of GaN-based lateral power devices. In an MIS-gate device, high D_{it} would result in severe threshold voltage (V_{th}) instability when these states undergo charging/discharging processes during switching operation or electrical/thermal stresses. [5]

Among the various treatment methods to improve the interface quality, the interface nitridation technique with repeatable feasibility and lower thermal budget stands out and has been validated to be a productive approach to reducing the D_{it} of GaN device and enhancing the dielectric/GaN interface quality by forming a nitridation interfacial layer (NIL). [6, 7]. Recently, we have reported the amendment of surface state distribution as a result of nitrogen adsorption on GaN surface by first principles calculation and photoelectron spectroscopy. [8, 9] However, the previous work has been limited to the surface rather than the SiN_x/GaN interface which is of high interests to GaN MIS-gate devices. The microscopic mechanism of the modification of interface trap density by nitridation at SiN_x/GaN interface is still not fully understood.

In this work, the SiN_x/GaN interface properties are systematically investigated by first-principles calculation. The amorphous-SiN_x (*a*-SiN_x) structure is generated to mimic the realistic dielectric in the calculation. The calculated results exhibit that both shallow and deep traps occur in a wide energy range within the GaN bandgap for the non-nitridized SiN_x/GaN interface. However, with proper nitridation prior to the dielectric deposition, the interface states are significantly

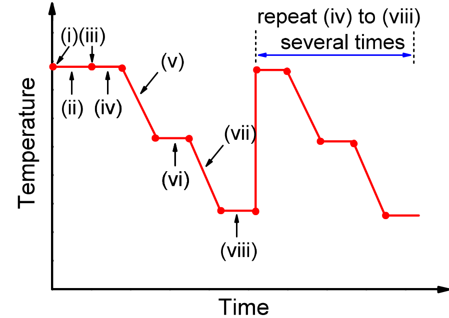

Fig. 1 The generation sequence of *a*-SiN_x. (i) crystal Si_3N_4; (ii) HT annealing at low density; (iii) density rescaling; (iv) HT annealing at normal density; (v) quenched to MT; (vi) MT annealing; (vii) quenched to LT; (viii) relaxation.

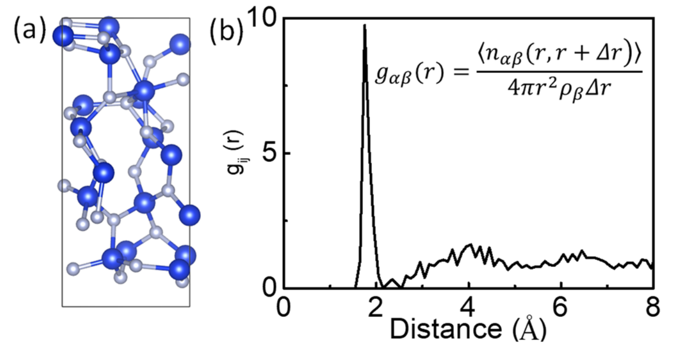

Fig. 2 (a) The atomic structure of *a*-SiN_x. Blue and gray balls represent Si, and N atoms, respectively. (b) RDF curve for the *a*-SiN_x obtained by AIMD calculation. The sharp peak around 1.76 Å corresponding to the average Si-N bond length, indicating a reasonable amorphous structure. The RDF functions are calculated according to the inserted equations.

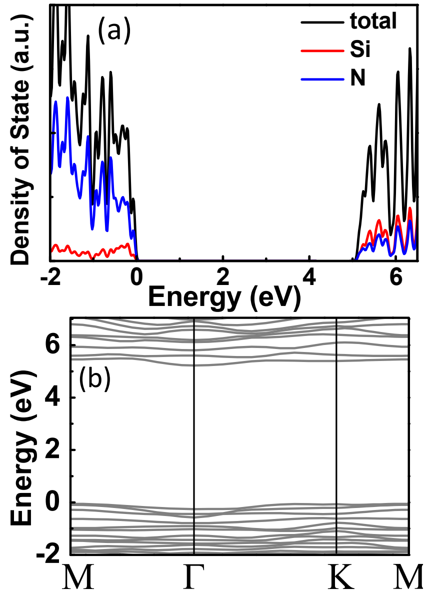

Fig. 3 The (a) density of states (DOS) and (b) band structure of *a*-SiN_x calculated with HSE functional.

suppressed, leading to enhanced V_{th} stability in the MIS-gate region.

CALCULATION METHOD

The calculations are implemented in the VASP code [10]. The detailed calculation parameters are the same as those reported in [9]. A defect-free *a*-SiN_x sample [Fig. 2(a)] with clean bandgap is generated by a repeated "melt and quench" scheme using *ab-initio* molecular dynamics (AIMD) [11], with the generation sequence depicted in Fig. 1. The radial-distribution function (RDF) curve for the *a*-SiN_x in Fig. 2(b) features a broad distribution of Si-N bond lengths with the average bond length of 1.76 Å and some pretty long interaction distances up to 2.2 Å, consistent with the previous reports, [12] which indicates a reasonable amorphous state. The SiN_x exhibits a bandgap of 5.2 eV by HSE functional correction. The pristine GaN (0001) surface in a 2×2 supercell is built from a wurtzite bulk unit cell. The electronic structures of GaN surface are depicted in Ref. [9]. The SiN_x/GaN interface is built by stacking SiN_x and GaN together with a 12 Å-thickness vacuum to avoid the image interaction. To obtain a realistic interface, the SiN_x slab is initially moved in x, y, and z directions relative to the GaN slab until the energy minima is found. Then the interface undergoes partial relaxation (to release initial artificial stresses), annealing (at 1100 K, around the deposition temperature of LPCVD-SiN_x), cooling (to 0K) and final relaxation (below a 0.05 eV/Å force tolerance level) to reach the stable structure.

RESULTS

Various *a*-SiN_x/GaN interfaces with different interface nitridation conditions are constructed. A Si-rich interface with only Si-Ga bonds at the interface (i.e., without interfacial N-Ga bonds) is specifically studied to understand the non-nitridized interface properties, thus providing reference to acquire the nitridation effects on the SiN_x/GaN interface. The density of states as well as the atomic structure of SiN_x/GaN without nitridation are demonstrated in Fig. 4 (a). We can see that only Si atoms are located at the interface, thus the Si-Ga bonds (with the average bond length of 2.49 Å) are formed at Ga-face GaN surface. Both shallow and deep traps are presented in a wide energy range within the bandgap of GaN. The interface states originate from the Si-Ga bonds at the interface. Such large amount of interface states in the gate region is detrimental to the stability of the gate-controlled channel in GaN MIS-FET.

When GaN surface undergoes nitridation before SiN_x deposition, N atoms can be adsorbed to the GaN surface, leading to modified SiN_x/GaN interfacial atomic arrangement. According to the previous reports, the most stable site to host N-adatom on Ga-face GaN surface is the *H*3 site (i.e., above the hollow site on GaN surface). [9] Various *a*-SiN_x/GaN interfaces with different interface nitridation conditions are constructed to examine the variation tendency with the increased nitridation coverage ratio. The nitridation effects on the interface properties are eminent and mainly reflected in the suppression of interface states. For the interface with nitridation [25% N-adatom coverage, as is shown in Fig. 4 (b)], the interfacial atomic arrangement is

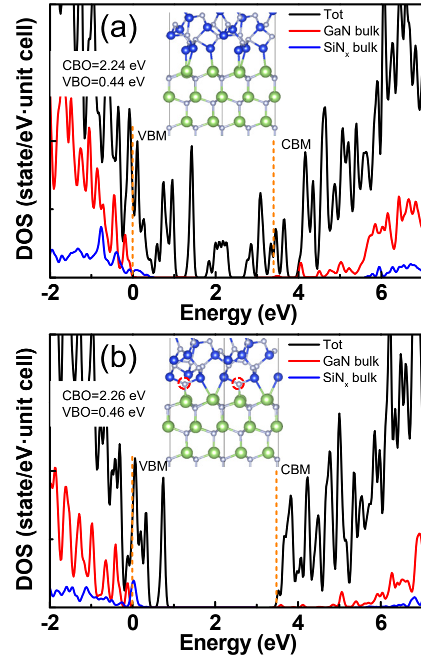

Fig. 4 DOS of *a*-SiN_x/GaN interface (a) without nitridation and (b) with nitridation (25% N-adatom coverage, highlighted by red circle). The black, red and blue lines represent DOS of the interface, GaN bulk and SiN_x bulk, respectively. The corresponding interface atomic arrangements are inserted. The VBM of GaN bulk is aligned at 0 eV.

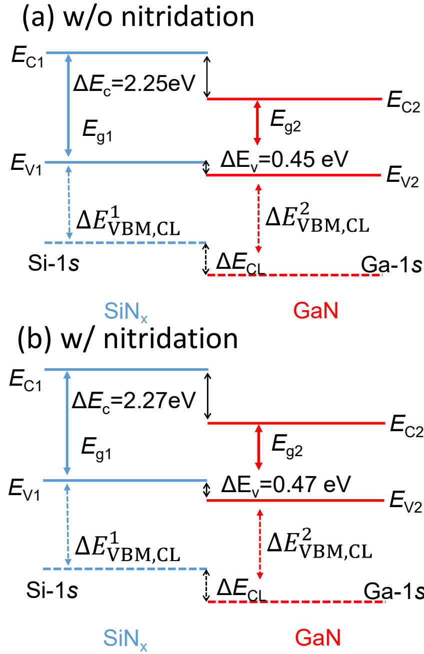

Fig. 5 Band alignments of *a*-SiN_x/GaN interface (a) without nitridation, (b) with nitridation derived by the core level scheme. Si-1*s* and Ga-1*s* core level are applied to align the band edge. The results agree with that obtained by the projected DOS scheme in Fig. 4.

modified. As a result, some of the interfacial Si atoms are passivated by the N-adatoms, thus forming the interfacial Si-N bonds instead of the initial Si-Ga bonds. Consequently, the shallow interface traps are significantly suppressed and the deep traps move downward and become located within a 0.9 eV energy range above the GaN valence band [Fig. 4(b)]. For the interface with higher N-adatom coverage (50%, 75% and even 100%, not shown here), a nitridation interfacial layer is formed and more interfacial Si atoms are passivated. The deep traps gradually merge into the valence band, and the shallow traps mostly disappear, leaving a "clean" interface with negligible trap density. According to the projected DOS of GaN bulk and SiN_x bulk, a type-II band alignment is obtained with a conduction band offset of 2.2~2.3 eV for all the interfaces (labelled in Fig. 4), agreeing with that obtained by electrical characterization [3] and XPS measurement [13]. A more precise band alignment obtained by the core level scheme [14] adopting the calculated Ga-1*s* and Si-1*s* energy level is derived in Fig. 5, which is in accordance with that obtained by the projected DOS results shown in Fig. 4.

The clean bandgap by nitridation indicates effectively suppressed shallow (as well as deep) interface traps in GaN MIS-gate devices. In such device, the interface trap distribution can be modified by nitridation treatment. Correspondingly, the V_{th} stability can be significantly influenced. The shallow traps above the Fermi-level can response to the switching gate control signals. The dynamic charging/discharging of these shallow traps could induce V_{th} instability. In the case of a nitridized interface, there are less shallow traps that can change their charge states during the device switching, leading to the enhanced V_{th} stability. The deeper interface traps are buried below the Fermi-level and behave as "fixed" charge, which less affect the V_{th} stability. This mechanism is exhibited in Fig. 6.

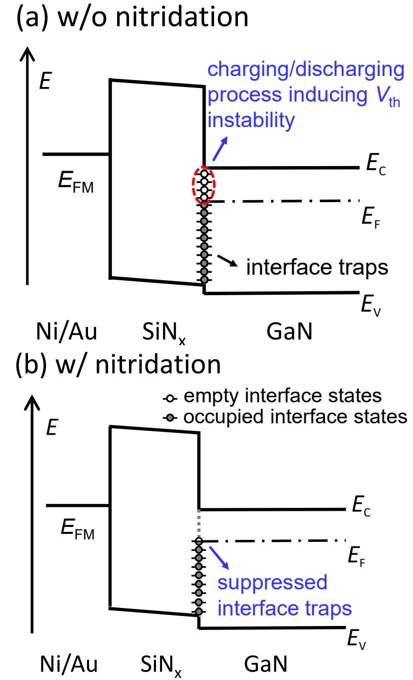

Fig. 6. Schematic band diagram of the metal/SiN_x/GaN MIS structure at *pinch-off* state for (a) without and (b) with interface nitridation. Compared with the interface that SiN_x directly deposited on GaN, density of shallow states of nitridized interface is effectively suppressed, resulting in the enhanced V_{th} stability.

The modification of SiN_x/GaN interface trap density was further verified by the *C-V* measurement in GaN MIS diode with nitridation, which was fabricated with fully recessed gate technique and 2-nm PECVD-SiN_x/17-nm LPCVD SiN_x as gate dielectric layer, as is mainly described in Ref. [3]. The nitridation process was carried out by applying low-energy N_2 plasma prior to the SiN_x deposition. [9] Compared with the diode without nitridation, the diode with nitridation shows remarkably reduced frequency dispersion [Fig. 7(a)]. The extracted D_{it} by conductance method [Fig. 7(b)] proves an effective suppression (more than one order of magnitude) of the interface traps in nitridized GaN MIS-diode. Thus, we can conclude that the nitridation at SiN_x/GaN interface can result in improved interface quality.

CONCLUSION

The microscopic understanding about the modification of interface trap density by nitridation treatment on *a*-SiN_x/GaN interface is revealed by first-principles calculation and verified by *C-V* measurement. The nitridation effects are noticeable and mainly reflected in the suppression of both shallow and deep interface traps by forming the interfacial Si-N bonds. With proper interface nitridation, a clean bandgap

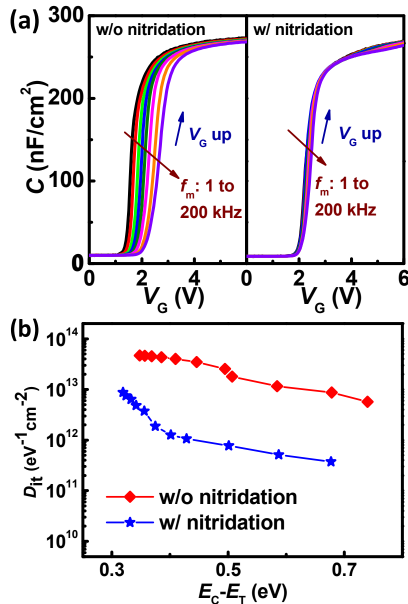

Fig. 7 (a) Measured frequency-dependent *C-V* characteristics of SiN_x/GaN MIS-diode without and with interface nitridation treatment. (b) D_{it}-E_T mapping of GaN MIS diode obtained from the conductance method.

interface structure is obtained. The reduced D_{it} proved by both theoretical calculation and experimental measurement well explains the improved threshold voltage stability in nitridized GaN MIS-gate power and RF device.

ACKNOWLEDGEMENTS

This work was supported in part by Shenzhen Science and Technology Innovation Commission under Grant JCYJ20160229205511222. We thank the technology support from the National Supercomputer Center in Guangzhou (NSCC-GZ) for providing computer resources that contributed to the results reported within this paper.

REFERENCES

[1] K. J. Chen, O. Haberlen, A. Lidow, C. L. Tsai, T. Ueda, Y. Uemoto, and Y. Wu, "GaN-on-Si Power Technology: Devices and Applications," *IEEE Trans. Electron Device,* vol. 64, no. 3, pp. 779-795, Mar. 2017.

[2] M. Ishida, T. Ueda, T. Tanaka, and D. Ueda, "GaN on Si Technologies for Power Switching Devices," *IEEE Trans. Electron Devices,* vol. 60, no. 10, pp. 3053-3059, Oct. 2013.

[3] M. Hua, Z. Zhang, J. Wei, J. Lei, G. Tang, K. Fu, Y. Cai, B. Zhang, and K. J. Chen, "Integration of LPCVD-SiN_x Gate Dielectric with Recessed-gate E-mode GaN MIS-FETs: Toward High Performance, High Stability and Long TDDB Lifetime," in *IEDM Tech. Dig.*, 2016, pp. 10.4.1-10.4.4.

[4] X. Hu, A. Koudymov, G. Simin, J. Yang, M. A. Khan, A. Tarakji, M. S. Shur, and R. Gaska, "Si_3N_4/AlGaN/GaN-Metal-Insulator-Semiconductor Heterostructure Field-Effect Transistors," *Appl. Phys. Lett.,* vol. 79, no. 17, pp. 2832-2834, Aug. 2001.

[5] S. Huang, S. Yang, J. Roberts, and K. J. Chen, "Threshold Voltage Instability in Al_2O_3/GaN/AlGaN/GaN Metal-Insulator-Semiconductor High-Electron Mobility Transistors," *Jpn. J. Appl. Phys.,* vol. 50, p. 110202, Sep. 2011.

[6] S. Huang, Q. Jiang, S. Yang, C. Zhou, and K. J. Chen, "Effective Passivation of AlGaN/GaN HEMTs by ALD-Grown AlN Thin Film," *IEEE Electron Device Lett.,* vol. 33, no. 4, pp. 516-518, Apr. 2012.

[7] S. Yang, Z. Tang, K. Wong, Y. Lin, C. Liu, Y. Lu, S. Huang, and K. J. Chen, "High-Quality Interface in Al_2O_3/GaN/AlGaN/GaN MIS Structures With In Situ Pre-Gate Plasma Nitridation," *IEEE Electron Device Lett.,* vol. 34, no. 12, pp. 1497-1499, Dec. 2013.

[8] Z. Zhang, B. Li, X. Tang, Q. Qian, M. Hua, B. Huang, and K. J. Chen, "Nitridation of GaN surface for power device application: A first-principles study," in *IEDM Tech. Dig.*, 2016, pp. 36.2.1 - 36.2.4.

[9] Z. Zhang, B. Li, Q. Qian, X. Tang, M. Hua, B. Huang, and K. J. Chen, "Revealing the Nitridation Effects on GaN Surface by First-Principles Calculation and X-Ray/Ultraviolet Photoemission Spectroscopy," *IEEE Trans. Electron Device,* vol. 64, no. 10, pp. 4036-4036, Oct. 2017.

[10] G. Kresse and J. Furthmuller, "Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set," *Phys. Rev. B,* vol. 54, no. 16, pp. 11169-11186, Oct. 1996.

[11] E. A. Chagarova and A. C. Kummel, "Ab initio molecular dynamics simulations of properties of a-Al_2O_3/vacuum and a-ZrO_2/vacuum vs a-Al_2O_3/Ge(100)(2×1) and a-ZrO_2/Ge(100)(2×1) interfaces," *J. Chem. Phys.,* vol. 130, p. 124717, Jan. 2009.

[12] L. E. Hintzsche, C. M. Fang, T. Watts, M. Marsman, G. Jordan, M. W. P. E. Lamers, A. W. Weeber, and G. Kresse, "Density functional theory study of the structural and electronic properties of amorphous silicon nitrides: Si_3N_{4-x}:H," *Phys. Rev. B,* vol. 86, p. 235204, Dec. 2012.

[13] T. E. Cook, C. C. Fulton, W. J. Mecouch, R. F. Davis, and G. Lucovsky, "Band offset measurements of the Si_3N_4/GaN (0001) interface," *J. Appl. Phys.,* vol. 94, no. 6, pp. 3949-3954, Jun. 2003.

[14] E. A. Kraut, R. W. Grant, J. R. Waldrop, and S. P. Kowalczyk, "Precise Determination of the Valence-Band Edge in X-Ray Photoemission Spectra: Application to Measurement of Semiconductor Interface Potentials," *Phys. Rev. Lett.,* vol. 44, no. 24, pp. 1620-1623, Jun. 1980.

ACRONYMS

MIS: metal-insulator-semiconductor
FET: field-effect-transistor
D_{it}: density of interface states
V_{th}: threshold voltage
LPCVD: low-pressure chemical vapor deposition