Supporting Information

Insight into the Near-Conduction Band States at the Crystallized Interface between GaN and SiNx Grown by Low-Pressure Chemical Vapor Deposition

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At a high forward gate bias, the conduction behavior of the MIS diodes is well described by Fowler–Nordheim (FN) tunneling model shown below. Hua et al. [1]

already have a systematic study on the temperature-dependent current-voltage (I-V) characteristics of LPCVD-SiN_x/AlGaN/ GaN MIS diodes. It was confirmed the Fowler-Nordheim (FN) tunneling accounted for the current transport mechanism at high forward gate bias.

$$J_{FN} = AE_{OX}^2 \exp(-B / E_{OX}) \quad (1)$$

$$A = 1.54 \times 10^{-6} (m^* \Phi_B)^{-1} \quad (2)$$

$$B = 6.83 \times 10^7 (m^*)^{1/2} (\Phi_B)^{3/2} \quad (3)$$

E_{ox} is the average E-field acrocess LPCVD-SiN_x dielectric, the m^* =0.5 [2,3] is the effective electron mass in the LPCVD-SiN_x and Φ_B is the conduction-band offset ΔE_C. The ΔE_C of 2.4 eV is determined in this work, which is silimar to 2.3 eV abtained by Hua's work.

According to the TEM image and the lattice constants of GaN and Si_2N_2O optimized in the text, five kinds of Si_2N_2O/GaN interfaces are built by combining the Si_2N_2O (100) and GaN(0001) surface. The crystallographic relationship between Si_2N_2O and GaN is $<001>_{Si2N2O}//<11\text{-}20>_{GaN}$ and $<010>_{Si2N2O}//<1\text{-}100>_{GaN}$. Two terminations are possible for the Si_2N_2O slab. For the SiO terminated Si_2N_2O, three stacking possibilities have been taken into account: (a) SiO-termi_TopGa, (b) SiO-termi_TopN, (c) SiO-termi_Hollow. The top stacking (SiO-termi_TopGa and SiO-termi_TopN, Figure S1(a1,b1)) is obtained by placing one of the O atoms in Si_2N_2O surface over the Ga and N atom respectively in the GaN surface. On the other hand, in the hollow stacking (SiO-termi_Hollow, Figure S1(c1)), one of the O atoms in the Si_2N_2O surface is placed at a distance d above the center of the Ga atom in the

GaN surface. For the SiNN terminated Si_2N_2O, two stacking possibilities have been taken into account: (d) SiNN-termi_TopN and (e) SiNN-termi_Hollow. For the top stacking (SiNN-termi_TopN , Figure S1(d1)), one of the N atoms in Si_2N_2O surface is placed above one of the N atom in GaN surface(Figure S1(d2)). For the hollow stacking (SiNN-termi_Hollow, Figure S1(e1)), one of the N atoms in Si_2N_2O surface is placed above the center of Ga atoms in GaN surface(Figure S1(e2)). The repeated distance along the <11-20> and <1-100> directions in GaN , 3×3.216Å and 5.57Å, are adopted as the initio lattice constants that parallel of the interface. Then, both of the size and the atom positions for all the five interfaces are relaxed until the force of each atom is less than $0.02eVÅ^{-1}$. The SiO-termi_TopN and SiO-termi_Hollow interfaces are relaxed to SiO-termi_TopGa interface spontaneously after the full relaxation. While the configuration of SiN-terminated interfaces (Figure S1(d1) and (e1)) are not stable after the fully relaxation. So the SiO-termi_TopGa interface is adopted as the initio model to exploring the electronic structures in this work.

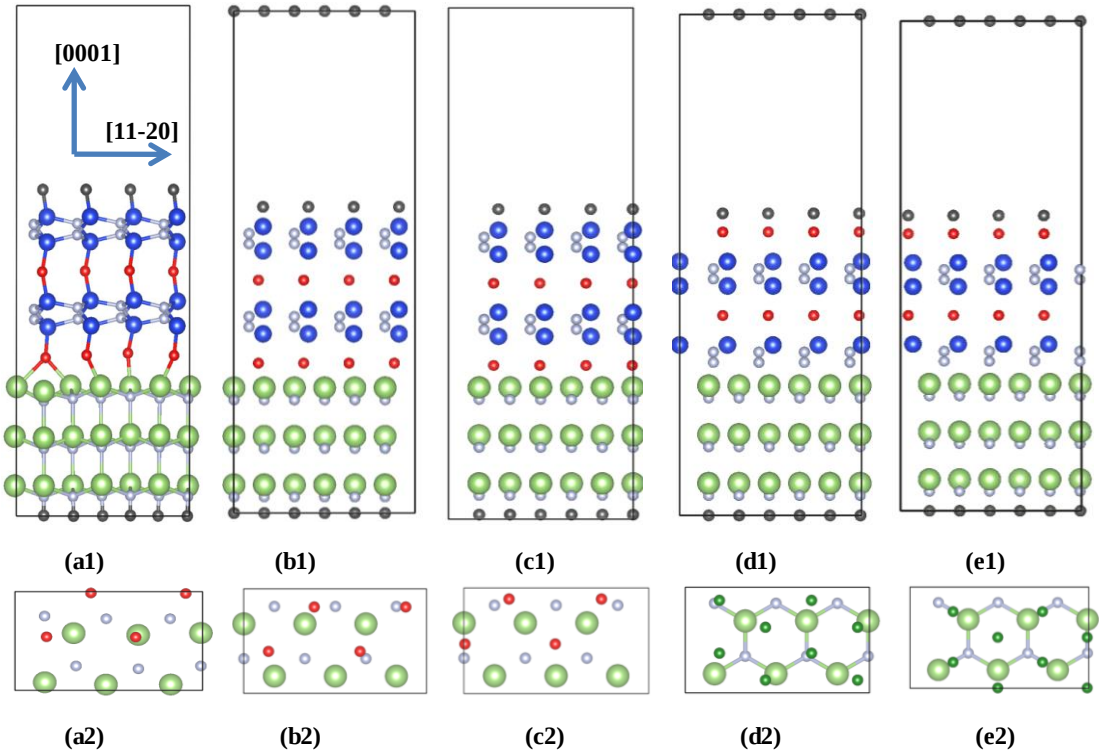

Figure S1. The side view(top) and top view(down) of Si_2N_2O/GaN interface configurations with different combination: SiO-termi_TopGa(a1,a2), SiO-termi_TopN(b1,b2), SiO-termi_Hollow(c1,c2), SiNN-termi_TopN (d1,d2) and SiNN-termi_Hollow(e1,e2). The black, blue, gray, red and green balls denote the H, Si, N, O and Ga toms respectively. In (d2) and (e2) the N atoms from Si_2N_2O are denoted as dark green balls to make the interface structure clearly.

Considering the time consuming of HSE functional in DFT, the pure interface with five GaN bilayers was simulated using the PBE functional to make the thickness test of GaN slab. Layer1&2 denote the first GaN bilayer in GaN surface, layer3&4 denote the second GaN bilayer in GaN surface and so on. As shown in Figure S2, the CBM of two interfaces differs little, while there is a down shift of VBM (about 0.42eV) of interface with five GaN bilayers compared with that contains three GaN bilayers. Both of the CBM of two interfaces are mainly contributed by the states of

first GaN layer. Besides, for the interface with 5 GaN bilayers, the states of 4th and 5th GaN bilayers contribute little to the CBM. The test results denote that the interface with 3 GaN bilayers is thick enough for our concern in this work (the origin of states near the CBM).

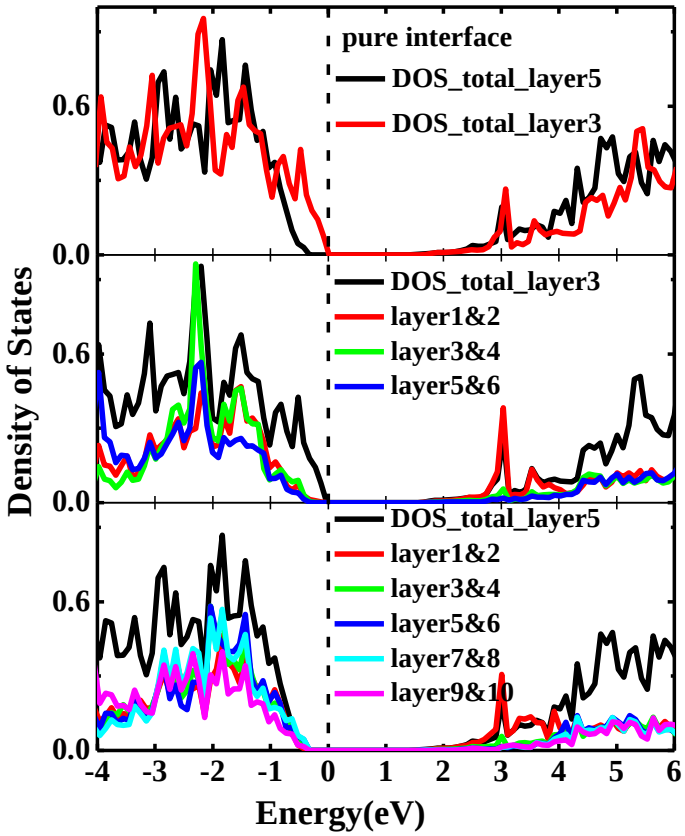

Figure S2. The density of states of Si_2N_2O/GaN interface model with 3 GaN bilayers (DOS_total_layer3) and 5 GaN bilayers (DOS_total_layer5). The vertical dashed lines denote the Valence Band Maximum (VBM) of the interface with 3 GaN bilayers. Here, we align the vacuum energy level of two interfaces.

Apart from the local DOS of the atoms in the vicinity of the Ga atom(Ga72 in Figure S3) with dangling bonds, the local DOS of the first GaN bilayer(including the vicinity N atoms) atoms in pure interface, $O_{GaN\text{-}N}$ and Ga_{Si} interfaces are plotted in Figure S3 to verify the source of the states near the CBM. It can be seen that, the

states of the atoms that far from the Ga72 have rather smaller contribution to the states near CBM compared with that of the main contributors, as shown in Figure 7 in our work.

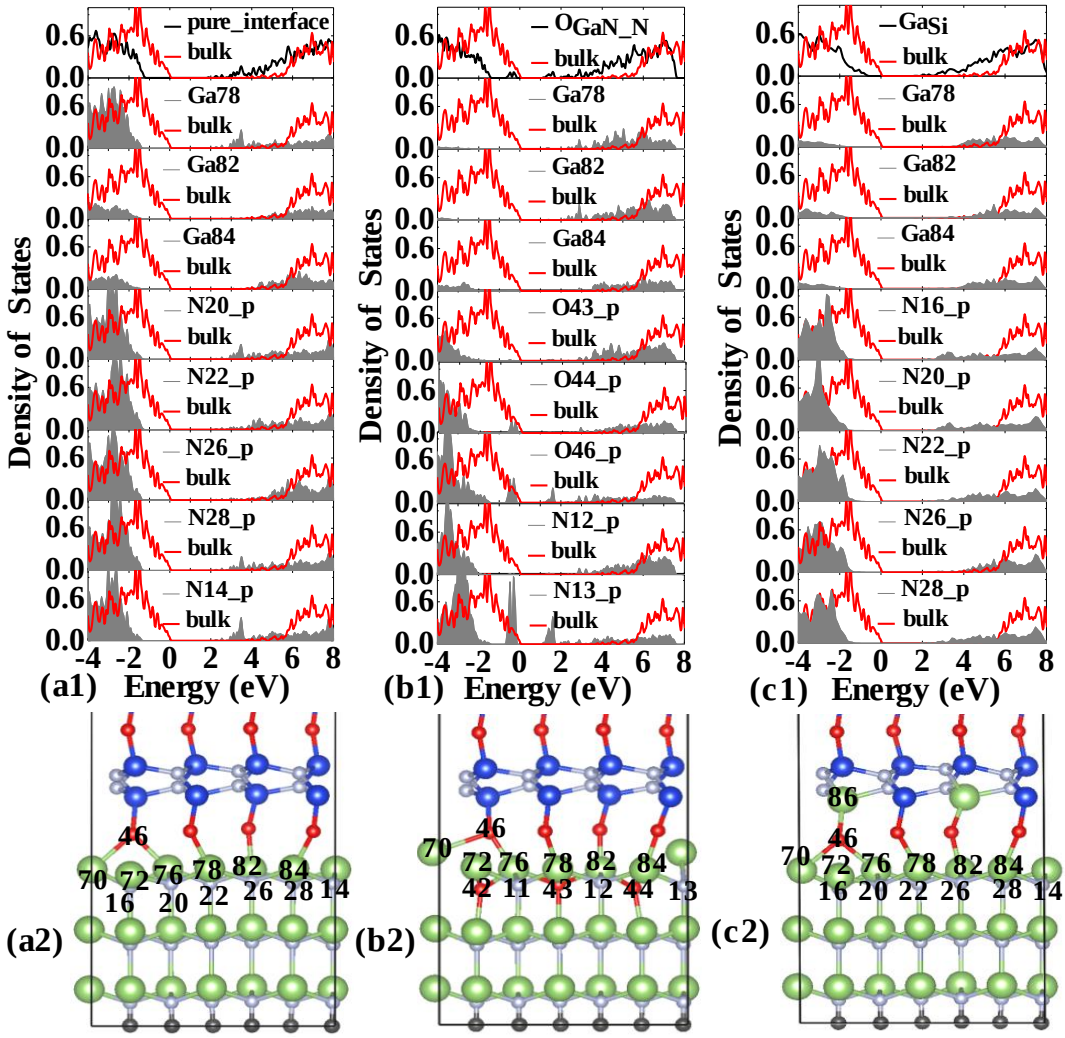

Figure S3. The local density of states of pure(a1), O_{GaN-N}(b1) and Ga_{Si}(c1) interfaces and their configurations of pure(a2), O_{GaN-N}(b2) and Ga_{Si}(c2) interfaces respectively. Here, the numbers on the elements denote the serial numbers of the corresponding atoms only. The density of states of N14 atom is not shown in (c1) as it is similar with that of N20 atom. The black, gray, blue, read and green balls denotes the H, N, Si, O and Ga atoms respectively.

Figure S4 indicates that there is little DOS near the CBM (~3.4 eV) in the Si_{Ga}

interface. Although this configurtion is of little help to analyze the origin of the NCB states, it doesn't mean that this kind of situation does not exist. The unsaturated bonds (Ga47 and Si55) and its vicinal atoms also contribute an important amount to the DOS far beyond the CBM and deep into the bandgap. It needs a further investigation.

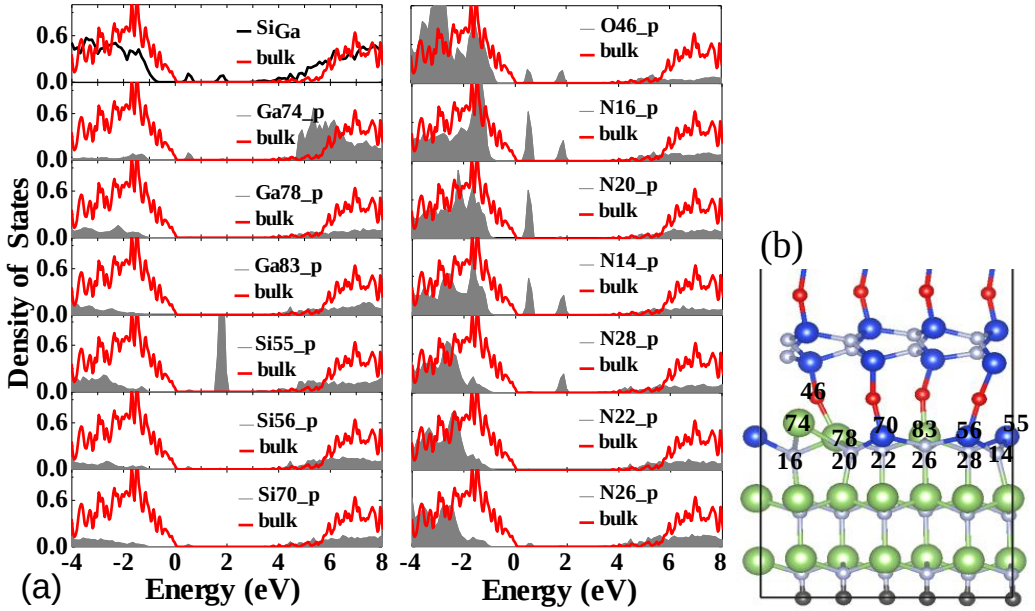

Figure S4. The local density of states of SiGa interface(a) and the configuration(b). Here, the numbers on the elements denote the serial numbers of the corresponding atoms only. The black, gray, blue, read and green balls denotes the H, N, Si, O and Ga atoms respectively.

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