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The Role of Ga(Gallium)-flux and AlN(Aluminum Nitride) as the Interface Materials, between (Ga-face)GaN and (Si-face)4H-SiC, through Molecular Dynamics Simulation

Srikanta Bose+, and Sudip K. Mazumder

Abstract**—**We report here, the results of molecular dynamics simulation of *p*-doped (Ga-face)GaN over *n*-doped (Si-face)(0001)4H-SiC hetero-epitaxial material system with one-layer each of Ga-flux and (Al-face)AlN, as the interface materials, in the form of, the total Density of States (DOS). It is found that the total DOS at the Fermi-level for the heavily *p*-doped (Ga-face)GaN and *n*-doped (Si-face)4H-SiC hetero-epitaxial system, with one layer of (Al-face)AlN as the interface material, is comparatively higher than that of the various cases studied, indicating that there could be good vertical conduction across the (Ga-face)GaN over (Si-face)(0001)4H-SiC hetero-epitaxial material system.

Keywords**—**Molecular dynamics, GaN, 4H-SiC, hetero-epitaxy.

I. INTRODUCTION

GaN and 4H-SiC as bulk materials (both have Space Group of $P6_3mc$ (186) with hexagonal Wurzite structure) offer great potentials for high-temperature and power-electronics applications due to their attractive material properties such as large bandgap energies, high breakdown fields and high thermal conductivities [1]-[4]. In addition, GaN has very good optical absorption coefficient and short carrier life time [1]-[4]. It would be preferable, if we have a semiconductor device which can possess excellent power handling capabilities, high thermal capacity and also can be optically controlled efficiently, to avoid any electro-magnetic-interference (EMI). In order to retain above qualities in a single device, direct hetero-epitaxial growth of GaN over 4H-SiC and vertical conduction, is the possible answer and we have already observed quite interesting features in our preliminary investigated simulation results [5], for a vertical *npn*-device, using above two materials.

The materials, GaN and 4H-SiC have a lattice mismatch of ~ 3.4%. So, to avoid this lattice mismatch, researchers have tried to grow GaN epitaxy, over a buffer layer of AlN [6]-[8] and studied the lateral conduction, which is entirely through GaN.

The authors are with the Laboratory for Energy and Switching-Electronics System, Department of Electrical and Computer Engineering, University of Illinois at Chicago, 851 South Morgan Street, Science and Engineering Office, Room No. 1020, Mail Code 154, Chicago, IL: 60607-7053 (+phone: 312-996-6548; fax: 312-996-6465; e-mail: sribose@ece.uic.edu).

But, investigations on vertical conduction are rarely available in the literatures [9]-[16]. In lateral devices, only the properties of GaN are exploited, however if we want to exploit the properties of 4H-SiC, as well, which are highly suitable for power-electronics applications, a vertical conduction approach has to be made. This is possible, if we can grow GaN directly above 4H-SiC without any buffer layer. To achieve this, Ga-flux has been used over (Si-face)(0001)4H-SiC, experimentally [15], [16], before actually growing GaN epitaxial layers.

In this work, we report, the total Density of States (DOS), for the *p*-doped (Ga-face)GaN over *n*-doped (Si-face)4H-SiC hetero-epitaxial material system with Ga-flux and (Al-face)AlN, as the interface materials, from the atomistic standpoint, by carrying out Molecular Dynamics simulations, using $DMol^3$ first-principle atomistic simulator [17] module of Material studio 5.0 [18], with the help of NCSA (National Center for Supercomputing Applications at University of Illinois Urbana-Champaign, US) Intel 64 Cluster Abe [19].

II. SIMULATION METHOD

While performing the Molecular Dynamics simulation (the supercell approach was adopted where the total no. of atoms in the cell was kept sixty and the atoms in (Si-face)4H-SiC were constrained whereas Ga, Al and N atoms were relaxed), the following major considerations were set in the $DMol^3$ first-principle atomistic simulator:

Ensemble: NVT
DFT exchange-correlation: LDA/PWC
Thermostat: Simple Nose-Hoover
External stress: 0 GPa
Temperature: 800 K (This value of temperature was considered in view of experimental setting [15], [16])
Given simulation time: 0.5 ps
Core-treatment: All-electron with Harris approximation
K-point set: Medium

III. RESULTS AND DISCUSSION

Fig. 1 shows a typical initial setup for Molecular Dynamics simulation for Ga-fluxed *p*-doped GaN over heavily *n*-doped (Si-face)4H-SiC hetero-epitaxial material system. Figs. 2(a),

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2(b), and 2(c) show the total density of states (DOS) of *p*-doped GaN over *n*-doped (Si-face)4H-SiC, heavily *p*-doped GaN over *n*-doped (Si-face)4H-SiC, *p*-doped GaN over heavily *n*-doped (Si-face)4H-SiC, hetero-epitaxial material systems, with one-layer of Ga-flux as the interface material whereas Figs. 3(a), 3(b), and 3(c) show the total density of states (DOS) of *p*-doped GaN over *n*-doped (Si-face)4-SiC, heavily *p*-doped GaN over *n*-doped (Si-face)4H-SiC, *p*-doped GaN over heavily *n*-doped (Si-face)4H-SiC, hetero-epitaxial material systems, with one-layer of (Al-face)AlN as the interface material. We replace the Ga-site with one Magnesium(Mg) atom for *p*-doped GaN and two Mg atoms for heavily *p*-doped GaN and similarly, C-site of 4H-SiC is replaced with one Nitrogen(N) atom for *n*-doped 4H-SiC and two N atoms for heavily *n*-doped (Si-face)4H-SiC. The energy unit has been converted from Hartree to ElectronVolt (1 Ha =~ 27.2 eV) while reporting the DOS value.

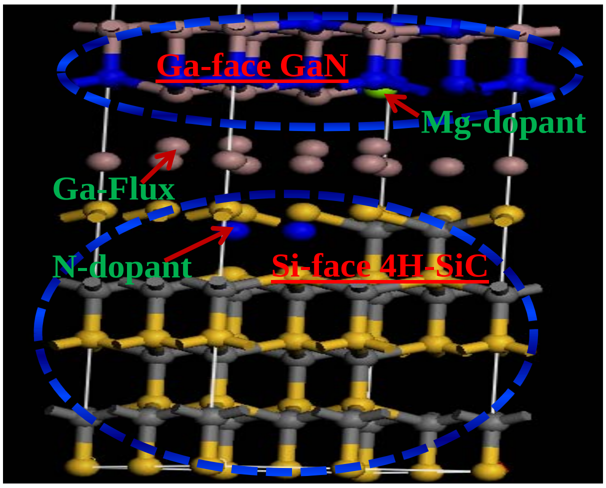

Fig. 1 A typical initial setup for Molecular Dynamics simulation for Ga-fluxed *p*-doped GaN over heavily *n*-doped (Si-face)4H-SiC hetero-epitaxial material system.

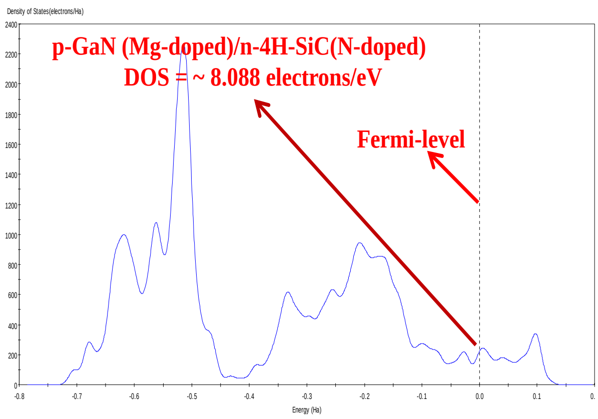

Fig. 2(a) The total density of states (DOS) of *p*-doped GaN over *n*-doped (Si-face)4H-SiC hetero-epitaxial material system, with one-layer of Ga-flux as the interface material.

Fig. 3(b) shows the maximum DOS at the Fermi-level for heavily *p*-doped GaN over *n*-doped (Si-face)4H-SiC hetero-epitaxial material system, with one-layer of (Al-face)AlN as the interface material. The element Mg has valence electrons in $3s^2 3p^0 3d^0$. That means the p and d-orbitals are vacant which means, these are holes (or minority carrier density) ready to be occupied by electrons. The maximum no. of electrons that can be accommodated in p and d- orbitals are 6 and 10, respectively. So, the minority carrier density is quite high in case of Mg-*dopant*. The element N has valence electrons in $2s^2 2p^3$, which means there are 3 unpaired electrons available out of which 2 will go to Si so that it can satisfy the Octet. So, the element N is left with 1 electron which will act as free electron i.e., the majority carrier density is quite low in case of N-*dopant*. The element Ga has valence electrons in $4s^2 4p^1 4d^0 4f^0$. The element Al has valence electrons in $3s^2 3p^1$. In case of Ga-flux *p+-n* hetero-epitaxial material system, the one unpaired electron from Ga will either go to Si or Mg, thereby reducing the DOS. In the absence of AlN, the *p+-n* hetero-epitaxial material system, has 2 Mg-*dopant* atoms whose p and d orbitals vacant and only one N-*dopant* atom. Since no free electrons are available in the one-layer of (Al-face)AlN material, it does not affect the DOS of the hetero-epitaxial material system and prevents the one freely available electron of N-*dopant* of 4H-SiC to be shared either by Mg-*dopant* or Ga of GaN.

IV. Conclusion

We have carried out the molecular dynamics simulation and provided the theoretical explanations in terms of total Density of States (DOS), for *p*-doped GaN over *n*-doped (Si-face)4H-SiC hetero-epitaxial material system with Ga-flux and (Al-face)AlN as the interface materials. We observed that the total DOS at the Fermi-level for heavily *p*-doped GaN over *n*-doped (Si-face)4H-SiC hetero-epitaxial material system, with one-layer of (Al-face)AlN as the interface material, exceeds the various other doped cases, signifying that there is a possibility of good vertical conduction across the (Ga-face)GaN over (Si-face)(0001)4H-SiC hetero-epitaxial material system with one-layer of (Al-face)AlN, as the interface material.

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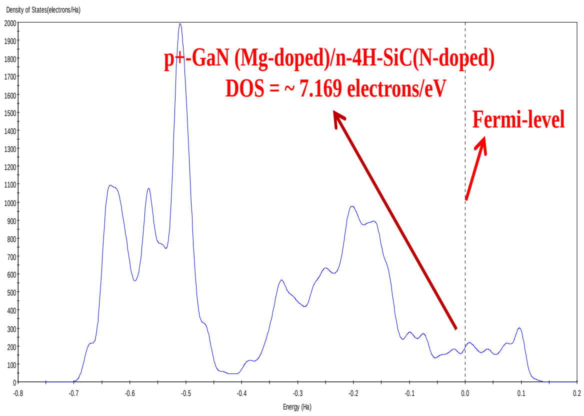

Fig. 2(b) The total density of states (DOS) of heavily *p*-doped GaN over *n*-doped (Si-face)4H-SiC hetero-epitaxial material system, with one-layer of Ga-flux as the interface material.

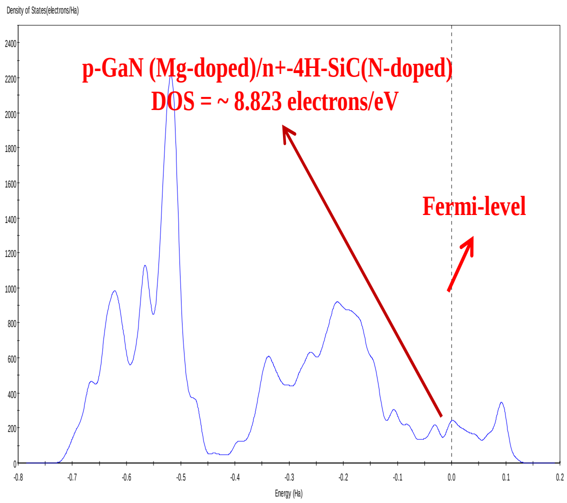

Fig. 2(c) The total density of states (DOS) of *p*-doped GaN over heavily *n*-doped (Si-face)4H-SiC hetero-epitaxial material system, with one-layer of Ga-flux, as the interface material.

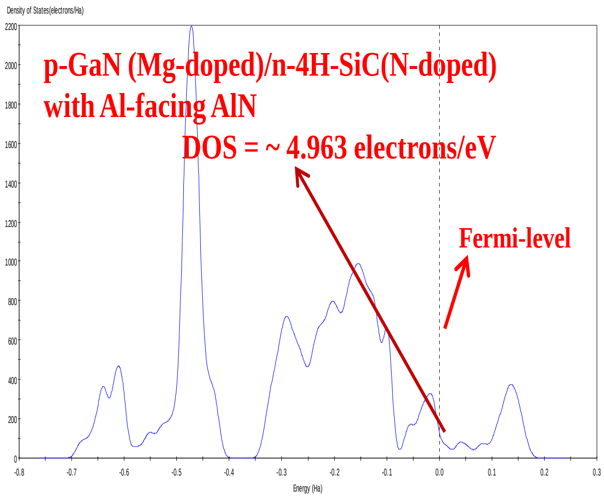

Fig. 3(a) The total density of states (DOS) of *p*-doped GaN over *n*-doped (Si-face)4H-SiC hetero-epitaxial material system, with one-layer of (Al-face)AlN as the interface material.

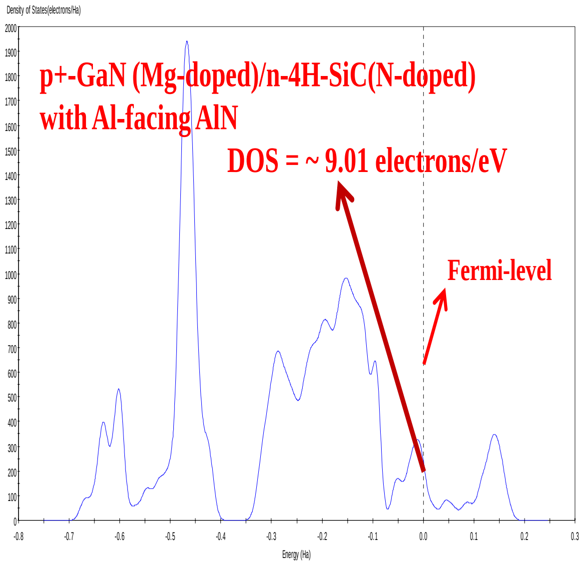

Fig. 3(b) The total density of states (DOS) of heavily *p*-doped GaN over *n*-doped (Si-face)4H-SiC hetero-epitaxial material system, with one-layer of (Al-face)AlN as the interface material.

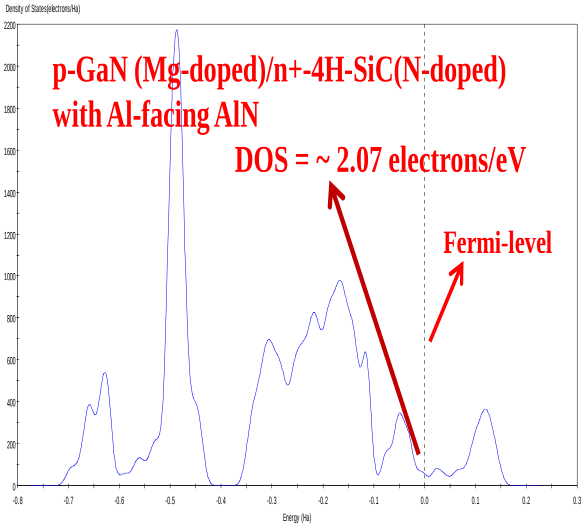

Fig. 3(c) The total density of states (DOS) of *p*-doped GaN over heavily *n*-doped (Si-face)4H-SiC hetero-epitaxial material system, with one-layer of (Al-face)AlN as the interface material.

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