Presented at the DLSU Research Congress 2017
De La Salle University, Manila, Philippines
June 20 to 22, 2017

First Principles Study of Structural and Electronic Properties of GaAs(001)- ß(2x4) Surface Defects

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Abstract: In this work, we investigate the defects located on the surface of GaAs(001)- ß(2x4), namely, As antisite (AsGa), Ga antisite (GaAs), and Ga vacancy (GaV). The changes in the atomic and electronic structure as compared to the clean surface are drawn using first principles calculations based on density functional theory (DFT). The DFT implementation within the projector augmented wave (PAW) potentials to describe the ion-electron interaction and within the hybrid exchange-correlation functional to show the electron-electron interaction gives surface geometries in good agreement with experiments. Significant changes in the geometry around the defects are noted. In terms of the electronic structure, states appear at the gap for all defects. However, the energy levels and the band widths are different. The presence of these distinct point defects introduced bound electrons and holes, which are manifested by the additional donor and acceptor defect levels in the band structure calculation. These results reveal that both atomic structure and energy levels, in terms of density of states (DOS) and band structure, can show definite changes depending on the defect nature on the surface.

Key Words: LT-GaAs; point defects; density functional theory

1. INTRODUCTION

The low-temperature-grown gallium arsenide (LT-GaAs) has been used for the generation and detection of terahertz (THz) radiation. Experimental and theoretical studies have been conducted to optimize its application in THz technology. One of the remarkable properties of LT-GaAs is the ability to absorb long wavelength signals (e.g., 1.55µm) when used as photoconductive (PC) antenna (Tani et al., 2000). It was suggested that this behavior is due to the two-step photon absorption mediated by midgap states, formed by defects (Tani et al., 2000). Recently, this sub-bandgap-optical-excitation induced photoconductivity

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(SOEP) using a 1560nm probe was also reported (Rämer et al., 2013). Particle-induced x-ray analysis revealed that LT-GaAs consists of 1-1.25 at % excess As (Liliental-Weber et al., 1991), which has been suggested as the source of EL2-like defect (0.68eV-0.8eV) (YU and Robinson, 1994). Several other deep-level defects were noted in many studies (Palovic and Desnica, 1998), which were believed to have originated from other type of point defects. The presence of these point defects and their role in the creation of deep-level states has been previously investigated (Schultz, 2016; Reddy et al., 1996), however, much remained unclear in the defect structure – electronic relationships due to the structural complexity of LT-GaAs. On the surface of LT-GaAs alone, various GaAs (001) phases have been observed (Schmidt and Bechstedt, 1996). However, the (2x4) reconstruction was noted to be prevalent. Specifically, β(2x4) was found to be one of the more energetically stable surface reconstructions for a wide range of arsenic chemical potential (Northrup and Froyen, 1993).

In this work, we examined the structural and electronic properties of GaAs(001)- β(2x4) with defects on the surface, namely, (1) As antisite (AsGa) or As occupying a Ga site; (2) Ga antisite (GaAs) or Ga occupying an As site; (3) and Ga vacancy (GaV) or Ga leaving its crystallographic site. Since, experimental characterization of these defects and their systematic influence on the electronic properties of the system are rare and that first-principles methods can now allow isolation of the complex defects characteristics and unambiguously determine effects on electronic structure, then this present study will provide the correlation between structural changes due to each of the defects and the consequent electronic properties.

2. MODELS AND COMPUTATIONAL METHOD

The present calculations are based on the DFT with the generalized gradient approximation by Perdew-Burke-Ernzerhof (GGA-PBE) (Perdew et al., 1996) function and within the projector-augmented-wave (PAW) (Blochl, 1994) pseudopotentials implemented in Vienna ab-initio simulation package (VASP) code. The system used to model the clean and the surface with point defects consist of 8 layers of alternating As and Ga atoms passivated with hydrogen. The β(2x4) corresponds to three As dimers at the top of GaAs(001) surface in As rich condition. The bottom half layer is frozen to mimic the surface of the bulk and a vacuum thickness of 12Å is used to separate the slabs.

3. RESULTS AND DISCUSSION

3.1 Structural Properties

The optimized structure of clean GaAs(001)-β(2x4) is shown in Fig. 1, where a dimerization of surface As atoms occurred. The surface dangling bonds buckle together to form the three As dimers with a bond distance (A-B) of 2.53Å. This is in excellent agreement with experiment (2.48 □ 0.2 Å) using reflection high-energy electron diffraction (RHEED) (Witte and G. Meyer-Ehmsen, 1995).

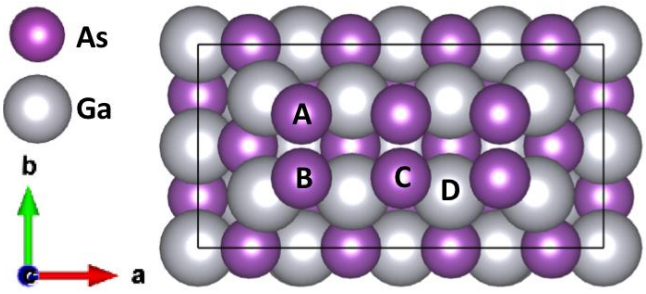

Fig. 1. Top view of the optimized clean GaAs(001)-β(2x4).

The introduction of various surface point defects resulted to significant geometrical changes in terms of dimer distance (A-B), dimer-dimer distance (B-C), and Ga-As distance (C-D). Among the defects,

the AsGa is found to be the most stable while the GaV is the least stable.

3.2. Electronic Properties

To further analyze the surface properties of GaAs(001)- ß(2x4), the electronic structure in terms of the DOS are investigated and the results are shown in Fig. 2.

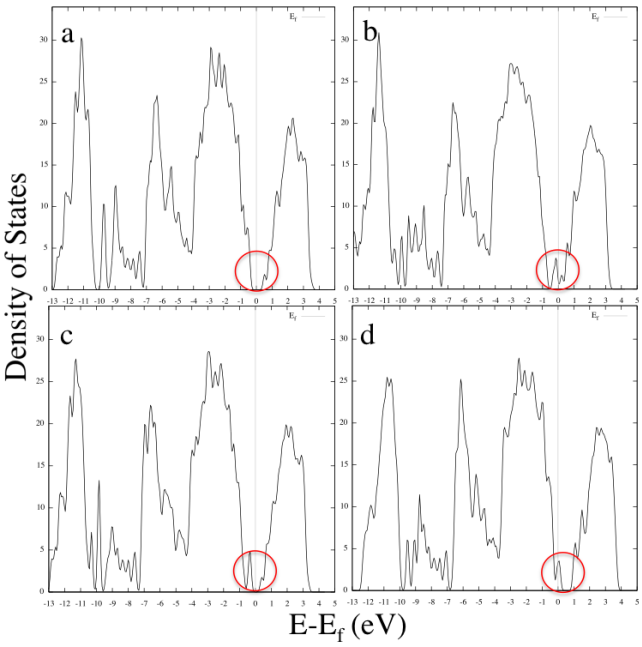

Fig. 2. Calculated DOS of (a) clean GaAs(001)- ß(2x4) and with (b) AsGa, (c) GaAs, (d) GaV points defects

The clean GaAs(001)- ß(2x4) surface exhibit a gap that is free of surface states. Shifting of states is observed upon introduction of point defects. This refers to the presence of several midgaps and shoulder peaks in Fig. 2. These peaks are mainly due to p orbitals as revealed by the calculated partial density of states. They also represent the localized bands in the projected band structure calculations as shown in Fig. 3.

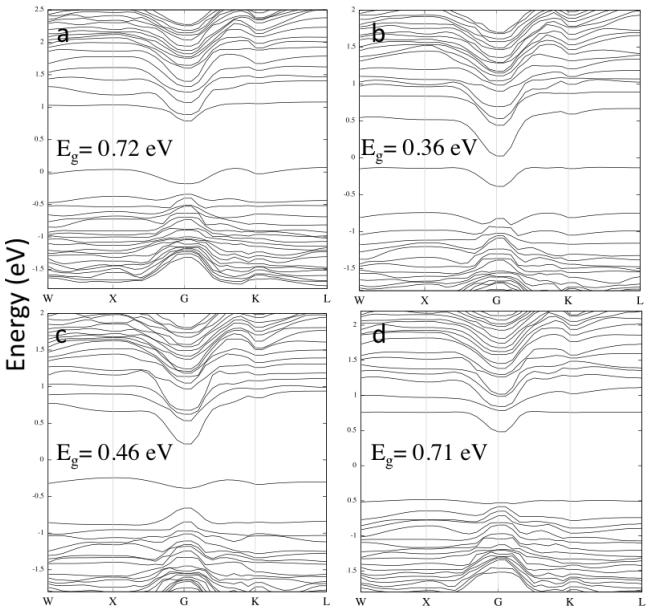

Fig. 3. Band structures for (a) clean GaAs(001)- ß(2x4) and with (b) AsGa, (c) GaAs, (d) GaV points defects.

The shifting of band gap is noticeable in the presence of various point defects as compared to the clean surface. Calculations on the partial charge distribution as seen in Fig. 2 revealed that such localized bands are primarily due to the atom in a particular point defect.

4. CONCLUSIONS

In this study, we have carried out the first principles calculations for the structural and electronic properties of GaAs(001)- ß(2x4) with AsGa, GaAs, and GaV point defects. Our calculated results showed that significant changes in the geometric structure, especially in terms of dimer distances, occurred upon the introduction of these point defects. These changes extend beyond the electronic structure, in terms of DOS and band structure calculations. The presence of these point defects shifted the energy levels. This research is significant in gaining helpful insights for application of LT-GaAs in low noise photoconductive detection and in efficient photoconductive emission in THz technology.

5. ACKNOWLEDGMENTS

This study is conducted using ACCMS Supercomputer in University of Kyoto and High Performance Computing Cluster of Fukui (HPCCF) of Escaño Research Group in University of Fukui, Japan under the financial support of Research Center for Development of Far-Infrared Region, Tenure-Track Program for Innovative Research, Center for information Initiative (CII), University of Fukui. D. B. acknowledges the Department of Science and Technology-Science Education Institute (DOST-SEI) and the Computational Materials Design Research Group of the Physics Department in DLSU for his graduate studies..

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