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Point Defect and Their Influence on the Atomic and Electronic Structure of β-$(Al_xGa_{1-x})_2O_3$ Alloys by STEM-EELS

Adrian Chmielewski[1], Sarah Deng[2], Parivash Moradifar[1], Leixin Miao[1], Kleyser Agueda Lopez[1], Akhil Mauze[3], Yuewei Zhang[3], James Speck[3], Wolfgang Windl[2] and Nasim Alem[1]

[1]Pennsylvania State University, University Park, Pennsylvania, United States, [2]The Ohio State University, Columbus, Ohio, United States, [3]University of California Santa Barbara, Santa Barbara, California, United States

β-Ga_2O_3 is considered an ideal material system for power electronics at extreme environments. Due to its high band gap, β-Ga_2O_3 has a high breakdown voltage (8 $MV.cm^{-1}$) and high resistivity to electric field and temperature. The electronic properties of β-Ga_2O_3 can be improved by incorporating a variety of dopants into the matrix such as Al, adding great flexibility to device design as in modulation doped field effect transistors of β-$(Al_xGa_{1-x})_2O_3/Ga_2O_3$ heterostructures [1].

In this study we use high resolution Annular Dark Field (ADF)-Scanning Transmission Electron Microscopy (STEM) and Electron Energy Loss Spectroscopy (EELS) to uncover the interfacial and electronic structure of β-$(Al_{0.2}Ga_{0.8})_2O_3$/β-Ga_2O_3 epitaxial film grown by molecular beam epitaxy technique. This investigation shows presence of various point defects across the interface in b-$(Al_{0.2}Ga_{0.8})_2O_3$/β-Ga_2O_3 interface. EELS is further used to understand how the electronic structure is modulated. This study further investigates the distribution and coordination of Al, as well as Al and Ga interstitials in β-$(Al_{0.2}Ga_{0.8})_2O_3$/β-Ga_2O_3 epitaxial film. Figure 1 shows a high resolution ADF-STEM image of the β-$(Al_{0.2}Ga_{0.8})_2O_3$/β-Ga_2O_3 interface. Interestingly the number of Al/Ga interstitials (highlighted by yellow circles) increases at the interface. In order to describe the effect of these defects on the electronic properties, we have performed EELS scan across the interface to probe the volume plasmon of Ga, as shown in Figures 1.b. We observed a blueshift in the volume plasmon energy which suggests that the free electron density across the β-$(Al_{0.2}Ga_{0.8})_2O_3$/β-Ga_2O_3 interface increases [2]. The increase in the electron density is due to the presence of Al/Ga interstitials across the interface and leads to presence of excess charges at the interface. .

Density functional theory (DFT) calculations have been carried out with the Vienna Ab initio Simulation Package (VASP), to get insight at atomic scale of the interstitial defect within the β-$(Al_{0.2}Ga_{0.8})_2O_3$ film [3]. Two initial β-$(Al_{0.2}Ga_{0.8})_2O_3$ structures were generated and studied. We considered both Ga interstitials and Al interstitials in the calculations. Ga interstitials induce distortion of certain nearest neighbors creating new interstitial atoms pushed from their initial positions acting as deep-level donor whereas distortions caused by Al interstitials creates a shallow donor state. These findings provide great insight into the fabrication of gallium-oxide based devices.

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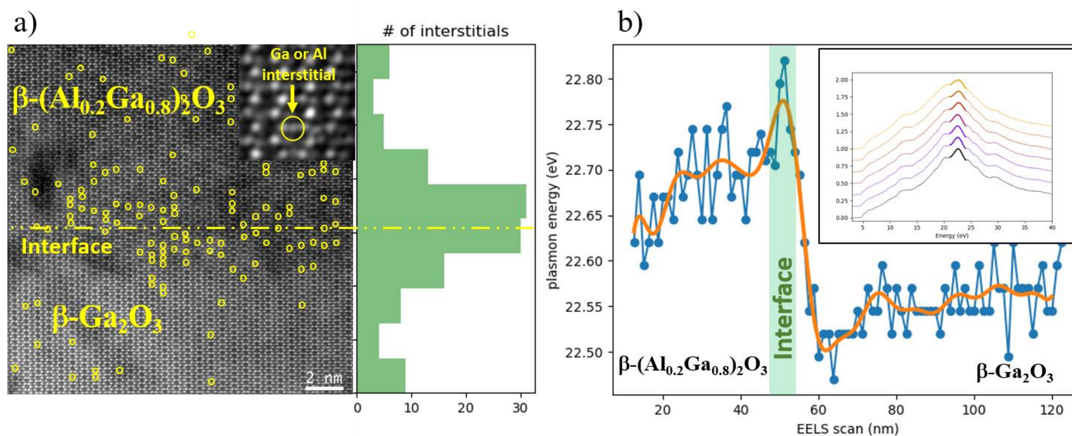

Figure 1. (a) HR-STEM image of the β-$(Al_{0.2}Ga_{0.8})_2O_3$/β-Ga_2O_3 interface in the [001] projection. Yellow circles are highlighting the Al and/or Ga interstitial as shown in the zoom-in image on the insert. (b) Plasmon energy variation across the β-$(Al_{0.2}Ga_{0.8})_2O_3$/β-Ga_2O_3 interface based on volume plasmon peak fitting as shown in the insert.

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