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Investigation of the Atomic and Electronic Structure of β-$(Al_{0.2}Ga_{0.8})_2O_3$ Alloys by STEM-EELS

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As a group III wide band gap (WBG) oxide, 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. In addition, β-Ga_2O_3 can serve as an ideal lattice-matched substrate for group III nitride optical applications while maintaining transparency. β-Ga_2O_3 has been intensively investigated as a wide band-gap semiconductor for solar-blind UV photodetectors [1] and high-power transistors [2]. Band gap engineering can be accomplished by incorporating a variety of dopants into the matrix, adding great flexibility to device design. Modulation doping of $(Al_xGa_{1-x})_2O_3/Ga_2O_3$ heterostructures can be used to spatially separate the ionized donors in the $(Al_xGa_{1-x})_2O_3$ film from the conduction electrons in the Ga_2O_3 film, highly increasing the electron mobility by suppressing scattering from the ionized impurities.

In this study we show the interfacial structure and the band gap modulation in a β-$(Al_{0.2}Ga_{0.8})_2O_3/\beta$-$Ga_2O_3$ epitaxial film using high resolution scanning/transmission (HR-S/TEM) imaging and electron energy loss spectroscopy (EELS). In addition, this study further investigates the distribution of the dopants, such as Al and Mg, as well as oxygen vacancies in β-$(Al_{0.2}Ga_{0.8})_2O_3/\beta$-$Ga_2O_3$ epitaxial film. Figure 1 shows a HR-STEM image of the β-$(Al_{0.2}Ga_{0.8})_2O_3/\beta$-$Ga_2O_3$ interface. β-$(Al_{0.2}Ga_{0.8})_2O_3/\beta$-$Ga_2O_3$ with a 20% concentration of Al is obtained by plasma assisted molecular beam epitaxy (PAMBE).

This study investigates the distribution of the dopants within the matrix to further uncover the oxygen vacancy cluster within the lattice in the β-$(Al_{0.2}Ga_{0.8})_2O_3$ film. Oxygen vacancies can modulate the band gap and electronic structures further affecting the efficiency of power devices. In order to measure the band gap of the β-$(Al_{0.2}Ga_{0.8})_2O_3$ and its variation with respect to the β-Ga_2O_3 substrate, we have performed EELS scan across the interface, as shown in Figures 1(b-c). Using a polynomial fitting, we observe a modulation and an increase in the band gap across the interface with the addition of Al in the lattice. This band gap modulation across the β-$(Al_{0.2}Ga_{0.8})_2O_3/\beta$-$Ga_2O_3$ interface is in a good agreement with the recent density functional theory calculations performed on β-$(Al_{0.2}Ga_{0.8})_2O_3$ [3]. This study uncovers the changes in the atomic and electronic structure in β-$(Al_{0.2}Ga_{0.8})_2O_3$ with the addition of dopants and substitutional elements. This understanding is the key for further design of electronic devices of this crystal.

References:

[1] T. Oshima, T. Okuno et al., Appl. Phys. Express **1** 011202 (2018)
[2] M. Higashiwaki, K. Sasaki et al., Appl. Phys. Lett. **100**, 013504 (2012)
[3] T. Wang et al, Phys. Rev. A. **10**, 011003 (2018)

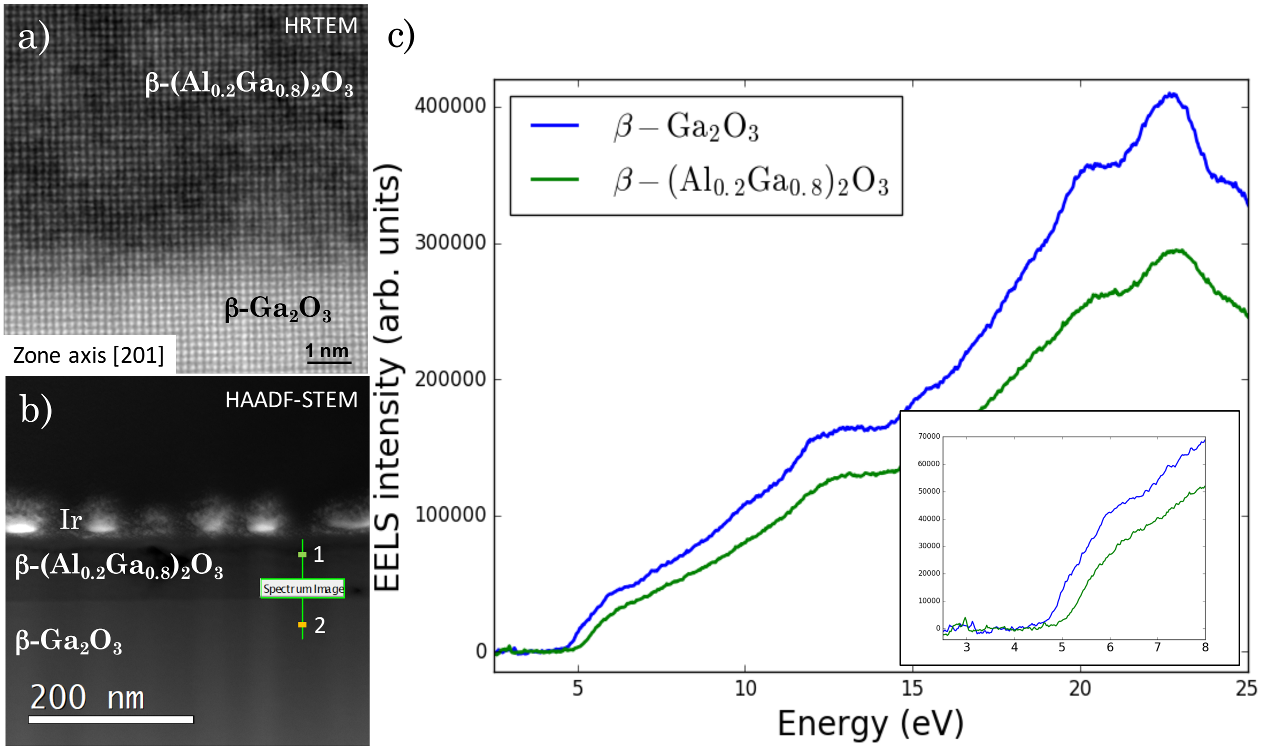

Figure 1. (a) HR-STEM image of the β-(Al$_{0.2}$Ga$_{0.8}$)$_2$O$_3$/β-Ga$_2$O$_3$ interface. (b) HAADF-STEM image of the β-(Al$_{0.2}$Ga$_{0.8}$)$_2$O$_3$/β-Ga$_2$O$_3$ sample under study. EELS line (in green) was performed to study the band gap offset between β-(Al$_{0.2}$Ga$_{0.8}$)$_2$O$_3$ (point 1) and β-Ga$_2$O$_3$ (point 2). (c) Green line: EELS spectrum corresponding to β-(Al$_{0.2}$Ga$_{0.8}$)$_2$O$_3$ (point 1 on Figure 1(b)). Blue line: EELS spectrum of β-Ga$_2$O$_3$ (point 2 on Figure 1(b)). Insert: Zoom-in on the band gap offset between β-(Al$_{0.2}$Ga$_{0.8}$)$_2$O$_3$ and β-Ga$_2$O$_3$.