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Point and Extended Defects in Ultra Wide Band Gap β-Ga_2O_3 Interfaces

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β-Ga_2O_3 has been recently gaining significant attention as a great candidate material for ultra wide band gap (UWBG) electronic, optical, and power device applications. Its ~ 4.9 eV band gap is nearly the highest among the known wide band gap materials [1], and it also has other unique advantages, including the high break down voltage, the transparency and conductivity up to ultraviolet region, and availability as inexpensive bulk-grown single crystal substrates. Despite these advantages, many of the basic properties of β-Ga_2O_3 are still not fully understood. The main issues include the lack of understanding on the exact origin of the intrinsic *n*-type behavior, low doping efficiency, difficulties in *p*-type doping, and the detailed connection between the impurities and the electronic/optical properties [2]. These issues are directly related to the point defects in β-Ga_2O_3, and therefore new understanding on the exact physical nature of the point defects and how they are related to the basic properties of the material will be required to control the properties of β-Ga_2O_3 and advance the material for high-performing, highly-efficient UWBG device applications. In particular, the detailed information on how the cation and oxygen vacancies are distributed, how the impurity atoms incorporate into the atomic structure and affect the extended defects, and how the point defects interact with each other and potentially form defect complexes or clusters need to be acquired (Fig. 1), and directly compared to the electrical, optical, and defect spectroscopy data to establish a direct relationship between the defects and important properties. Recently, thin film growth of β-Ga_2O_3 on various substrates has also been explored [3], but the detailed understanding of the common extended defects in these interfaces and how they affect the device properties has been largely lacking.

Characterization of defect structure will require a technique that combines high resolution and precision, and can determine the detailed structure and positions of the individual point and extended defects in materials. Here we show the microscopic investigation on the individual point and extended defects that directly connect to the electronic and optical properties of β-Ga_2O_3, both bulk-grown substrates and MBE grown interfaces, using scanning transmission electron microscopy (STEM). We will especially focus on two important technical aspects of the β-Ga_2O_3 characterization: (*i*) the imaging of point defects using electron channeling contrast method that we recently developed [4], and (*ii*) TEM sample preparation of β-Ga_2O_3. The channeling contrast method detects the de-channeling of the electron caused by individual point defects, including vacancies and impurity atoms, using multiple narrowly selected detection angles in STEM. The technique is highly promising as it can be used to determine the structure and positions of the individual point defects that directly connect to the electronic and optical properties of β-Ga_2O_3 materials and interfaces (Fig. 2a). However it requires very thin (less than ~10 nm) TEM samples with clean surfaces. Focused ion beam may not be the best method for preparing such samples, as the milling rate is very slow due to the high hardness of β-Ga_2O_3 (only slightly lower than Sapphire) and re-deposition of the material. Mechanical wedge polishing can generally produce very thin samples with clean surfaces [5], but because of the preferred cleavage plan in β-Ga_2O_3, the TEM sample can only be prepared in limited number of orientations. However, the preferred cleaving orientation can produce β-Ga_2O_3 membranes that can be as thin as ~10 nm [6]. We will discuss the results from all three preparation methods – FIB-prepared, wedge polished, and membrane samples.

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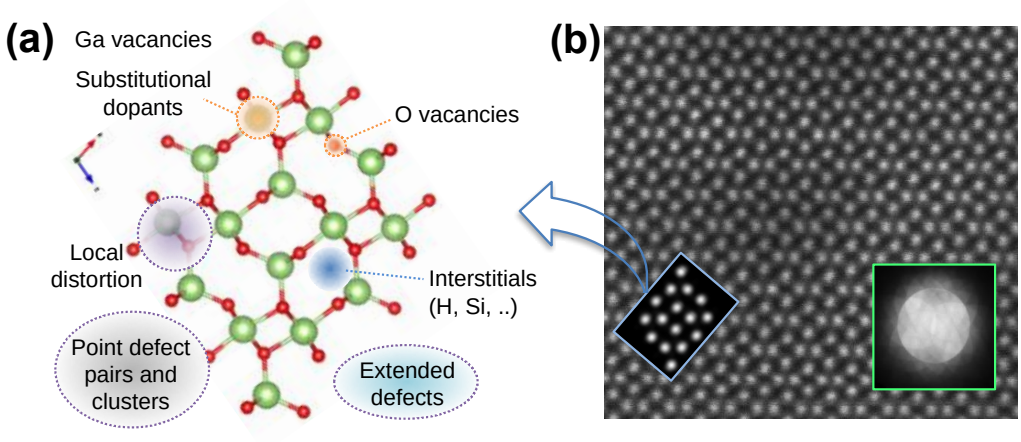

Figure 1. CBED (a) Potential defects in β-Ga_2O_3 under investigation. (b) An experimental STEM HAADF image of β-Ga_2O_3. Inset (left) is the simulated image that matches the structure in (a), and (right) is the experimental position averaged convergent beam electron diffraction pattern taken from a unit cell of β-Ga_2O_3.

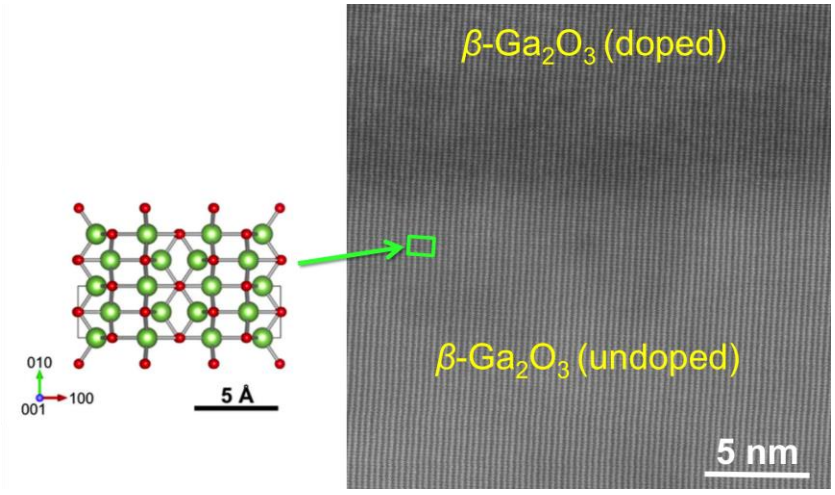

Figure 2. High angle annular dark field image showing the interface between doped and undoped β-Ga_2O_3 from monoclinic 001 orientation. Variation in the contrast at the interface indicates the presence of strain and potential extended defects.

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