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Point Defects and Complexes in Gallium Oxide Materials and Devices

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Beta gallium oxide (Ga_2O_3) has received much attention recently as a viable candidate for the next-generation material for power electronics and photonic applications, with its unique advantages, such as the wide bandgap (~ 4.9 eV), high breakdown voltage, and optical transparency up to UV range. Recent advances in high quality Ga_2O_3 thin film growth, such as using molecular beam epitaxy or chemical vapor deposition, combined with the material's availability as inexpensive bulk substrates have opened new exciting opportunities for the fabrication of novel Ga_2O_3 devices. Despite the advances, many of the fundamental properties of Ga_2O_3 are yet to be understood clearly. As in many other oxide-based transparent semiconductors, point defects and their complexes can dictate the properties of Ga_2O_3. Various spectroscopic methods as well as theoretical calculations have provided useful insights on the nature of the point defects and complexes in Ga_2O_3. Regardless, what has been missing in the field is the detailed information on the atomic scale structure of the defects and complexes in Ga_2O_3. Such information is crucial to determine how the atomic scale defects relate to many of the unanswered questions regarding the unique properties of Ga_2O_3, including how point defects and impurity atoms influence the formation of trap states, how the dopant atoms are compensated, and what is the exact origin of the difficulty in doping of Ga_2O_3 (especially p-type).

We use quantitative scanning transmission electron microscopy (STEM) to investigate the detailed structure of the point defects and their complexes in Ga_2O_3 [1]. Our quantitative analysis of STEM images has confirmed that the defect complexes, each of which involves 2 cation vacancies and 1 interstitial Ga atom (and therefore named as interstitial-divacancy complex), are present within the beta-Ga_2O_3 structure (Fig. 1). Our STEM observation is in fact consistent to what has been previously suggested by DFT calculation [2]. The concentration of the complex increases as the doping (e.g. Sn) concentration increases, suggesting that the doping facilitates the formation of Ga vacancies, which in turn increases the concentration of the interstitial-divacancy complex. This trend is also consistent with the increase in the concentration of the defect trap state measured at $E_c - 2$ eV using deep level optical spectroscopy, which strongly implies that the complex is responsible for the trap state.

We also found that the increase in the cation vacancy concentration (and therefore the increase in the interstitial-divacancy complex) can also lead to further relaxation of the atomic structure, resulting in the local lattice distortion that resembles gamma-Ga_2O_3 phase (Fig. 2a and 2b), which may further influence the electronic properties. Higher concentration of defect complexes is observed when the chemical heterogeneity of the material increases either by doping or alloying ($Al_{1-x}Ga_xO$), which may also develop into extended defects within the device heterostructures (Fig. 2c). In summary, our STEM results provide new important insight on the material's unique response to the impurity incorporation that can significantly affect their properties, which can offer important guidance to the development of Ga_2O_3 devices for novel applications. We acknowledge support by the Department of Defense, Air Force Office of Scientific Research GAME MURI Program (Grant No. FA9550-18-1-0479).

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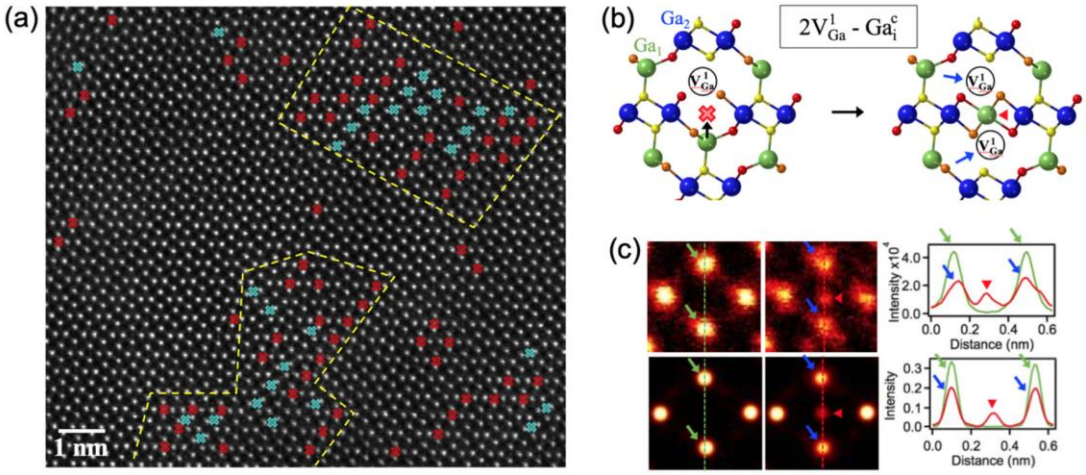

Figure 1. (a) Low magnification STEM image showing the locations of ib-type (blue X) and ic-type (red X) interstitials. (b) Formation of interstitial-divacancy complex suggested by DFT simulation. (c) Experimental STEM image (top row) compared to image simulation (bottom row), confirming the DFT-predicted complex shown in (b).

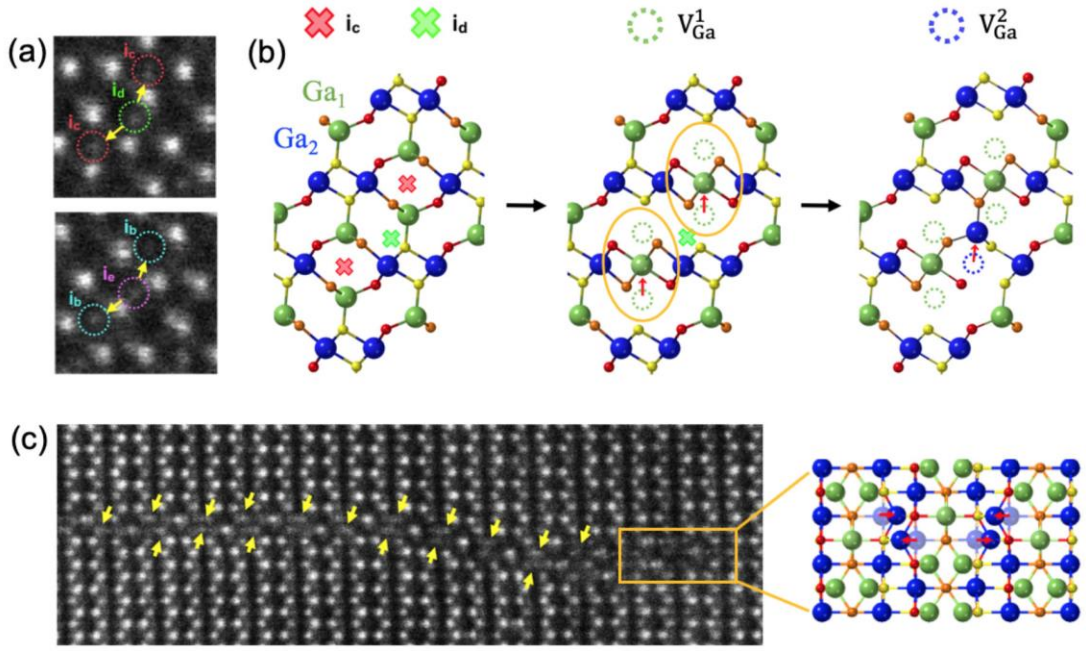

Figure 2. (a) id interstitial paired with 2 ic interstitials (top) and ie interstitial paired with 2 ib interstitials. (b) Formation mechanism of id interstitial by clustering of the interstitial-divacancy complex revealed by STEM. The resulting structure resembles the relatively stable gamma-Ga2O3 phase. (c) Extended defect formed by the alignment of the complexes along the direction perpendicular to the growth direction of the Al1-xGaxO thin film.

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