The electronic structure of oxygen-related defects in non-stoichiometric amorphous In-Ga-Zn-O

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Recently, Zn-based amorphous oxide semiconductors such as amorphous In-Ga-Zn-O (a-IGZO) have attracted much attention because these semiconductors are used as channel materials in transparent thin-film transistors (TFTs). Although oxide-based TFTs exhibit superior properties such as flexibility, transparency, and high field-effect mobility, as compared to amorphous Si-based devices, the reliability of a-IGZO TFTs still remains as one of important issues. Especially, a-IGZO TFTs suffer from a high density of charge traps which cause large shifts of threshold voltage (Vth) under various stress conditions. Under negative bias illumination stress (NBIS), Vth is shifted negatively up to about -18 V: this phenomenon is called the NBIS instability. Based on first-principles theoretical calculations, we suggested that O-vacancy defects (VO) in a-IGZO are responsible for the NBIS instability [1-3]. On the other hand, when a-IGZO TFTs are under positive bias stress (PBS), the PBS instability takes place, with positive shifts of Vth. In our recent study [4], we investigated the atomic and electronic properties of O interstitial defects in a-IGZO and showed that these defects act as electron traps in the channel region when the Fermi level is close to the conduction band edge. Thus, it was proposed that interstitial O atoms cause positive shifts of Vth under PBS in a-IGZO TFTs.

In the previous studies [1-4], O-related defects were generated by eliminating host O atoms or introducing excess O atoms in the predefined amorphous model of a-IGZO, which was obtained from stoichiometric crystalline IGZO with the composition ratio of In:Ga:Zn:O = 1:1:1:4. Here we study the electronic properties of O-related defects in different amorphous samples. We consider non-stoichiometric IGZO samples with excess O atoms or O deficiencies and generate amorphous structures as well as O-related defects through melt-and-quench ab initio molecular dynamics simulations. We compare the electronic properties of O-related defects with the previous results [1-4] and discuss their roles in the device stability of a-IGZO TFTs.


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