Ab initio investigation of source of instability in amorphous semiconducting oxides

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Ultra-definition, large-area displays with three-dimensional visual effects represent megatrend in the current/future display industry. On the hardware level, such a "dream" display requires faster pixel switching and higher driving current, which in turn necessitate thin-film transistors (TFTs) with high mobility of 30~50 $cm^2/V \cdot s$. The traditional a-Si TFT performs far below than this requirement and amorphous semiconducting oxides (ASOs) such as In-Ga-Zn-O are poised to enable the high-mobility TFTs. However, the device instabilities under various stress conditions such as voltage, temperature, and light become the main hurdle against the massive commercialization of the AOS-based TFTs.[1] Therefore, the microscopic understanding on the device instability is highly demanded at this moment.

In this presentation, I will summarize our recent ab initio calculations on the source of instability in ASO, mainly focusing on the defects and impurities introduced during the thin-film growth. To explain various instability sources, we calculated the absorption spectrum of ASO, the interface between ASO and SiO_2,[2] and the oxygen vacancies.[3] In addition, through the combined study with experiments, we investigated the device instability more directly[4] and proposed how to improve the stability.[5,6]

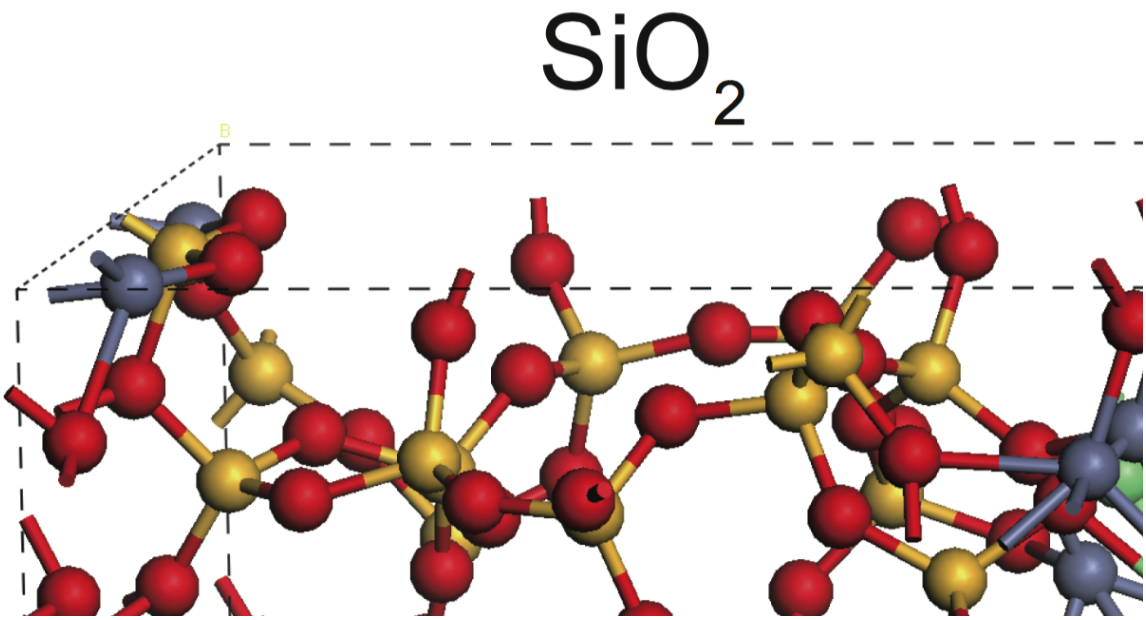

Fig. 1. A representative of amorphous IGZO- SiO_2 interface model

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