

ANALYSIS OF IGZO CRYSTALLINE STRUCTURE AND ITS STABILITY BY FIRST-PRINCIPLES CALCULATIONS

Tomonori Nakayama, Semiconductor Energy Laboratory Co., Ltd., Japan
tn1231@sel.co.jp

Masahiro Takahashi, Tomosato Kanagawa, Toshimitsu Obonai, Kenichi Okazaki, and Shunpei Yamazaki,
Semiconductor Energy Laboratory Co., Ltd., Japan

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In-Ga-Zn oxide (IGZO), an oxide semiconductor, has been actively researched as a semiconductor material having features different from those of silicon in recent years [1]. IGZO is used as a transistor material in backplanes of commercially available displays. Transistors including crystalline IGZO have high stability and thus are suitable for mass production [2].

Our previous studies revealed that the selected area diffraction pattern of an IGZO film formed at room temperature by sputtering is a halo pattern, whereas diffraction spots are observed in the diffraction pattern obtained by nanobeam electron diffraction with a probe diameter of 1 nm [3,4]. These results suggest that the IGZO film has rather nanometer-sized crystalline structures than a completely amorphous structure. We named this film “nano-crystalline IGZO (nc-IGZO) film.” Other researchers have reported that the nc-IGZO film has a crystalline-cluster composite structure, according to the analysis results obtained by grazing-incidence X-ray diffraction, anomalous X-ray scattering, and reverse-Monte-Carlo simulation [5].

In this study, an IGZO structure having a minute crystalline region, which was considered to exist in nc-IGZO as a local structure, was created by first-principles calculations and its stability was analyzed. The IGZO model having a crystalline region used in this study was obtained by a melt-quench method in the following manner. Note that the initial structure had a hexagonal-prism crystalline region at the center and an amorphous region (random atomic arrangement) around the crystalline region. The composition ratio was In:Ga:Zn:O = 1:1:1:4 and the density was 6.1 g/cm³. First, for structural relaxation with the crystalline region maintained, the amorphous region was fused in quantum molecular dynamics simulation (3500 K, 6 ps) while the atomic arrangement of the crystalline region was fixed, and the structure was cooled to 500 K at a rate of 500 K/ps and held at 300 K for 5 ps. Finally, the entire structure including the crystalline region was optimized towards the target structure (Fig. 1). An amorphous model was also created for reference. The amorphous model was obtained by quantum molecular dynamics simulation of the entire structure under similar temperature conditions without fixing the atomic arrangement of the crystalline region, followed by structural optimization. The comparison between the two models showed that the total energy of the IGZO model having a crystalline region was lower than that of the amorphous model (not having a crystalline region). This suggests that the crystalline region contributes to structure stabilization.

For more detailed thermal stability analysis of the IGZO structure having a crystalline region, quantum molecular dynamics simulations were performed at several temperatures. The results will be available at the conference.

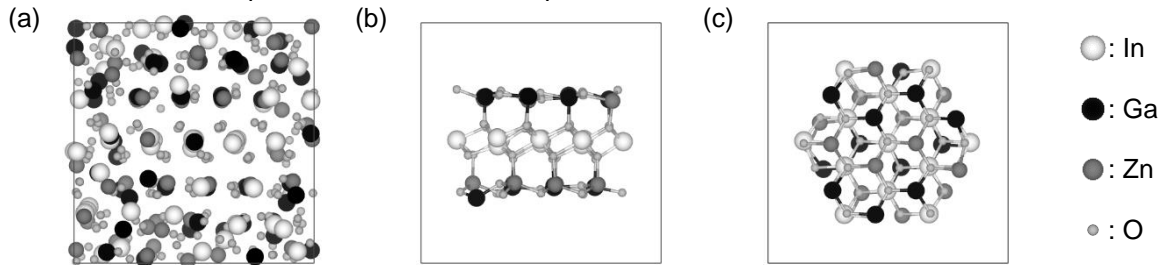


Figure 1 – The model having a crystalline region obtained by first-principles calculations: (a) the entire structure; (b) a portion initially set as a crystalline region; and (c) a 90° rotated view of (b).

References

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