A 3D Structural Study of Hydrogenated and Non-hydrogenated Amorphous In-Ga-Zn-O Thin Films

NIMS/SPring-8 [1], MSL Tokyo Tech [2], MCES Tokyo Tech [3]

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Amorphous indium-gallium-zinc oxide (a-IGZO) semiconductor as a TFT channel layer exhibits advantages over other semiconductor channel materials such as high field-effect mobility, small subthreshold swing, excellent uniformity, very large on/off ratio, and low temperature fabrication [1]. The mobility of an a-IGZO film is comparably large to its crystalline phase. Since the continuous carrier transport paths in a-IGZO are formed due to the overlap of the vacant *s*-orbitals with neighboring similar isotropic *s*-orbitals of the heavy post transition metal cations, which is insensitive to the metal-oxygen-metal bond angles [2].

Here we prepared a-IGZO films using a polycrystalline $InGaZnO_4$ target at room temperature with standard (STD, the base pressure ~10^{-4} Pa) and ultrahigh vacuum (UHV, ~10^{-7} Pa) radio frequency magnetron sputtering systems with different oxygen-containing atmospheres (see e.g. [3]). The structures of a-IGZO were analyzed using high-energy X-ray diffraction (HEXRD) combined with fluorescence extended X-ray absorption fine structure (EXAFS) data, atomic pair distribution function (PDF) analysis, and reverse Monte Carlo (RMC) modeling methods. We performed HEXRD and EXAFS measurements in the BL04B2 and BL01B1 beamlines at the SPring-8, respectively.

From the structural models generated by RMC, we obtained significant different partial pair correlation function, $g(r)$, for STD and UHV a-IGZO films e.g. in Zn-O and In-O correlations (Fig. 1(a,b)). The obtained RMC models are shown in Figure 1(c), which have network regions of edge-sharing In-O polyhedra and local inhomogeneity. The present HEXRD coupled to the PDF and RMC structure-modeling methods distinguishes different atomic scale structures of a-IGZO films with different impurity hydrogen.

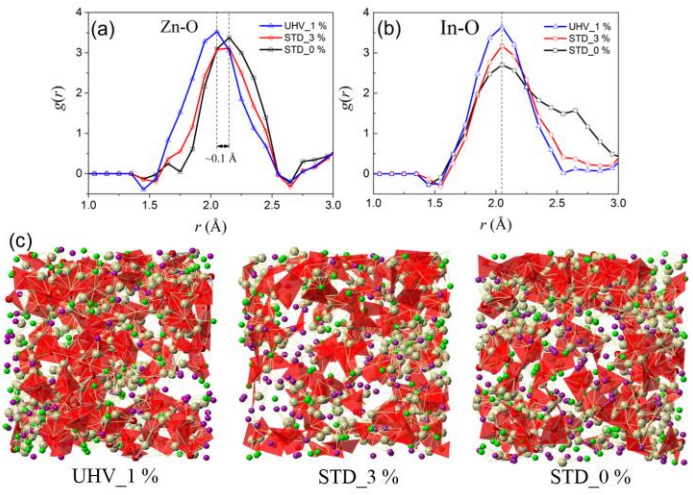

FIG. 1. Partial $g(r)$ of (a) Zn-O and (b) In-O correlation, and (c) distribution of InO_n polyhedral (wheat: O, magenta: Zn, Green: Ga, red: In).

(1) J. S. Park *et al.* Appl. Phys. Lett. 90 (2007) 262106.

(2) K. Nomura *et al.* Nature 432 (2004) 488.

(3) H. Tang *et al.* J. Appl. Phys. 118 (2015) 205703.