Characterization of the crystal structure of In-Ga-Zn-O materials via Precession Electron Diffraction

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Indium-Gallium-Zinc-Oxide (IGZO) compounds have been regarded as attractive material for the channel in transparent thin-film transistors (TFTs), with low leakage in the off-state and high mobility. IGZO-based materials belong to the class of high band-gap semiconductors and their crystallographic properties are the key characteristic determining the final performances of the electronic devices. Amorphous IGZO, for example, is easy to grow and has good electron mobility, in contrast to other semiconductors such as Si and Ge in the amorphous state. However, in the perspective of the fabrication of electronic devices, amorphous IGZO TFTs suffer from electrical instability. Crystalline IGZO mostly exists in two polytypes having spaces group $R\bar{3}m$ (160) and P63/mmc (194), and has showed improved electrical performances. There is also an intermediate crystal phase where the periodicity is kept only in the c-axis, while being structureless in the a and b-axis. This phase is called CAAC (c-axis aligned crystalline) IGZO and it is less prone to defect formation. More sophisticated configurations have been employed in TFTs: for example, a double layer design, constituted of amorphous and CAAC-IGZO, has shown good device stability [1]. To further enrich the family of IGZO compounds, a new a spinel polytype has been recently demonstrated, which can be grown via PVD using intermediate conditions derived from the growth of amorphous and CAAC-IGZO, and exploiting a Ga2ZnO4 (GZO) layer as a seed [2].

In such a complex panorama, there is a need for an appropriate technique to characterize the huge diversity of crystal phases in IGZO-based TFTs. To this end, we referred to Precession Electron Diffraction (PED) [3] executed via a Transmission Electron Microscope (TEM) in scanning (STEM) mode. In fact, standard electron diffraction, due to sample thickness, is significantly affected by multiple/dynamic scattering, which leads to diffracted intensities not easy to be interpreted. PED was introduced to solve this issue and analyze crystal structures with better sensitivity. In PED, the electron beam is rocked at a fixed angle to the optic axis above the sample, forming a hollow cone, and then it is de-rocked below the sample. It can be demonstrated that the final diffraction pattern has many more reflections than in the case of an unprecessed beam, having intensities unaffected by dynamic scattering. We applied scanning PED to the study of IGZO thin (about 20 nm) films having spinel structure and grown on GZO layers having different thickness (from 2 to 10 nm). We prove the possibility to correctly identify materials with similar electron diffraction patterns, such are IGZO and GZO, using PED and Phase &

Orientation mapping of the scanned area (ASTAR, NanoMEGAS) [4]. We demonstrate that high sensitivity can be achieved to properly resolve even narrow GZO layers, as thin as 2 nm, from the above IGZO. This can be inferred from Figure 1, which shows the combination of phase map and indexation for two different IGZO samples, grown on GZO having thickness of 10 nm (a) and 2 nm (b), respectively. Moreover, phase and orientation mapping allowed us to study the grains structural properties in IGZO grown on GZO layer with different thickness. We show that, as expected, IGZO grows epitaxially on the GZO seed layer. Moreover, IGZO grain growth is related to the thickness of the underlying GZO layers: size of the IGZO grains is coarse when GZO has higher thickness, while columnar growth of narrower and IGZO grains is reached when thin GZO is used. For GZO having 2 nm thickness, IGZO and GZO present texture, with growth of IGZO/GZO along the <111> direction. Finally, we study the case where thermal annealing in a hydrogen atmosphere reduces the IGZO film and induces the formation of In-rich grains dispersed in the IGZO matrix. In this context, we study the crystal structure of these grains and their matrix.

This study is preliminary to the characterization of TFTs devices employing complex design and based on IGZO compounds as channel material. In general, these results can open the way to the study of different devices, where the common feature relies in the close link between the crystallographic structure and the final performances.

Graphic:

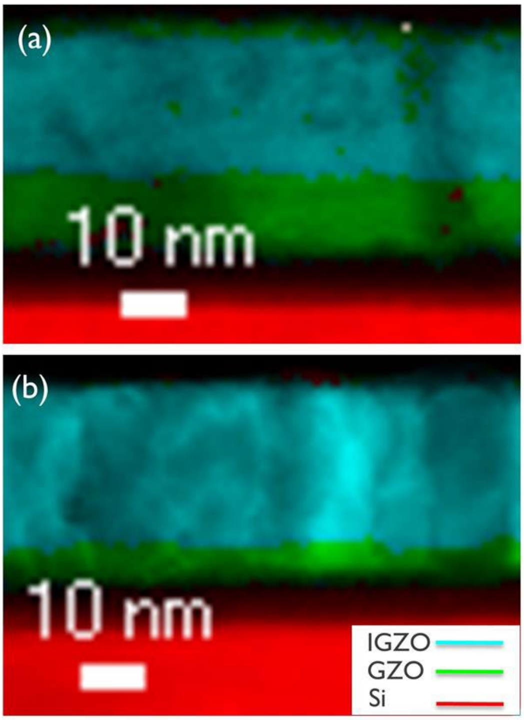

Figure 1. Combination of Phase Map and Index Map for (a) IGZO grown on 10-nm GZO and (b) IGZO grown on 2-nm GZO.

Keywords:

In−Ga−Zn oxide, Precession Electron Microscopy

Reference:

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