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Atom Probe Tomography Study of In-doped ZnO

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In-doped ZnO is a highly promising material for thermoelectric (TE) applications. In contrast to other materials purposed for that application (i.e Si−Ge alloys, transition metal disilicides, and B-based compounds), the $In_2O_3(ZnO)_k$ structure (where k is an integer) possess several unique advantages. It has high chemical and structural stability at high temperatures, a wide band gap which prevents thermal excitation of carriers and hence allows the figure of merit, ZT, increase with temperature. In addition, the In-doped ZnO forms compositionally dependent superlattice which sometime referred to as homologous series. The superlattice structure creates phonon scattering interfaces which offer additional mechanism for the reduction of the thermal conductivity.

The unique structure of $In_2O_3(ZnO)_k$ has been the focus of numerous studies. X-ray diffraction, Transmission Electron Microscopy (TEM) and Scanning TEM have shown before the existence of polytypoid structure of ZnO wurtzite slabs separated by single octahedrally-coordinated InO_2 sheets lying on the basal plane, while the spacing depends on composition [1]. In addition, another structure of “Zig-Zag” was found to exist in the system [2]. However, the concentration and distribution of the In atoms in the ZnO slabs still remain unclear. A control on the In inside the ZnO slabs, can contribute to the thermal, optical and electrical properties of the material and therefore is much of an interest.

In this study, we have used Atom Probe Tomography (APT) in order to analyze the composition profile of $In_2O_3(ZnO)_k$ structure. First, In-doped ZnO samples were prepared using commercial high purity nitrate powders, $Zn(NO_3)$ and $In(NO_3)_3$ by molecular mixing with organic materials and combustion process, followed by calcination, densification (using current assisted system) and post-annealing. Then APT tips were prepared from the annealed $(Zn_{1-x}In_x)O$ (x=0.1) using a Focused Ion Beam Scanning Electron Microscope (FIB-SEM) [3]. The tips were then studied using laser pulse Local Electrode Atom Probe (LEAP) system.

Three different configurations of the materials were observed from the APT measurements. A complete random distribution of In, Zn and Oxygen, a superlattice structure of In/ZnO slabs separated by Indium Oxide sheets and a “Zig-Zag” Structure as can be seen in Fig. 1. The reconstruction and composition analysis of the different structures provide the information on the distribution of the In inside the ZnO slabs and in the sheets.

In this work, we demonstrate the preparation and the analysis of atom probe tips from bulk In-doped ZnO. The APT provides chemical and structural analysis of the system which was compared with previous TEM results and the different models of the superlattice structure. In addition, a correlation with of the APT results and the thermal conductivity was done.

References:

[1] Y Yan, S J Pennycook, J Dai, R P H Chang, A Wang and T J Marks, Applied Physics Letters, **73(18)**, (1998), p. 2585.
[2] C Ii, Y Bando, M Nakamura, and N Kimizuka, Journal of Electron Microscopy **46(2)** (1997), p. 119.
[3] M K Miller, K F Russell, K Thompson, R Alvis, and D J Larson, Microscopy and microanalysis **13(6)** (2007), p. 428.
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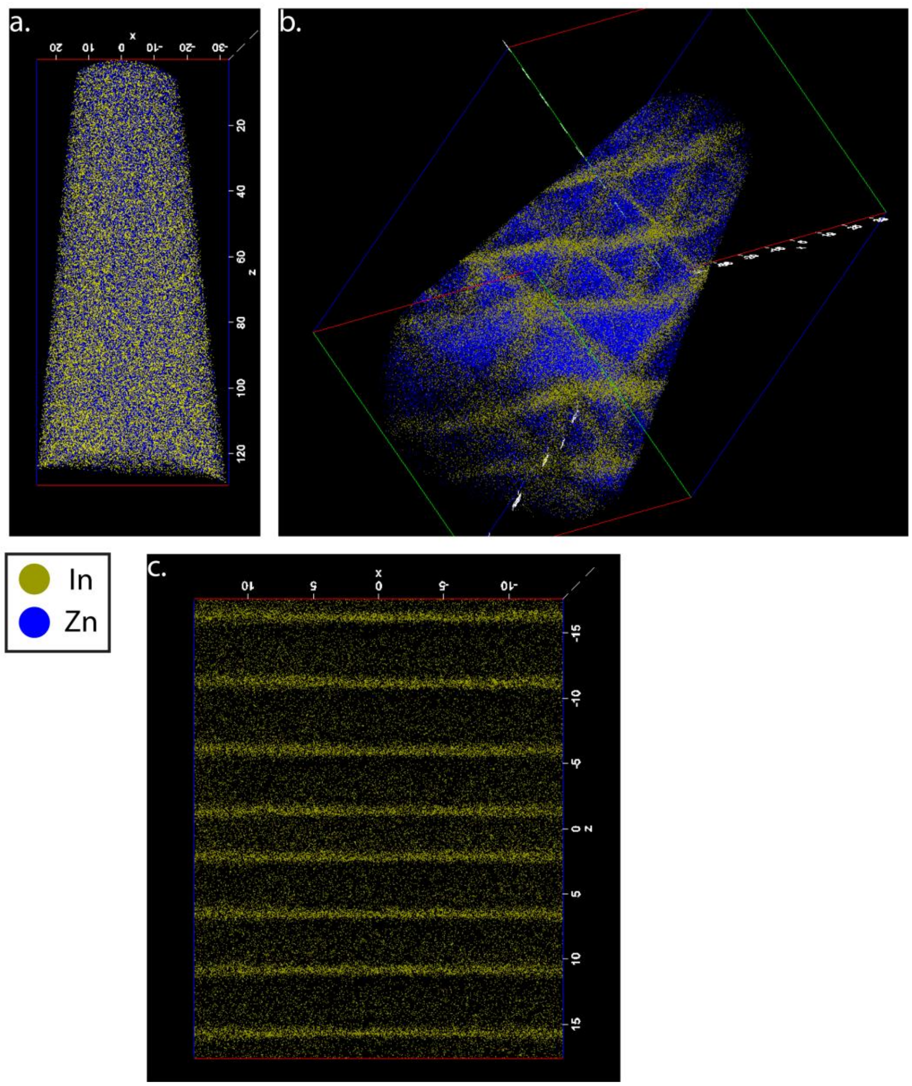

Figure 1. Three different configurations of the In/ZnO structure a. Completely random distribution of In, Zn b. In and Zn in a“Zig Zag” Structure and c. Distribution of Indium in a superlattice structure of Indium Oxide sheets between ZnO slabs.

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