Limitation of Multiphases Study with Anomalous X-ray Diffraction Technique for Similar Lattice Spacings in TLS & TPS

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Abstract

To study the phase change among various metallic material such as TbDyFe, it is essential to know the contribution of each element among various observed diffraction peaks. In order to achieve this, the anomalous X-ray diffraction technique has been carried out since it provides the opportunity to differentiate among elements with almost similar scattering factor such as Tb, Dy and multiphases with similar d-spacings, such as Tb_2O_3 and Dy_2O_3 in oxidized TbDyFe sample. We also utilized this method by analysis the solar cells materials CZTSe to understand the antisite formation which affects the efficiency of the solar cell devices. XRD results revealed that the existence of multiple phases in the CZTSe based films. To understand the defect formations or swapping of Cu and Zn into and out of the system, it is therefore essential to take the peaks contributing only due to CZTSe peak. However, in our cases, the anomalous technique faces the issue of weak elastic diffraction peak which lead to poor signal to noise ratio of anomalous signal of CZTSe samples. The systematic error contributes by the fluctuation of incident X-ray intensity in TLS is about 10% when compared to the dispersive of f' of Cu and Zn elements resulting a poor anomalous signal which is only 6-7% difference in intensity. In additional, a high fluorescence background after the K-edge overwhelms the elastic scattering signal. The problem of this high fluorescence background can be overcome with the help of the utilizing crystal analyzer which has been applied in TPS09A and enhanced twice the signal to noise ratio. Alternatively, using solid state detector could also avoid the fluorescent signal. In a final remark, anomalous scattering serves as an efficient tool for thin film samples, even though the neutron could also serve for this purpose based on different scattering cross section for various elements. Neutron scattering is difficult to be applicable for a thin film of only nm thickness.

Keywords - anomalous X-ray diffraction, amorphous, solar cells, thin films.