Investigation of Reaction between Cu_2Se and In_2Se_3 during Temperature Ramping by In-Situ X-ray Diffraction

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Chalcopyrite α-$CuInSe_2$(CIS) and its alloys with Ga or S, have been proven to be absorbed materials for high efficiency thin film solar cells. The purpose of this work is to investigate the reaction between Cu_2Se and In_2Se_3 during temperature ramping by in-situ XRD. The reaction between Cu_2Se and In_2Se_3 can be expressed as the following equation,

$$Cu_2Se + In_2Se_3 \rightarrow 2CuInSe_2 + 2Se(vapor)$$

Since the evaporation pressure of selenium is higher than Cu and In individual elements, the extra Se powders were added on the top of the mixture of In_2Se_3 and Cu_2Se powders. Figure 1 shows the XRD pattern of the individual powders of In_2Se_3, Cu_2Se and its physical mixture. From the JCPDS database, it indicates that the structures of In_2Se_3 and Cu_2Se are hexagonal and orthorhombic, respectively. Figure 2 shows the structure evolution of the mixture of the Cu_2Se and In_2Se_3 powders during temperature ramping with a ramp rate of 10 ^oC/min. When temperature is increased, the phase is starting to change. All of In_2Se_3 and Cu_2Se peaks are transformed to $CuInSe_2$ (112)、(204)、(116) alloy, and the peaks for the In_2Se_3 and Cu_2Se powders gradually disappear. A detailed understanding of the phase equilibria and formation kinetics of CIS and its sub-ternaries would greatly assist the development of robust process models to optimize high performace and cost-effective commercial process

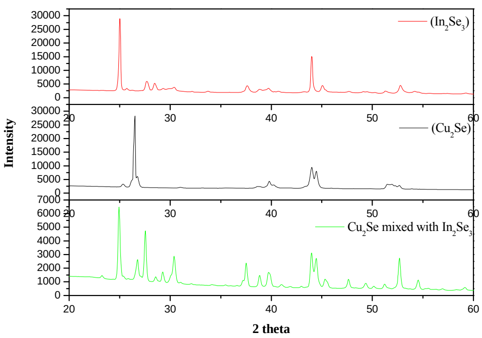

Figure 1. XRD pattern of prinstine In_2Se_3, and Cu_2Se powders as well as their mixture.

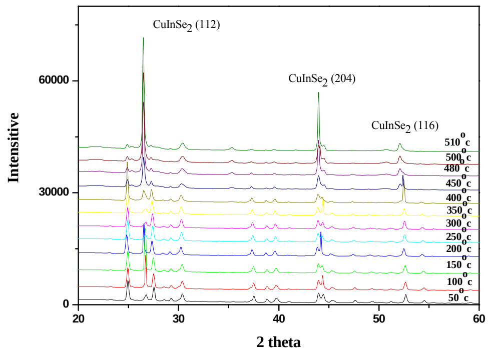

Figure 2. Evolution of XRD patterns of the mixture of Cu_2Se and In_2Se_3 powders during ramping temperature. Ramp rate = 10 ^oC/min from 60 ^oC to 510 ^oC