Dose Dependent Structural Properties of Fe Ion Implanted $CuInSe_2$ Thin Film

Li-Jung Liu (劉禮榮), Ming-Zhe Lin (林銘哲), Yen-Fa Liao (廖彥發), and Chih-Hao Lee (李志浩)

Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan

The I-III-VI_2 compound are the most promising thin film photovoltaic cell. Because of their highest absorption coefficient and the best thermal stability, $CuInSe_2$ thin film solar cells are the most popular material applied in photovoltaic cells. Based on the band structure simulation of the Fe doped $CuInSe_2$ [1], it is believed the generated photocurrent and the output voltage of the operating cells will be higher.

The $CuInSe_2$ thin films were prepared by an MBE system. The concentrations of implanted Fe were from $2*10^{14}$ to $1*10^{17}$ (cm^{-2}) at 72 keV. The annealing process was taken under $6.2*10^{-2}$ torr at 400 ℃.

From the X-ray diffraction spectra (see Fig.1), there is no detectable secondary phases in all the dose of $CuInSe_2$ samples and also no Fe clusters segregated on the surface of the $CuInSe_2$ thin film. From the enlarged spectra, the peak shifts were observed at [312] diffraction peaks. It may indicate that the iron atoms would replace the copper atom sites because of the shorten d-spacing of lattice plane, [312].

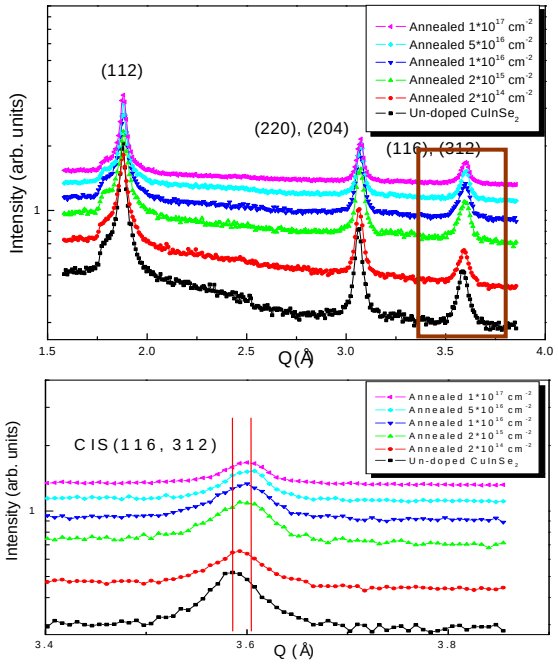

Figure 1. X-ray diffraction spectra of all implnated samples

Fig 2 shows the d-spacing was decreased as the implanted dose increased. It might indicate that the iron atoms of high dose implanted iron atoms would be segregated. From the X-ray absorption spectra (Fig. 3), the energy of absorption edge indicates that the valence state of iron atoms in light dose implanted $CuInSe_2$ thin films is +2. We can speculate that the light dose implanted iron atoms might form the Fe_{Cu} substitutional atoms. Fig. 4 shows the X-ray absorption spectra of Fe K-edge at high dose. The valence state of iron of high dose implanted $CuInSe_2$ thin film is 0. It means that the iron atoms segregated from $CuInSe_2$ matrix and form iron clusters.

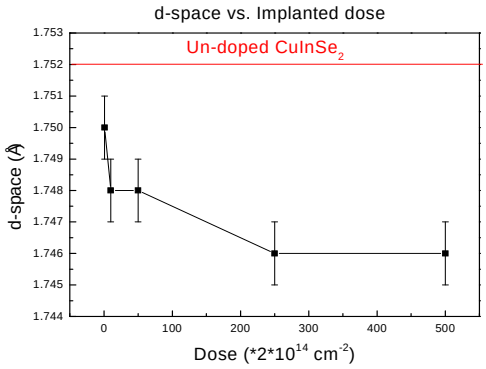

Figure 2. The variation of d-spacing of lattice plane, [312]

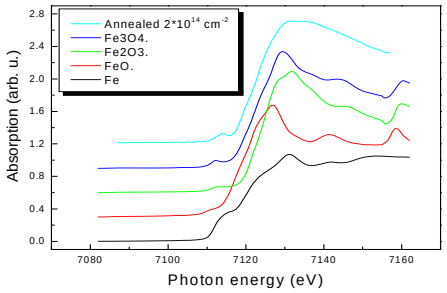

Figure 3. The X-ray absorption spectra of iron of $2*10^{16}$ cm^{-2} Fe implanted $CuInSe_2$ thin film.

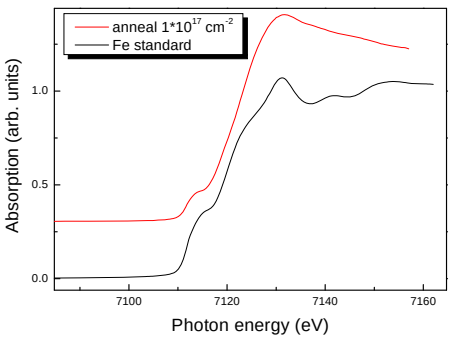

Figure 4. The X-ray absorption spectra of the Fe K-edge of the high dose ($1*10^{17}$ cm^{-2}) implanted $CuInSe_2$ thin film.

References：

[1] Jean-Marc Raulot, Christophe Domain, and Jean-François Guillemoles, Phys. Rev. B **71**, 035203 (2005).