Study of Te Substituted $CuGaS_2$ ($CuGa(S,Te)_2$) Thin Films Deposited by Chemical Pyrolysis

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Introduction $CuGaS_2$ (CGS) and similar chalcopyrite compounds are considered potential semiconductors for thin film photovoltaic devices given their high optical absorption coefficient and adjustable wide bandgap. However, vaporization of sulfur atoms during fabrication of CGS thin films at high temperatures results in defect formation and degrades the material properties. Post deposition ex-situ sulfurization may minimize S deficit, but it is still challenging to control S content due to its high vapor pressure. This work, therefore, investigated the effect of partial Tellurium (Te) doping during deposition on the crystallinity and optical properties of CGS, expecting relatively low vapor pressure of Te helps stabilizing CGS structure.

Methods $CuGaS_2$ ($CuGaS_{2(1-x)}Te_{2x}$) thin films were prepared via chemical spray pyrolysis method at 250 °C. Thin films were characterized by X-ray diffraction (XRD), and photoluminescence (PL) with excitation source of 405 nm laser at room temperature.

Results and Discussion XRD measurements indicates formation of CGS structure without such binary phases as Cu_2S, CuO, and Ga_2S_3 (Fig. 1). From the calculated crystallite size using Scherrer's equation, it can be inferred that Te doping even stimulates larger grain growth. Crystallite size has increased from 19.9 nm without doping (x=0) to 47.7 nm with doping (x=0.15).

PL measurement shows that Te doping of x=0.15 induces recovery of CB-VB transition peak and enhancement of shallow state around 2 eV (Fig. 2). Although it is not from band-edge, enhancement of shallow state while maintaining the intensity around the band-edge may imply longer carrier lifetime and better optical property.

Conclusion This research has revealed Te doping of x=0.15 positively affects crystallinity and optical property of CGS. Further studies on intrinsic shallow effect of CGS and the interaction between the defect and Te would help understanding the behavior of Te in CGS.

Acknowledgment This work is supported by JSPS Kakenhi (No. 18K04224).

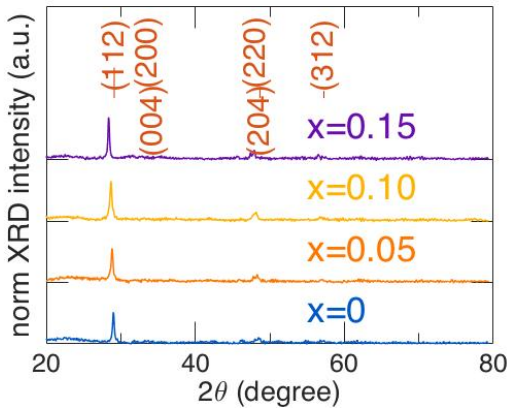

Fig. 1: XRD results of $CuGaS_{2(1-x)}Te_{2x}$ films

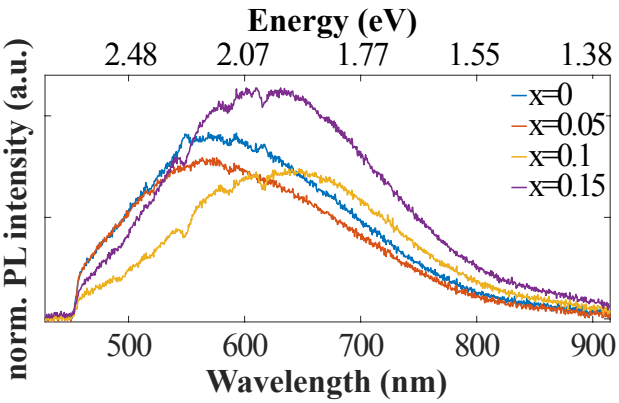

Fig. 2: PL spectra of $CuGaS_{2(1-x)}Te_{2x}$ films