Cu-doping into $ZnSnN_2$ film: Structural, Electrical and Optical Properties

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***INTRODUCTION*:** Zinc tin nitride ($ZnSnN_2$) can be regarded as a pseudo-III-nitride semiconductor. The bandgap was theoretically predicted to be (1.42±0.1) eV [1], which is ideal for both photovoltaic absorbers and visible light-active photocatalysts. Thus $ZnSnN_2$ can be an excellent material for such applications. However, reported electron densities (n_e) as high as ~10^{21} cm^{-3} [1] were consistent with heavy donor doping. Such high n_e are mainly attributed to the unintentional oxygen doping. In this work, we examined the Cu(I)-doping to compensate the oxygen donors.

***FILM GROWTH*:** The reactive RF magnetron sputtering technique was applied to grow $ZnSnN_2$ thin films on alkali-free glass substrates at room temperature. We used a metal Zn:Sn target (Zn:Sn ratio = 1:1) and N_2 concentrations were fixed at 80% during the film growth. Cu-doing was done by putting Cu chips on the target.

***RESULTS & DISCUSSION*:** Figure 1 presents the X-ray diffraction (XRD) patterns for a $ZnSnN_2$:Cu and $ZnSnN_2$ films. As seen from this figure, all the diffraction peaks were assigned to $ZnSnN_2$ even for the $ZnSnN_2$:Cu film and no impurity phase was detected. The Hall coefficients of our films were negative, indicating *n*-type conductivity. While the $ZnSnN_2$ film had free electron density of 2.8 × 10^{19} cm^{-3}, Cu-doping effectively lowered the electron density down to 3.5 × 10^{18} cm^{-3}. This indicates that Cu served as an effective electron killer in $ZnSnN_2$ films. The Tauc-plots for films are shown in Fig. 2. The linear extrapolations resulted in direct optical bandgaps of 2.4 eV for the undoped film. On the other hand, the bandgap of the $ZnSnN_2$:Cu film had a smaller value of 2.3 eV, which also suggests that Cu-doing decreases free electron density, in terms of the Burstein-Moss effect. In our presentation, we will discuss more in detail including Cu concentration, Zn/Sn ratios and annealing effect, *etc.*.

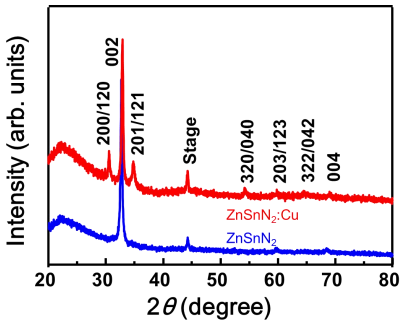

Fig.1 θ-2θ XRD patterns for typical $ZnSnN_2$ films.

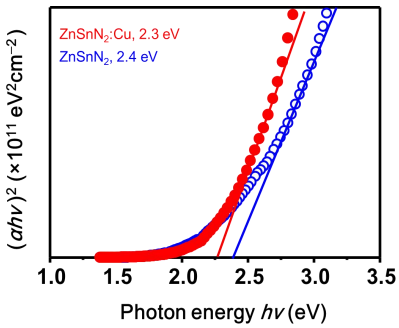

Fig.2 Tauc-plots for typical $ZnSnN_2$ films.

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***REFERENCES*:** [1] L. Lahourcade *et al.*, Adv. Mater., **25**, 2562 (2013).