Effective mass and bandgap of $ZnSnN_2$ earth-abundant solar absorber

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***INTRODUCTION*:** $ZnSnN_2$, comprised wholly of earth-abundant elements, can be regarded as a solar absorber material due to its high optical absorption coefficient in the solar spectrum region and tunability of bandgap. However, the important basic properties such as the effective mass and intrinsic bandgap are far from quantitatively determined. In this work, we will analyze and discuss the optical absorption of disordered $ZnSnN_2$ degenerately doped with oxygen (*i.e.*, $ZnSnN_{2-x}O_x$) in the ultraviolet to infrared region to determine the conduction-band effective mass (m_c^*) and intrinsic bandgap (E_g).

***FILM GROWTH & CHRACTERIZATION*:** Disordered $ZnSnN_2$ epitaxial films were grown on YSZ(111) substrates by reactive radio-frequency magnetron sputtering technique using $Zn_{0.5}Sn_{0.5}$ alloy target. Films were grown under N_2 partial pressure ranging from 1.0 to 2.0 Pa , and at substrate temperatures ranging from 250 to 350 °C. Optical transmittance and reflectance in the wavelength range of 0.3−5.0 μm were collected using a UV-Vis-NIR spectrophotometer and FTIR spectrometer.

***RESULTS & DISCUSSION*:** Figure 1 presents optical transmittance (T) and reflectance (R) spectra for one typical $ZnSnN_{2-x}O_x$ epilayer in the ultraviolet to infrared region. Owing to the large n_e values on the order of 10^{20} cm^{-3}, free-electron absorption and reflection are clearly seen in the infrared region. We analyzed the free-electron absorption/reflection using the double Tauc-Lorentz and Drude model to determine the conduction-band effective mass (m_c^*) of disordered $ZnSnN_2$, see Fig. 2. We thus revealed the m_c^* value to be $(0.37 \pm 0.05)m_0$, combing the reported data ($0.5m_0$) from [1], indicating that the theoretical values are probably underestimated. The T/R spectra, representatively shown in Fig. 1, also enables us to determine the optical bandgap (E_g^{opt}) values from calculation of the optical absorption coefficient α of the $ZnSnN_2$ epilayers. The blue shift of the E_g^{opt} was analyzed in the framework of the Burstein-Moss effect. Our E_g^{opt} values as well as literature values showed a universal 2/3-power dependence on the electron density n_e. From this dependence, the E_g of disordered $ZnSnN_2$ was determined to be 0.90 eV.

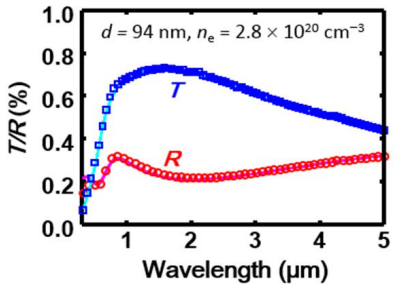

Fig.1. Optical transmittance (T) and reflectance (R) spectra for one typical $ZnSnN_{2-x}O_x$ epilayer.

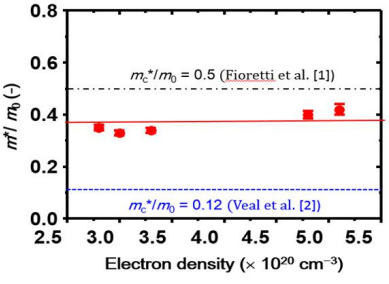

Fig.2. Conduction-band effective mass (m_c^*/m_0) of disordered $ZnSnN_2$ as a function of n_e.

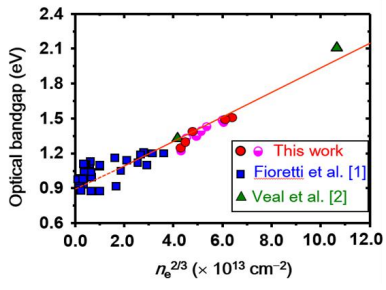

Fig.3. Optical bandgap of disordered $ZnSnN_2$ films as a function of 2/3-power of n_e.

***REFERENCES*:** [1] A. N. Fioretti *et al.*, J. Mater. Chem. C, **3**, 11017 (2015).
[2] T. D. Veal *et al.*, Adv. Energy Mater., **5**, 1501462 (2015).

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