Area: 2. Thin-Film Compound Semiconductor PV

FORMATION OF A NOVEL MG-P-ZN TERNARY SEMICONDUCTOR: A KEY MATERIAL OF EFFICIENCY ENHANCEMENT IN Zn_3P_2-BASED SOLAR CELLS

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Introduction

Zinc phosphide (Zn_3P_2) is considered as a potential non-toxic and earth-abundant alternative to CdTe because of the similarity in applicable manufacturing processes [1]. The highest efficiency of Zn_3P_2-based solar cells (6.08%) was reported with Mg/p-Zn_3P_2 junction by Catalano et al. [2]. In the previous studies on the device, it was suggested that diffusion of Mg into Zn_3P_2 led to formation of Mg-doped n-type Zn_3P_2 [3] or Mg-P-Zn alloy [4]. However, there are no reports on nanoscopic observation of Mg/p-Zn_3P_2 interface and the interface structure is still controversial. In the present study, we thus analyzed Mg/p-Zn_3P_2 junctions by a transmission electron microscope (TEM) on and reveal that a Mg-P-Zn ternary compound semiconductor, not Mg-doped Zn_3P_2 nor Mg-P-Zn alloy, is formed at the interface.

Experimental procedure

The Zn_3P_2 bulk crystals were fabricated by the physical vapor transport method [5]. The grown crystals were mechanically processed into the wafers with mirror surfaces. The wafers exhibit a p-type conductivity with a hole concentration in the range of 10^{16} cm^{-3}. Prior to the deposition of the electrodes, the wafers were chemically etched in bromine water diluted 20 times with ultra-pure water for 10 min and then ultrasonic washed in ultra-pure water. Mg and Ag electrodes were prepared on the Zn_3P_2 wafers by thermal evaporation. Some samples were annealed at the temperatures in the range from 100 to 300 °C for 1 h in sealed quartz ampules under a pressure of 10^{-2} Pa. Cross-sectional scanning transmission electron microscopy (STEM), energy dispersive X-ray spectrometry (EDS), and selected area electron diffraction (SAED) analyses were carried out for thin samples prepared by focused Ga^+ ion beam.

Results and Discussions

Figure 1 shows the cross-sectional images by STEM-EDS of the Mg/p-Zn_3P_2 interfaces after annealing at 300 °C. The area including Mg, P, and Zn with a thickness over 1 μm is observed at the interface. SAED patterns shown in Fig. 2 (a) and (b) indicate that the Mg-P-Zn layer has a different crystal structure to that of Zn_3P_2. As the results of the STEM-EDS and the SAED analyses, the Mg-P-Zn layer consists of a ternary compound $Mg_xZn_yP_2$ which have similar structure to that of $Mg_{1.75}Zn_{1.25}P_2$ as shown in Fig. 2(d).

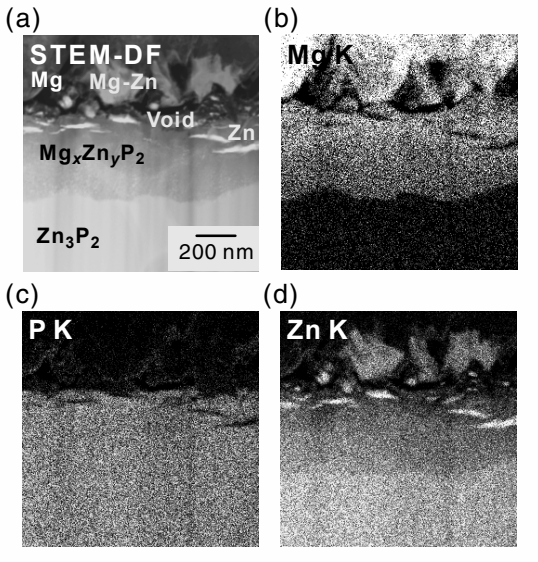

Figure 1: (a) STEM-dark field image and EDS mappings for (b) Mg K, (c) P K, and (d) Zn K of the Mg/p-Zn_3P_2 interfaces annealed at 300 °C.

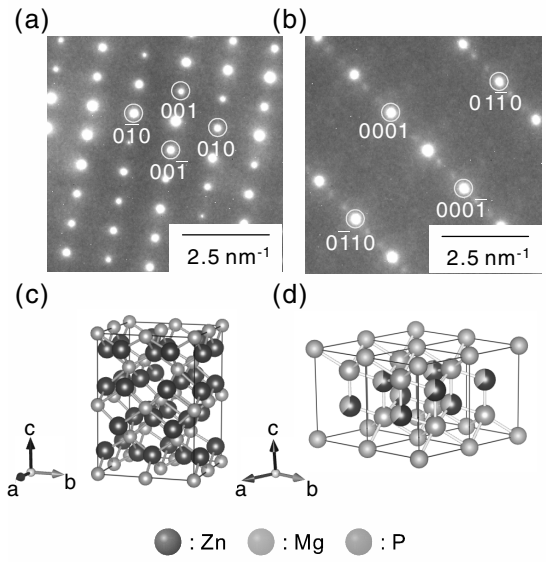

Figure 2: (a) SAED pattern from the area of (a) Zn_3P_2 (b) $Mg_xZn_yP_2$ in Fig. 2(a), and crystal structures of (c) Zn_3P_2 and (d) $Mg_{1.75}Zn_{1.25}P_2$.

Reference

[1] J. Collier et al., *Energy* (2014). [2] A. Catalano et al., *Proc. 2nd E. C. PVSEC* (1979). [3] A. Catalano and M. Bhushan, *Appl. Phys. Lett.* (1980). [4] G. M. Kimball et al., *Proc. 37th IEEE PVSC* (2011). [5] R. Katsube and Y. Nose, *J. Mater. Chem. C* (2017).