Area: 6 Advanced Concepts and New Emerging Materials for Future PV.

DEVELOPMENT OF PREFERRED ORIENTATION IN EVAPORATED $BASI_2$ FILMS ON SI(100) BY CONTROLLING THE NEAR-INTERFACE STRUCTURE

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$BaSi_2$ is an emerging absorber-layer material for thin-film solar cells with earth-abundant elements. The highest reported power conversion efficiency of solar cells using $BaSi_2$ is 9.9%, which was achieved with a p-type $BaSi_2$/n-type Si heterojunction structure [1,2]. Since $BaSi_2$ has a band gap of 1.3 eV and high absorption coefficients ($> 10^4$ cm^{-1}), a higher conversion efficiency reaching 25% is theoretically possible with a $BaSi_2$-based structure [3]. Thermal evaporation of $BaSi_2$ is a simple and effective method to prepare $BaSi_2$ films. Films with long carrier lifetime up to 5 μs can be formed even at a high deposition rate around 1 μm/min [4]. For the application of evaporated $BaSi_2$ films to solar cells, highly-oriented films are preferable to suppress the spatial distribution of electrical properties. So far, almost *a*-axis oriented $BaSi_2$ films were formed by thermal evaporation by increasing the substrate temperature to 700 ˚C [5]. The mechanism of preferred orientation is, however, not elucidated. In this study, we investigated the effects of the processing conditions influencing the near-interface structure on the crystal orientation of evaporated $BaSi_2$ films and discuss the mechanism of *a*-axis-oriented growth.

Approximately 500-nm-thick $BaSi_2$ films were prepared by thermal evaporation of $BaSi_2$ granules on Si(100) substrates at a substrate temperature of 650 ˚C in a high-vacuum chamber. Si substrates were cleaned by organic solvents and diluted HF solution before loading into the chamber. To investigate the effects of surface oxidation of substrate by the residual gas in the vacuum chamber on the crystal orientation of $BaSi_2$ films, the substrate heating duration before starting evaporation was changed from 0 to > 30 min. While evaporation proceeds, the vapor composition changes from Ba-rich to Si-rich. We also investigated the effects of the initial Ba-rich vapor by keeping the shutter close for 4 s after evaporation started.

Figure 1 shows the 2θ–ω X-ray diffraction (XRD) patterns of the evaporated $BaSi_2$ films together with the simulated powder pattern of $BaSi_2$. The $BaSi_2$ film deposited including the initial Ba-rich vapor after substrate heating for more than 30 min shows strong peaks of 211/103/202, 111/102, and 123/222 diffractions. On the other hand, the 600 diffraction is very weak and 200 and 400 diffractions are not observed, indicating that the fraction of *a*-axis-oriented grains is small. By decreasing the substrate heating duration to 0 min, an increase in 600 peak intensity is observed. The block of the initial Ba-rich vapor further increases the relative intensity of 600 diffraction. In this case, the 200 and 400 diffractions are also clearly observed. Auger electron spectroscopy (not shown) indicated that oxygen concentration around the interface decreased either by the decrease of the substrate heating duration or by blocking the initial Ba-rich vapor. The increase in the fraction of *a*-axis-oriented $BaSi_2$ grains is, therefore, probably related to the suppression of oxygen incorporation around the interface. In the presentation, the relationship between oxidation and oriented growth of $BaSi_2$ will be further discussed.

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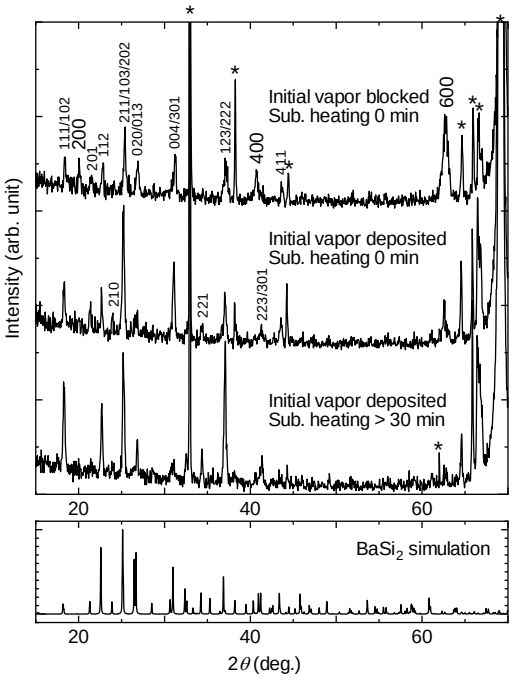

Figure 1: 2θ–ω XRD patterns of $BaSi_2$ evaporated films deposited at 650 ˚C. Peaks with * symbols derive from Si substrate.

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