Electron paramagnetic resonance lines of *a*-axis-epitaxial $BaSi_2$ thin-film

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【 Introduction 】

We have paid a special attention to barium disilicide ($BaSi_2$) consisting of earth-abundant Ba and Si. $BaSi_2$ possesses an indirect bandgap of 1.3 eV, which is more suitable than crystalline Si for a single-junction solar cell. Recent experiments have revealed that $BaSi_2$ has a sufficiently large minority carrier diffusion length (L ~ 10 μm) and a large minority carrier lifetime (τ ~ 10 μs) for thin-film solar cells. In addition, $BaSi_2$ has high absorption coefficients exceeding 3×10^4 cm^{-1} at 1.5 eV, since its direct transition edge is located higher by only 0.1 eV than the band gap[1]. Thus, conversion efficiency (η) exceeding 25% is expected by utilizing outstanding properties of $BaSi_2$ for the light absorber layers in thin-film solar cells[2]. To the end of attain such high η, high-quality film is required. We revealed that the deposition rate ratio R_{Ba}/R_{Si} affects the quality of the films strongly[3]. We attribute these results to native point defects inside $BaSi_2$ films. Thus, in this study, we employ electron paramagnetic resonance, (EPR), in order to investigate the defects inside the films.

【 Experiment 】

A 450-nm-thick $BaSi_2$ with R_{Ba}/R_{Si} = 2.2 film was fabricated on a Fz-Si(111) substrate by MBE after growing a $BaSi_2$ template layer by RDE. We then formed a 3-nm-thick amorphous Si, which acts as a surface passivation layer. Out-of-plane and in-plane x-ray diffractions and Raman scattering using 532 nm laser were measured to characterize the sample. The CW-EPR measurements were performed at 5 - 50 K with a microwave frequency of 9.56 GHz (X-band). Angular dependent EPR measurements were performed by varying an angle θ between the direction of static magnetic field B and the direction of the crystallographic *a*-axis of *a*-axis-orientated epitaxial $BaSi_2$ film.

【 Result and discussion 】

As shown in Fig. 1(a), at θ = 0°, two EPR lines were observed in the $BaSi_2$ film on the Fz-Si (111) substrate at 10 K. Compared with the result on the Si substrate under the same measurement condition, we suggest that the observed additional line (an arrow shown in Fig. 1(a)) originates from the $BaSi_2$ film, not from the Si substrate. In order to confirm that the additional line is due to the $BaSi_2$ film, we performed further experiments with different microwave power. The results showed that the two lines possessed different origins since they display different MW power saturation. In addition, we observed the resonance field of the film attributed to the $BaSi_2$ layer change with orientation ($\Delta g \approx 0.0075$, $\Delta B \approx 0.13$ mT) while the line from the substrate is isotropic (Fig. 1(b)). We attribute this angular dependence to symmetry of the films which possess 3 epitaxial variants in the plane, although furthermore investigations would be needed.

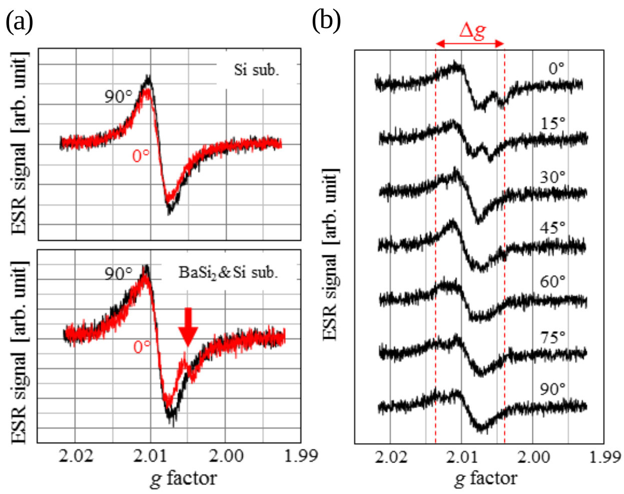

Fig. 1(a) EPR lines from Si substrate (upper) and *a*-axis-orientated epitaxial $BaSi_2$ film on Si substrate (lower) at 10 K. (b) The angular dependence of the EPR lines measured at 20 K.

【 Reference 】

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