Investigations of defects inside bulk and thin-film $BaSi_2$ by EPR

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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 attain such high η, high-quality films are required. Therefore, we have investigated defects inside $BaSi_2$ by using electron paramagnetic resonance, (EPR). In the last autumn meeting, we reported EPR lines which are originated from defects in $BaSi_2$ thin-films[3]. In this study, we perform EPR for bulk $BaSi_2$ in order to obtain furthermore information on their defects. Compared present results with those of film samples, we try to clarify the defects of $BaSi_2$.

【 Experiment 】

We powdered bulk samples whose nominal composition ratio are Ba : Si = 1: 1.88 (Ba-rich), 1 : 1.94 (near-stoichiometric), and 1 : 2.06 (Si-rich) in an agate mortar and then placed in EPR tubes and sealed in an Ar atmosphere. All procedures mentioned above were carried out in a globe box to prevent samples from degradation and oxidation in air. EPR measurements were performed at 5 - 50 K. We employed different microwave frequencies (X-band; 9.65 GHz, Q-band; 34.0 GHz, and Higher-field; 331.2 GHz) in order to determine precise g factors which characterize each paramagnetic center.

【 Result and discussion 】

As shown in Fig.1 (a), EPR lines were observed at 10 K in all samples. In non-stoichiometric Ba-rich and Si-rich samples, the EPR lines consist of two components. One of the two has $g \approx 2.003$ (shown as red lines in Fig.1 (a) and (b)), which is almost consistent between X-band (Fig.1 (a)) and Q-band (Fig.1 (b)). Furthermore, the value of this line seems to correspond to results of thin-film samples (Fig.1 (c)). The other component is broad line at lower g factor. Its behavior at Q-band seems different from each other. Further investigation including effects of hyperfine interaction have been performed for the moment. Interestingly, in a case of near-stoichiometric sample, we observed that an EPR line with $g \approx 1.98$ increased (shown as an orange line in Fig.1 (a)). Through investigation of present bulk results, we discuss the origins of EPR lines observed in thin-films.

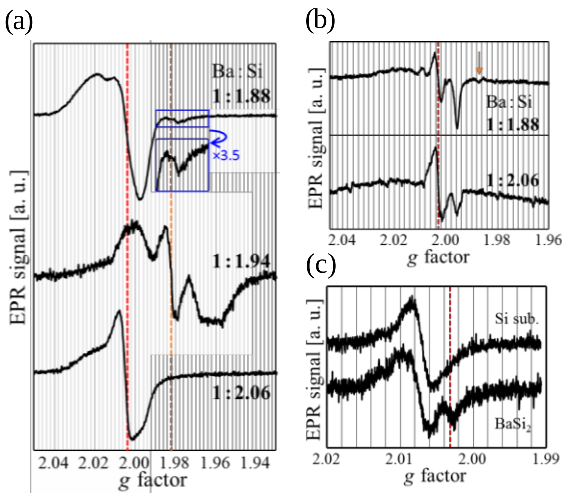

Fig.1 (a) X-band EPR lines (at 10 K) of Ba-rich, near-stoichiometric, and Si-rich from top to bottom, respectively. (b) Q-band EPR lines (at 10 K) of Ba-rich (upper) and Si-rich (lower). (c) X-band EPR lines of Si substrate (upper) and $BaSi_2$ film (lower). In all figures, red lines and an orange line (an arrow) indicate that $g \approx 2.003$ and 1.98, respectively.

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【 Reference 】

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