Investigation of hydrogen states in semiconducting $BaSi_2$ by muon spin rotation

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Introduction

$BaSi_2$ has advantages over other solar cell materials from the viewpoints of a suitable band gap of 1.3 eV, a large absorption coefficient of 3×10^4 cm^{-1} at 1.5 eV, exceeding those of CIGS, and a large minority-carrier diffusion length of ca. 10 μm [1]. The electrically active defect levels of the order of 10^{13} cm^{-3} were detected even in high-quality $BaSi_2$ films by deep-level transient spectroscopy, and they were considered to originate from Si vacancies (V_{Si}) in $BaSi_2$ [2]. According to the first-principle calculations by Kumar *et al.*[3] that V_{Si} are most likely to occur as point defects in $BaSi_2$. In the previous research, we passivated these V_{Si} using atomic H by radio-frequency (RF) plasma generator. The photoresponsivity of $BaSi_2$ passivated with atomic H is higher by one order of magnitude than the highest value previously reported, and the minority carrier lifetime was also improved to 14 μs, equivalent to its bulk carrier lifetime. These results show that atomic H is an effective method to passivate V_{Si} [4]. Motivated by such a major role of H in $BaSi_2$, we plan to clarify the physical and electronic structure of isolated H centers via their muonium (Mu) analog as performed in GaN [5]. This is the first time to apply muon spin rotation (μSR) measurement to $BaSi_2$.

Experiment

We performed μSR measurements on 2-inch polycrystalline $BaSi_2$ bulk at Japan proton acceleration research complex (J-PARC), MLF S1 Spectrometer. The temperature was varied from 4 to 300 K under longitudinal (LF) or transverse (TF) magnetic fields.

Results & Discussions

Two typical μSR asymmetry time spectra are shown in Figs. 1 (a) and 1(b), measured at 21 K and 222 K, respectively, under the transverse magnetic field (TF) of 20 G. The amplitude of the precession signal under TF increases with increasing temperature, indicating that the appearing parts forms a Mu state. The activation energy for Mu ionization was found to be approximately 31 meV by fitting the date in Fig. 2 over the temperature range from 60 to 200 K using the equation of $\alpha + \beta\exp(-E_a/k_BT)$. It represents a direct transition from the defect level to the conduction band minimum, suggesting strongly suggest that shallow Mu states exist in $BaSi_2$.

Acknowledgment

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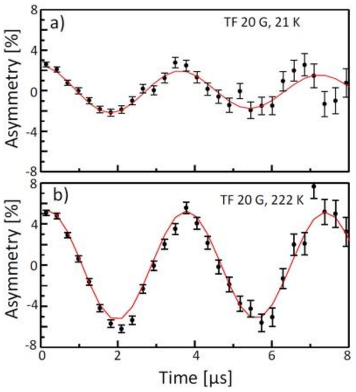

Fig. 1. Muon spin rotation in $BaSi_2$ at (a) 21 K and (b) 222K under TF mode of 20 G.

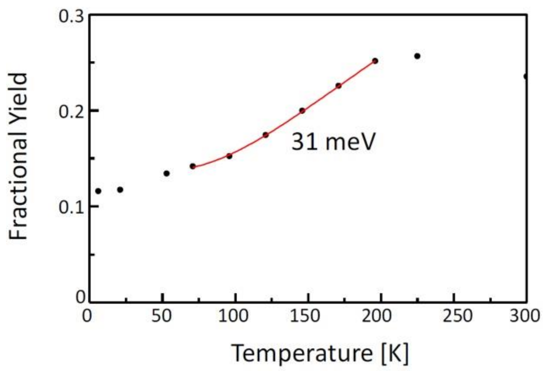

Fig. 2. Temperature dependence of fractional yield of muon. Solid curve is a fitting result. The activation energy was deduced to be approximately 31 meV.