Effects of hydrogen on trap neutralization in BaSi2 with interstitial silicon atoms

Sho Aonuki,

Kaoru Toko,

Andrew B. Filonov[1],

Dmitri B. Migas[1],

Takashi Suemasu

2023

[1] Belarusian State University of informatics and radioelectonics, 220013, Minsk, 6 P. Brovki str.

Keywords: Barium disilicide, thin film, molecular beam epitaxy, solar cell, photoresponsivity, trap neutralization, ab initio calculations.

Abstract: Semiconducting barium disilicide (BaSi2) is one of emerging materials for solar cell applications. Therefore, defect neutralization is very important for improving its solar cell performance. Herein, the effect of atomic hydrogen (H) on the photoresponsivity of 500-nm-thick undoped n-BaSi2 films grown under Si-rich conditions by molecular beam epitaxy was examined, wherein interstitial Si atoms were likely to exist instead of common Si vacancies. The photoresponsivity reached a maximum of ∼1.3 A W−1 at room temperature (about twice as large as that for as-grown films) in BaSi2 films exposed to an atomic H for 10 s. This H treatment time is much smaller than that for BaSi2 films grown under stoichiometric conditions, indicating that interstitial Si atoms provide a smaller trap concentration with respect to the case of Si vacancy domination and incorporation of H atom can neutralize traps. The inverse logarithmic slope (E0) of the Urbach tail was investigated to discuss the dependence of the photoresponsivity of BaSi2 films on H treatment time.

There was a clear negative correlation between E0 and photocurrent density obtained from the photoresponsivity. The detailed picture on how interstitial Si atoms affect the electronic structure of BaSi2 by defect state formation and how H atom incorporation modifies the structure is revealed by ab initio calculations that allowed interpreting and understanding of all experimentally observed trends.

Effects of hydrogen on trap neutralization in BaSi2 with interstitial silicon atoms / Sho Aonuki [et al.] // Thin Solid Films. – 2023. – Vol. 773. – P. 139823.