Marked enhancement of the photoresponsivity and minority-carrier lifetime of $BaSi_2$ passivated with atomic hydrogen

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2019

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Keywords: Barium disilicide, H passivation, Photoconductivity, Minority-carrier lifetime.

Abstract: Passivation of barium disilicide ($BaSi_2$) films is very important for their use in solar cell applications. In this paper, we demonstrated the effect of hydrogen (H) passivation on both the photoresponsivity and minority-carrier lifetime of $BaSi_2$ epitaxial films grown by molecular beam epitaxy. First, we examined the growth conditions of a 3-nm-thick hydrogenated amorphous silicon (a-Si) capping layer formed on a 500-nm-thick $BaSi_2$ film and found that an H supply duration (*t*a-Si:H) of 15 min at a substrate temperature of 180 °C sizably enhanced the photoresponsivity of the $BaSi_2$ film. We next supplied atomic H to $BaSi_2$ epitaxial films at 580 °C and changed supply duration (*t*BaSi;H) in the range of 1–30 min, followed by capping with an a-Si layer. The photoresponsivity of the films changed considerably depending on *t*BaSi;H and reached a maximum of 2.5 A/W at a wavelength of 800 nm for the sample passivated for *t*BaSi;H = 15 min under a bias voltage of 0.3 V applied to the front-surface indium-tin-

oxide electrode with respect to the back-surface aluminum electrode. This photoresponsivity is approximately one order of magnitude higher than the highest value previously reported for $BaSi_2$. Microwave photoconductivity decay measurements revealed that the minority-carrier lifetime of the $BaSi_2$ film with the highest photoresponsivity was 14 μs, equivalent to its bulk carrier lifetime ever reported. We performed theoretical analyses based on a rate equation including several recombination mechanisms and reproduced the experimentally obtained decay curves. We also calculated the total density of states of $BaSi_2$ by *ab initio* studies when one Si vacancy existed in a unit cell and one, two, and three H atoms occupied Si vacancy or interstitial sites. A Si vacancy caused a localized state with two energy bands to appear close to the middle of the band gap. In certain cases, H passivation of the Si dangling bonds can markedly decrease trap concentration. From both experimental and theoretical viewpoints, we conclude that an atomic H supply is beneficial for $BaSi_2$ solar cells.

This article published in: Marked enhancement of the photoresponsivity and minority-carrier lifetime of BaSi2 passivated with atomic hydrogen / Z. Xu [and others] // Phys. Rev. Mater. – 2019. – Vol. 3, № 6. – P. 065403. – https://doi.org/10.1103/PhysRevMaterials.3.065403.

Internet link to the article:

https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.3.065403.