Atomic hydrogen passivation for photoresponsivity enhancement of boron-doped p-$BaSi_2$ films and performance improvement of boron-doped p-$BaSi_2$/n-Si heterojunction solar cells

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Abstract: Semiconducting barium disilicide ($BaSi_2$) is an emerging material for solar cell applications, and therefore, defect passivation is critical forimproving its solar cell performance. Herein, the effect of atomic hydrogen (H) on the photoresponsivityof 500 nm-thick boron (B)-dopedp-$BaSi_2$ films was examined. The photoresponsivity reached ~4 A/W (about twice the highest reported value for H-passivated undoped $BaSi_2$films) in B-doped p-$BaSi_2$ films exposed to an atomic H supply for 5 − 10 min because of an increased minority-carrier lifetime, as measuredby the microwave-detected photoconductivity decay. Furthermore, a ≥15 min atomic H supply was found to degrade photoresponsivity.Ab initio studies were used to interpret and understand experimental observations by analyzing states in the gap region, which can act as traps,in B-doped p-$BaSi_2$ with H incorporation. The effect that atomic H had on the performance of B-doped p-$BaSi_2$/n-Si heterojunction solar cellswas also studied. The saturation current density was found to decrease by three orders of magnitude with the atomic H supply, and the conversionefficiency was increased up to 6.2%. Deep-level transient spectroscopy revealed a reduction of defect densities induced by the atomic Hsupply. Both experimental and theoretical viewpoints show that an atomic H supply is beneficial for $BaSi_2$ solar cells.

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