Recent Progress Toward Realization of High-Efficiency $BaSi_2$ Solar Cells: Thin-Film Deposition Techniques and Passivation of Defects

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Abstract: Safe, stable, and earth-abundant materials for solar cell applications are of particular importance to realize a decarbonized society. Semiconducting barium disilicide ($BaSi_2$), which is composed of nontoxic and earth-abundant elements, is an emerging material to meet this requirement. $BaSi_2$ has a bandgap of 1.3 eV that is suitable for single-junction solar cells, a large absorption coefficient exceeding that of chalcopyrite, and inactive grain boundaries. This review is started by describing the recent progress of $BaSi_2$ thin-film deposition techniques using radio-frequency sputtering and discuss the high photoresponsivity

of $BaSi_2$ thin films. Special attention is paid to passivation of the defects in $BaSi_2$ films by hydrogen or carbon doping. Ab initio studies based on density-functional theory are then used to calculate the positions of the localized defective states and the Fermi level to discuss the experimentally obtained passivation effects. Finally, the issues that need to be resolved toward realization of high-efficiency $BaSi_2$ solar cells are addressed.

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