Effects of lattice parameter manipulations on electronic and optical properties of BaSi2

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Abstract: We present comprehensive experimental and theoretical investigation on a band-gap engineering and modification in optical properties of BaSi2 – a new and very promising material for solar cell fabrication. BaSi2 thin films have been synthesized by molecular beam epitaxy with various deposition rates of Si and Ba. Changes in their band gaps and shifts in absorption edges with respect to alteration in the a lattice parameter have been investigated by optical

measurements. It is possible to shrink a by about 0.003 nm (or 0.3%), while the other lattice parameters are locked by the epitaxial relationship with a Si(111) substrate, that leads to the gap reduction from 1.28 eV to 1.20 eV. By means of ab initio calculations we explore a possibility to manipulate band-gap values in BaSi2 along with the corresponding shift in the absorption edge by changing its a, b and c lattice parameters. It is revealed that an increase in any of the lattice parameters provides band-gap enlargement while the opposite trend is observed when decreasing the lattice parameters. Numerically uniaxial lattice strain of 3% can provide variations in the band gap up to 0.1 eV. We also discuss possible reasons for a variation and applicability of the band-gap engineering in BaSi2 by strain.

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