Influence of lattice expansion on the topological band order of $InAs_xSb_{1-x}$ (x=0, 0.25, 0.5, 0.75, 1) alloys

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Abstract

The topological band structures of $InAs_xSb_{1-x}$ (x=0, 0.25, 0.5, 0.75, 1) alloys have been investigated using density functional theory by utilizing the Wien2k package. These alloys are in a topologically trivial phase in their unstrained states and exhibit a small band gap. Since in small band-gap cubic semiconductors the nontrivial topological phase can be achieved by lattice expansion, we investigate the effect of hydrostatic and biaxial lattice expansion on band inversion strength and band order of these alloys. It is found that under reasonable hydrostatic lattice expansion, $InAs_xSb_{1-x}$ (x=0, 0.25, 0.75, 1) alloys with cubic symmetry and $InAs_{0.5}Sb_{0.5}$ alloy with tetragonal symmetry, are converted to nontrivial topological semiconductors with zero band gap and non-zero band gap, respectively. In order to convert $InAs_xSb_{1-x}$ (x=0, 0.25, 0.75, 1) alloys into topological semiconductors with non- zero band gap, we let the systems of $InAs_xSb_{1-x}$ (x=0, 0.25, 0.75, 1) alloys undergo a biaxial lattice expansion. Thus by breaking the cubic symmetry in these alloys, not only they are converted to topologically nontrivial phase but also a small band gap is opened at Γ point.