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Origin of the unusually large band gap bowing and the breakdown of the band-edge distribution rule in the SnxGe1-x alloys WAN-JIAN YIN, XIN-GAO GONG, Fudan University, Shanghai, China, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado, USA — Most semiconductor alloy AxB1-x has a non-linear dependence of its band gap Eg(x) as a function of the alloy composition x, and the variation is usually described by a parabolic function Eg(x) = xEg^A+ (1-x)Eg^B - bgx(1-x), where Eg^{A}and Eg^B are the band gaps of A and B at their respective equilibrium lattice constants and bg is the so-called bowing parameter. The conventional band-edge distribution of bg is usually described by the equation bVBM(CBM) = ΔEVBM(CBM)/ΔEgbg , where ΔEVBM(CBM) and ΔEVBM(CBM) are VBM and CBM natural band offsets. Using first-principles calculations, we investigate the unusual nonlinear behaviors of the band gaps in SnxGe1-x alloys. We show that the large bowing of the direct band gap is induced by the disordering effect. Moreover, we calculated individual contribution of the band edge states and find that the bowing of the conduction band edge is much larger than the bowing of the valence band edge, although the natural valence band offset between Ge and Sn is larger than the natural conduction band offset. The breakdown of the band-edge distribution rule is explained by the large lattice mismatch between Ge and Sn and the large deformation potential of the band edge states.

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