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Bowing in the Compositional Dependence of Optical Transitions in GeSn alloys VIJAY D' COSTA, ANDREW CHIZMESHYA, CANDI COOK, JOHN KOUVETAKIS, JOSE MENENDEZ, Arizona State University — Recent ellipsometric measurements provide a detailed picture of the band structure of GeSn alloys. In particular, the compositional dependence of the strongest interband optical transitions was determined in the compositional range x $<$ 0.2. The results show very strong deviations (bowing) from a linear interpolation between the band structures of pure Ge and α-Sn. In this presentation we analyze the bowing parameters for GeSn alloys and compare them with similar parameters for the SiGe system. The possibility of a comparative study of bowing between these two systems is exciting due to their isoelectronic nature and the similarities in their structural relaxation parameters. Following the theory of Bernard and Zunger [J.E. Bernard and A. Zunger, PRB 36, 3199 (1987)], the bowing is described as the sum of three terms, involving volume deformation, charge redistribution, and internal relaxation. The first and third mechanisms are expected to scale with the lattice constant mismatch, which is much larger in the Ge-Sn system. The second mechanism is proportional to the electronegativity difference, which is also larger in Ge-Sn. The parameters needed for quantitative predictions are obtained from measured volume dependencies of optical transitions or from calculated band structures for Si, Ge, α-Sn, SiGe, and GeSn as a function of volume.

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