Abstract Submitted
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Surface phase stability and surfactant behavior of InAsSb alloy surfaces.[1] EVAN M ANDERSON, ADAM M LUNDQUIST, Materials Science and Engineering, University of Michigan, CHRIS PEARSON, Computer Science, Engineering, and Physics, University of Michigan-Flint, JOANNA M MILLUNCHICK, Materials Science and Engineering, University of Michigan — InAsSb has the narrowest bandgap of any of the conventional III-V semiconductors: low enough for long wavelength infrared applications. Such devices are sensitive to point defects, which can be detrimental to performance. To control these defects, all aspects of synthesis must be considered, especially the atomic bonding at the surface. We use an *ab initio* statistical mechanics approach that combines density functional theory with a cluster expansion formalism to determine the stable surface reconstructions of Sb (As) on InAs (InSb) substrates. The surface phase diagram of Sb on InAs is dominated by Sb-dimer termination α2(2x4) and β2(2x4) and c(4x4). Smaller regions of mixed Sb-As dimers appear for high Sb chemical potentials and intermediate As chemical potential. We propose that InAsSb films could be grown on (2x4), which maintain bulk-like stoichiometry, to eliminate the formation of typically observed n-type defects. Scanning tunneling microscopy and reflection high energy electron diffraction confirm the calculated phase diagram. Based on these calculations, we propose a new mechanism for the surfactant behavior of Sb in these materials.

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