Influence of hydrogen surface passivation on Sn segregation, aggregation, and distribution in GeSn/Ge(001) materials

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Abstract

Plane-wave density functional theory is used to investigate the impact of hydrogen passivation of the p(2×2) reconstructed $Ge_{1-x}Sn_x$ surface on Sn segregation, aggregation, and distribution. On a clean surface, Sn preferentially segregates to the surface layer, with surface coverages of 25%, 50%, and 100% for total Sn concentrations of 2.5%, 5.0%, and 10.0%, respectively. In contrast, a hydrogen passivated surface increases interlayer migration of Sn to subsurface layers, in particular, to the third layer from the surface, and results in surface coverages of 0%, 0%, and 50% corresponding to Sn concentrations of 2.5%, 5.0%, and 10.0%, respectively. Hydrogen transfer from a Ge-capped surface to the one enriched with increasing Sn surface coverage is also an unfavorable process. The presence of hydrogen therefore reduces the surface energy by passivating the reactive dangling bonds and enhancing Sn interlayer migration to the subsurface layers. For both clean and hydrogenated surfaces, aggregation of Sn at the surface layer is also not favored. We explain these results by considering bond enthalpies and the enthalpies of hydrogenation for various surface reactions. Our results thus point to reduced Sn segregation to the surface in a $Ge_{1-x}Sn_x$ epitaxial thin film if CVD growth, using hydride precursors in the hydrogen limited growth regime, is used. This would lead to a more abrupt interface and is consistent with recent experimental observation. Hydrogenation is therefore a promising method for controlling and manipulating elemental population of Sn in a $Ge_{1-x}Sn_x$ epitaxial thin film.

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