Implications for SiGeSn growth from the surface science of Sn on Si

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SiGeSn is a promising alloy for optoelectronic applications due to having a simpler path for integration into silicon semiconductor manufacturing than compound semiconductors. A direct bandgap has been predicted theoretically, but has not been definitively observed experimentally. This discrepancy is thought to result from the atoms in the lattice not forming a random alloy, but exhibiting short range order. Curiously, SiGe has the same underlying atomic- and mesoscopic-scale forces, i.e. bonding and strain, but is a random alloy. The goal of this research is to understand what is driving short range ordering in SiGeSn alloys. We collected data with scanning tunneling microscopy (STM), analyzing growth in a step-by-step fashion where sub-monolayer Sn is deposited on to a Si(100) substrate, and then annealed. Step-by-step tuning of growth and annealing variables can be analyzed *in situ* with STM.

Atomic scale analysis of the Sn:Si surface gives insight into what drives ordering of group IV alloys. Our data shows Sn deposited on Si forms 2x1 dimer chains, but, unlike Si deposited on Si, they don't pack closely together due to steric repulsion. After annealing, Sn both assembles into islands at the surface as well as incorporates into the topmost layer of Si atoms in the substrate, but with a 3x2 periodicity (Fig 1). The change implies an interaction between the local strain inherent to the dimer rows, bonding, and steric repulsion. Sn coverage, annealing time, and annealing temperature collectively change the appearance of structures above the atomic scale – e.g. the length of the chains. Meanwhile, only the long-range periodicity of these features is dictated by the strain. Atomic positions from the experimental data will be compared to predictions from modeling.

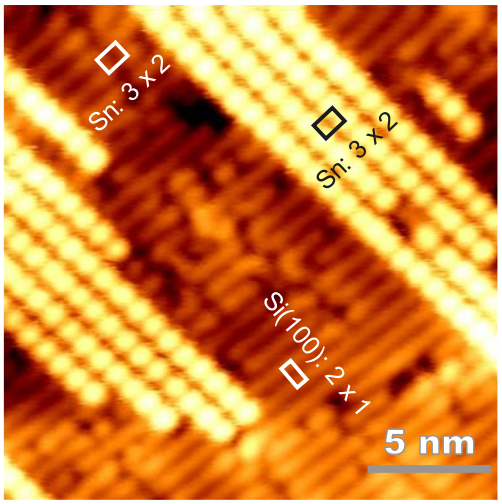

Figure 1. STM image of <ML Sn deposited on Si(100). After annealing, Sn organizes into islands on the Si surface and incorporates into the substrate, appearing as vacancy lines. Sn inherently segregates as illustrated by the Sn 3x2 phase coexisting with the Si 2x1 phase.

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