It is necessary to understand Nb-Sn-O intermolecular interactions to inform optimal Nb-Sn growth procedures. Recently, there has been significant progress in understanding the relationship between Nb-Sn-O film quality and cavity performance. With the goal of developing predictive Nb-Sn growth models, combined experimental and computational efforts have revealed the relationship between Sn adsorption and diffusion behavior and the underlying oxidized Nb substrate. Such information is essential when developing optimal Nb-Sn growth procedures.

Sn adsorption and diffusion behavior on (3×1)-O/Nb(100): 0.25 ML equivalence deposited at $T_{\text{sample}} = 24 \, ^\circ\text{C}$

STM data of 0.25 ML Sn/(3×1)-O/Nb(100)

- Sn adsorbs along (3×1)-O ladder columns at room temperature
- Annealed for 5 min at temperatures relevant to Nb-Sn growth procedures
- Sn diffusion is guided by the underlying substrate
- Sn desorption by 900 °C

STM and STS data of 0.25 ML Sn/(3×1)-O/Nb(100)

- Sn islands have a wider surface bandgap relative to the underlying (3×1)-O surface
- Taller Sn islands have a narrower surface bandgap compared to average height Sn islands

In situ sample preparation and surface characterization using UHV surface science techniques

- Electron beam (e-beam) evaporation source
- Quartz crystal microbalance (QCM)
- Auger electron spectroscopy (AES)
- Temperature programmed desorption (TPD)
- X-ray photoelectron spectroscopy (XPS)
- Scanning tunneling microscopy (STM)
- Scanning tunneling spectroscopy (STS)

The underlying oxide structure influences Sn adsorption and diffusion behavior

Sn adsorption and diffusion on (3×1)-O/Nb(100): 1.1 ML equivalence, $T_{\text{sample}} = 24 \, ^\circ\text{C}$

STM data of 0.25 ML Sn/(3×1)-O/Nb(100)

- Hexagonal Sn structure
- Rectangular Sn structure
- Both align with ladder rows

DFT calculations of Sn adsorption energies

- Edge site adsorption energies are, on average, lower energy than along ladder rungs
  - 0.88 eV min, 1.49 eV max
- Ladder site adsorption energy is minimized at the center point of the ladder width
  - 0.89 eV min, 2.88 eV max

Calculated (3×1)-O/Nb(100) surface

The lower adsorption energy for ladder edge sites may explain observed Sn adsorption and diffusion behavior

Investigating Sn adsorption and diffusion behavior on (3×1)-O/Nb(100) enhances our understanding of Sn-Nb-O interactions and the role of large-scale defects on alloy growth

This work was supported by the U.S. National Science Foundation under Award PHY-1549132, the Center for Bright Beams.