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Deconvoluting Initial Nb-Sn-O Interactions: Spatially Resolved Electronic Characterization of Sn Reconstructions on (3×1)-O Nb(100)

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The potential for lowered operating costs and higher quality factors (Q) motivate efforts to implement Nb₃Sn based superconducting radio frequency cavities. These benefits are contingent upon the continued optimization of coating procedures resulting in smooth, homogeneous A15 Nb₃Sn films. Specifically, the efficiency of Nb₃Sn cavity coatings is limited by the presence of surface defects including micron scale surface roughness and atomic dislocations such as Sn desegregation, high grain boundary density, and the persistence of surface oxides and subsurface oxygen. Fabricating pristine Nb₃Sn coatings requires a thorough understanding of the surface chemistry driving Nb₃Sn growth. Experimental data that outlines fundamental Nb-Sn-O surface interactions and Nb₃Sn alloying mechanisms would not only augment theoretical models detailing the superconducting and electronic consequences of various Nb₃Sn defects, but ultimately inform cavity Sn deposition procedures.

The atomic-scale interactions guiding Sn adsorption and diffusion behavior on oxidized Nb are probed using a well characterized (3×1)-O Nb(100) metal single crystal surface. An ultra-high vacuum chamber equipped with an electron beam evaporation source and quartz crystal microbalance, for precise metal deposition, paired with scanning tunneling microscopy/spectroscopy (STM/STS) enable in situ deposition, heat treatment, and analysis of the Sn/Nb interface. The (3×1)-O Nb(100) surface was exposed to precisely calibrated sub-monolayer (ML) quantities of Sn and was subsequently held at temperatures ranging from 500 – 900 °C to promote lateral Sn diffusion. STM images taken between annealing treatments reveal the morphology of Sn aggregates and the underlying NbO ladders. Room temperature STS spectra reveal electronic distinctions between multiple Sn reconstructions and the underlying NbO surface, demonstrating the electronic consequences of Sn adsorption and diffusion on oxidized Nb with atomic-scale spatial resolution. Ongoing work aims to elucidate the distinct structural and electronic features of Sn reconstructions as a function of Sn atomic %, temperature, and length of heat treatment. In addition to the experimental data obtained through this work, concomitant efforts using machine learning algorithms will be used to support observed surface structures and phases. Experimental observations of Sn adsorption and diffusion on a (3×1)-O Nb(100) surface aids in deconvoluting the complex surface chemistry mediating Nb-Sn alloying dynamics and mechanisms during Nb₃Sn formation.

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