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Spatially Resolved Adsorption Structures and Diffusion Dynamics of Sn on (3×1)-O Nb(100)

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Nb_3Sn has been identified as a promising next-generation material for superconducting radio frequency (SRF) cavities and there is significant interest in developing protocols resulting in pristine Nb_3Sn coatings. Recent work has shown that Nb_3Sn surface structure and composition significantly affects the cavity quality factor (Q) of Nb_3Sn SRF cavities; Sn homogeneity, surface roughness, and alloy thickness must be well controlled to achieve optimal cavity performance. There is not, however, a fundamental understanding of the surface mediated Sn diffusion and alloying mechanisms influencing pristine Nb_3Sn growth. In order to develop growth protocols resulting in smooth, homogeneous Nb_3Sn films, necessary for optimal Nb_3Sn cavity performance, fundamental studies investigating Sn adsorption and diffusion behavior must be conducted to identify deleterious Nb_3Sn growth mechanisms. Spatially resolved structural information of Sn adsorption structures and diffusion dynamics on oxidized Nb surfaces are needed to determine Nb_3Sn growth mechanisms resulting in heterogeneous Nb_3Sn coatings with low Q factors.

Using a combination of *in situ* ultra-high vacuum (UHV) surface science techniques, we aim to elucidate the spatially resolved Sn adsorption and diffusion behavior on oxidized Nb(100). Sample preparation and analysis was conducted in a custom built UHV experimental apparatus equipped with an electron beam (e-beam) evaporation source and quartz crustal microbalance (QCM), X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), scanning tunneling microscopy (STM), and scanning tunneling spectroscopy (STS) capabilities. Following deposition of 0.10 - 0.50 monolayers Sn, calibrated via QCM, on the (3×1)-O Nb(100) substrate, the initial Sn adsorption structure was determined using room temperature STM (RT-STM). The Sn/Nb(100) sample was then annealed at 500 ℃, 600 ℃, 700 ℃, 800 ℃, and 900 ℃ to promote Sn diffusion at temperatures relevant to the production of actual Nb_3Sn SRF cavities. RT-STM analysis following the annealing procedure revealed the formation of temperature dependent Sn adlayers on the (3×1)-O Nb(100) surface. Ongoing experimental and computational work is investigating the thermodynamic and kinetic parameters influencing the formation of the observed Sn adlayers on (3×1)-O Nb(100). The spatially resolved mechanistic information gleaned through this work is essential to guide the development of predictive Nb_3Sn growth models advancing current Nb_3Sn growth procedures.

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