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Correlating Atomic-Scale Structure with Superconducting Properties for Metallic, (3x1)-Oxidized, and Nitrogen-Dosed Nb(100)

Superconducting radio frequency (SRF) cavities are the fundamental accelerating components of linear particle accelerators. Niobium is the material of choice for SRF cavities due to its high malleability, thermal conductivity, and superconducting critical temperature (T_C). Despite Nb having a T_C of ~ 9 K, the practical operating temperature of a Nb SRF cavity is ~ 2 K, below the boiling point of He and consequently quite expensive to operate. The improvement of Nb SRF cavities and the lowering of operating costs has been focused primarily on the development of new materials on the Nb surface. Due to the ~ 100 nm superconducting penetration depth of Nb, only ~ 1 micron of material need be deposited onto the Nb surface to completely change its superconducting properties. One of the primary limitations to both Nb SRF cavities and the new materials under study is the presence of a thermally stable and robust oxide. Understanding the formation, stability, and dynamics of the oxide and its effects on the operation of Nb SRF cavities requires study both of material superconducting properties and atomic-scale surface material chemistry. Helium atom scattering (HAS) is a surface diffraction technique that has the ability to probe surface structure, bonding, and dynamics. The chemically inert He and an ultra-high vacuum (UHV) environment make HAS an ideal probe for the chemically reactive and sensitive Nb surface. Furthermore, experts in the field have developed theory involving the He-electron interaction and the surface electron-phonon interaction to formulate an equation by which HAS data can be used to determine an electron-phonon coupling (EPC) constant (λ) for the surface (λ_S). These data can then be used to find surface analogues for T_C along with other superconducting properties relevant to SRF cavity operation. We study the Nb(100) surface for its recognizable and stable (3x1)-O NbO oxide reconstruction. We find a λ_S of 0.50 ± 0.08 for the metallic Nb(100) versus a bulk λ of ~ 1 , demonstrating that the superconducting state is significantly modified at the surface. We also find a λ_S of 0.20 ± 0.06 for the (3x1)-O reconstruction. Lower λ_S corresponds to lower T_C and overall poorer superconducting performance. Therefore, our studies strongly corroborate a strong body of previous literature that has hypothesized that the oxide diminishes superconducting performance for both bare Nb and new materials built atop it. From this fundamental starting point, we look towards understanding better how and why nitrogen-dosed cavities improve superconducting performance. Currently, we know trace nitrogen is helpful for SRF cavity performance while thick NbN layers are not. Preliminary findings begin to show some information for how nitrogen diffuses into the surface and how nitrogen dosing affects EPC behavior.

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