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Surface Chemistry of Niobium Involving Oxygen, Hydrogen, and Nitrogen Relevant to the Performance of Superconducting RF Accelerator Cavities

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Superconducting radio frequency (SRF) technology is the key enabler for current and future high-energy and high-beam-power accelerators. Performance of SRF cavities for accelerators is characterized by their quality factor, Q_0 , a measure of their efficiency of operation, and the maximum accelerating field, E_{acc} , that they can sustain before their quality factor degrades. Chemical and structural defects at the surface and in the near-surface region of niobium SRF cavities can negatively or positively affect cavity performance. We investigate the surface structure, chemistry, and oxidative states of single-crystal niobium samples as well as technical grade polycrystalline SRF cavity samples using scanning tunneling microscopy (STM and STS), atomic force microscopy (AFM), Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS). These tools allow us to study processes such as the adsorption and dissolution of common elements such as oxygen and nitrogen onto and through the niobium surface and into the bulk, and how changes in local surface structure (such as crystal face, step edges, and domain boundaries) affect these processes. At atmospheric pressure, the niobium surface is completely covered in an insulating pentoxide overlayer. At relatively low temperatures, the pentoxide is reduced and dissolves into the bulk; we present kinetic results on this process. The orientation of the single-crystal surface significantly affects surface structure following reduction and dissolution of the pentoxide. After the dissolution of Nb_2O_5 , NbO is the thermally stable oxidative state and 3-5 layers remain on top of the bulk niobium. The NbO is thermally stable up to highly elevated temperatures where it desorbs from the surface. The orientation of the single crystal surface significantly affects the surface order exhibited by the NbO/Nb interface. The (111) face does not form long-range ordered surface structures even after high-temperature annealing for extended periods. The (100) face forms highly-organized ($n \times 1$) ladder-like features that cover the NbO(100) surface. We discuss the stability and interconversion of these ladder structures following thermal cycling with and without the presence of gas phase molecular oxygen, with particular focus on oxygen dissolution through the NbO(100) surface induced by relatively low-temperature annealing of the substrate following oxygen exposure. Inspired by recent discoveries at the Fermi National Accelerator Laboratory that involve the benefits of nitrogen-doping that enhance the operating characteristics of accelerator cavities, we also explore the possible relationship between nitrogen-doping and nanoscale hydride surface precipitation. Hydrides are known to form on cavity surfaces during cooldown to operational temperatures. These hydrides are non-superconducting and correlate strongly with diminished cavity performance. It is possible that nitrogen-doping serves as a hydrogen “trap” preventing hydrogen from migrating from the bulk to the surface during cooldown, and we investigate this possibility by studying polycrystalline samples cut from SRF cavities used at Fermi National Accelerator Laboratory. It is with pleasure that we acknowledge support from DOE and the NSF-MRSEC program at the University of Chicago.

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