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Atomic-scale chemical analyses of niobium for superconducting radio-frequency cavities

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Niobium is of great interest to the high-energy accelerator community due to its high transition temperature, high critical magnetic field, and high residual resistance ratio, which are required properties for increasing the accelerating field of a particle accelerator [1]. In addition, it is easy to fabricate niobium sheets into cavities with a complicated shape. There are many factors that determine the properties of the cavities. From a materials science point-of-view, the interstitial impurities in niobium, such as H, C, N, and O, are the most important ones. They are detrimental to the performance of the cavities, since they scatter electrons and reduce the width of superconducting gap. Little is known, however, concerning where all the impurities ultimately reside in the microstructure and what their concentrations and spatial distributions are.

Atom-probe tomography (APT) [2, 3] provides chemical information of analyzed materials on an atomic-scale utilizing time-of-flight (TOF) mass spectrometry, where the atoms are field evaporated on an atom-by-atom basis using pulse electric fields or laser pulses. We employ local-electrode atom-probe (LEAP) tomography [4, 5] to analyze the chemistry of niobium tips from the surface, which contains different oxides of niobium to the underlying bulk niobium.

A three-dimensional reconstruction of the experimental results is shown in Figure 1, containing 0.5 million atoms in a volume that is 36x36x49 nm^3. Niobium atoms are displayed in pink, O atoms in cyan, and H atoms in black. This figure demonstrates that the niobium oxide is on the surface of the bulk niobium. An isoconcentration surface of 50 at.% niobium is used to identify the oxide/bulk interface and calculate a proximity histogram, which presents the compositional information with respect to distance from the heterophase interface, Figure 2. The Nb/O ratio of 0.4 suggests that the surface oxide has the stoichiometry Nb_2O_5. This figure displays the wide oxide/bulk interface, approximately 10 nm in thickness, and a significant amount of O, ca. 20 at.%, in near surface oxide region.

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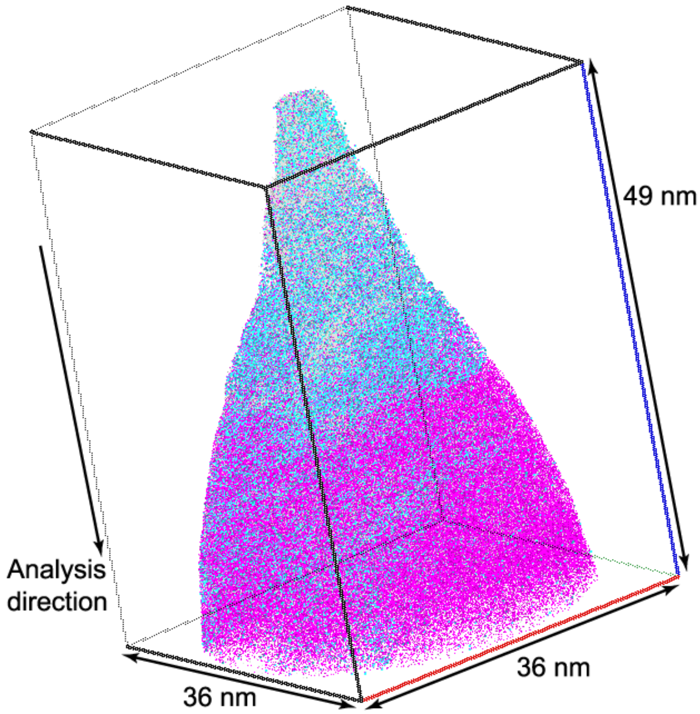

Figure 1. Three-dimensional atomic reconstruction of an oxide layer on the surface of a niobium tip. The overall reconstruction dimensions are 36x36x49 nm^3 (50279 nm^3); the volume contains ca. 500,000 atoms. Niobium atoms are displayed in pink, oxygen atoms in cyan, and hydrogen atoms in black.

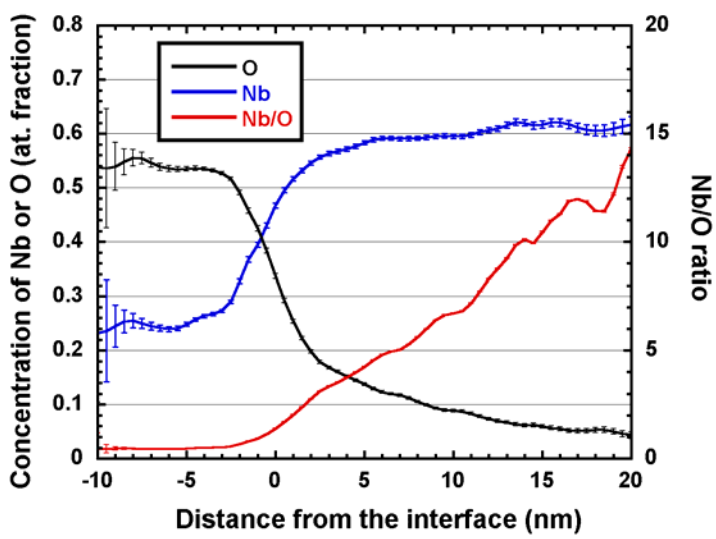

Figure 2. Proxigram showing quantitative concentration profiles associated with the atomic reconstruction shown in Figure 1. The transition from oxide to metal is marked by a rapid increase in the Nb/O concentration ratio. The Nb/O ratio of 0.4 in the oxide suggests that the surface oxide has the stoichiometry Nb_2O_5.

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