

In-Situ Study of Nb Hydride for SRF Cavity Applications Using Aberration-Corrected STEM and Electron Energy Loss Spectroscopy

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Niobium is a type-II superconducting material with the highest critical temperature ($T_c = 9.2$ K) and generally used to fabricate superconducting radio-frequency (SRF) cavities for linear particle accelerators. We present an atomic-resolution study of the effects that a 48 hour bake at 120 °C in vacuum has on the high-field properties of Nb-based SRF cavities. This bake results in a significant increase in high-field quality factor Q . However, an 800 °C bake for 2 hour reduces the H_{c3}/H_{c2} -ratio of cavities. Several mechanisms have been proposed to explain this contrary behavior, including an increased NbO_x surface layer thickness and the precipitation of $NbHy$. [1]

Using a combination of atomic-resolution Z-contrast imaging and electron energy-loss spectroscopy with in-situ heating and cooling experiments, we examine the atomic and electronic structures of Nb and related oxides/hydrides near the cavity surface. Also, we demonstrate that hydrogen atoms, incorporated into the Nb crystal by forming β -NbH precipitates, can be directly visualized using annular bright field imaging in our aberration-corrected JEOL ARM-200CF as shown in Figure 1(a). Image calculations of the β -NbH phase are performed using the STEM image simulation code by Kirkland, which employs the fast-Fourier-transform multislice algorithm. Figure 1(b) shows the experimental and calculated intensity profile for β -NbH [110]. [2]

Atomic resolution imaging can also be achieved during in-situ cooling. Figure 1(c) shows the ABF image of Nb [100] at LN_2 temperature. We can see a weak image contrast at the center of the square formed by the Nb atomic columns. Next, we use EEL spectroscopy to quantify the hydride phases, in particular the β , ϵ and ζ -phases, which have different crystal structures and hydrogen concentrations. In Figure 2, the spectrum at room temperature shows the typical metallic Nb features with the broad peak at 10.5 eV, however, at LN_2 temperature the peak at 10.5 eV disappears and is replaced by a peak at 7.8 eV.

In an effort to further improve the performance of Nb SRF cavities, a wide range of treatments are attempted during the manufacture process, which result in different defect structures at the Nb surface, as well as variety of impurities. Such defects and impurities will further reduce the superconductivity of the Nb cavities. Figure 3(a) shows ABF and HAADF images of Nb from the cavity surface after growing thin NbN layer on the inside of the cavity. We find that the 5 nm thick oxide layer is still present, and, from high-resolution ABF image shown in Figure 3 (b), the nitrogen atoms are visible inside of Nb crystal. Image simulation will also be presented.

In this presentation we will examine the effects of impurities and defects on the atomic and electronic structures of Nb as a function of the different treatment methods. Our results are helpful for predicting SRF cavity performance and to evaluate future manufacturing processes. [3]

Reference

1. R. Tao, R. F. Klie et al, Journal of Applied Physics, 110, Issue 12, (2011)

2. Y.J. Kim, R. Tao, R.F. Klie and D. Seidman, ACS nano 7 (1), pp 732–739, (2013)
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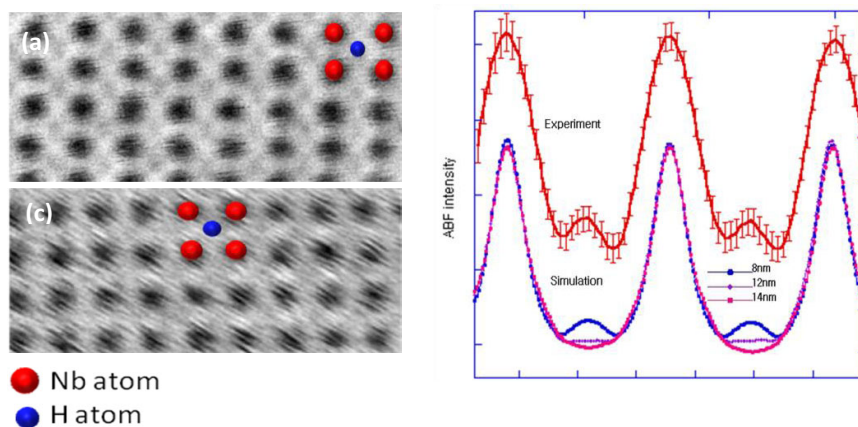


Figure 1: (a) ABF image of [10] direction β -NbH phase with visible Hydrogen atoms, (b) intensity profile plot comparison between experimental and simulation results, (c) ABF image of Nb [100] direction at LN₂ temperature

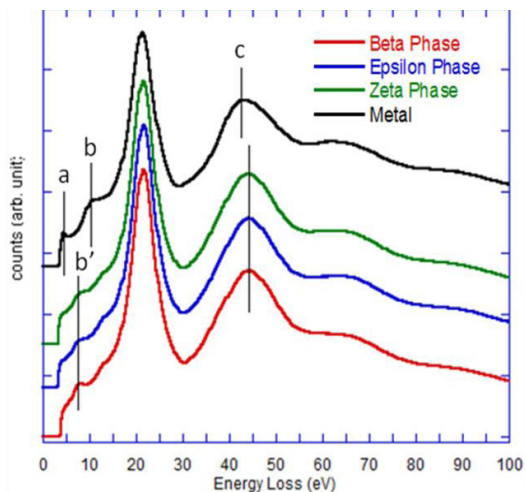


Figure 2: summary of Nb metal and three NbH phases low-loss peak after extracting zero-loss peak

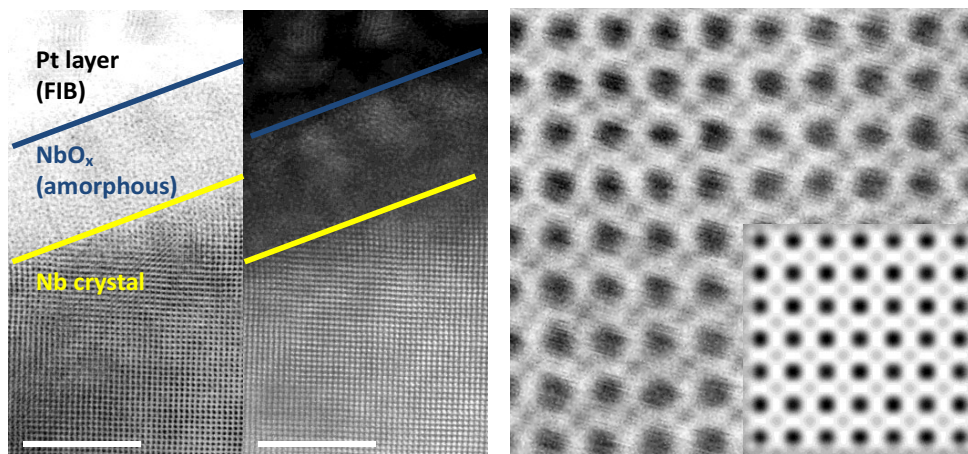


Figure 3: (a) ABF and HAADF image of Nb cavity surface after attempting at growing thin NbN layer, (b) ABF image shows visible nitrogen atoms in Nb crystal of NbN and corresponding Kirkland code simulation of image