Interfacial Oxidation in Niobium Films Probed by HAXPES

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Niobium (Nb) thin films are widely used in superconducting quantum circuits owing to their relatively high superconducting transition temperature (T_c) and compatibility with microfabrication processes [1,2]. Device performance, however, is often limited by dielectric losses originating from interfacial oxides in which two-level systems introduce parasitic energy dissipation [2,3]. A deeper understanding of the structural and chemical evolution of Nb oxides, as well as their depth distribution, is therefore critical for improving thin-film quality and coherence in superconducting devices. In this presentation we demonstrate the deposition of Nb thin films using DC magnetron sputtering. The oxidation behavior and interfacial chemistry of the films were investigated using laboratory-based X-ray photoelectron spectroscopy (XPS) together with variable-photon-energy Hard X-ray Photoelectron Spectroscopy (HAXPES) performed at the NSLS-II synchrotron. HAXPES measurements spanning photon energies from 2000–5500 eV enabled non-destructive, depth-resolved analysis from the surface oxide to the metallic Nb bulk. Quantitative fitting of the Nb 3d and O 1s core-level spectra revealed multiple suboxide species (Nb_2O_5, NbO_2, and NbO_x) and their gradual evolution across the Nb/NbO_x interface [2,4]. The variable-energy approach provided nanometer-scale insight into oxidation gradients and interfacial structure that are inaccessible to conventional XPS, highlighting the power of synchrotron-based depth profiling for complex superconducting thin films. Electrical transport measurements confirmed a T_c of approximately 9 K, demonstrating that high-quality superconducting properties can be achieved using sputtered Nb growth. The integrated structural, spectroscopic, and transport characterization establishes a framework for understanding interfacial oxidation mechanisms in Nb thin films and provides guidance for mitigating oxide-related losses in superconducting and quantum device technologies.

[1] Joshi et al Physical Review Applied. 2023 Aug 1;20(2):024031.
[2] Murthy et al. ACS nano. 2022 Sep 26;16(10):17257-62.
[3] Verjauw et al. Physical Review Applied. 2021 Jul 1;16(1):014018.
[4] Burnett et al. arXiv preprint arXiv:1512.02553.

Supplementary information:

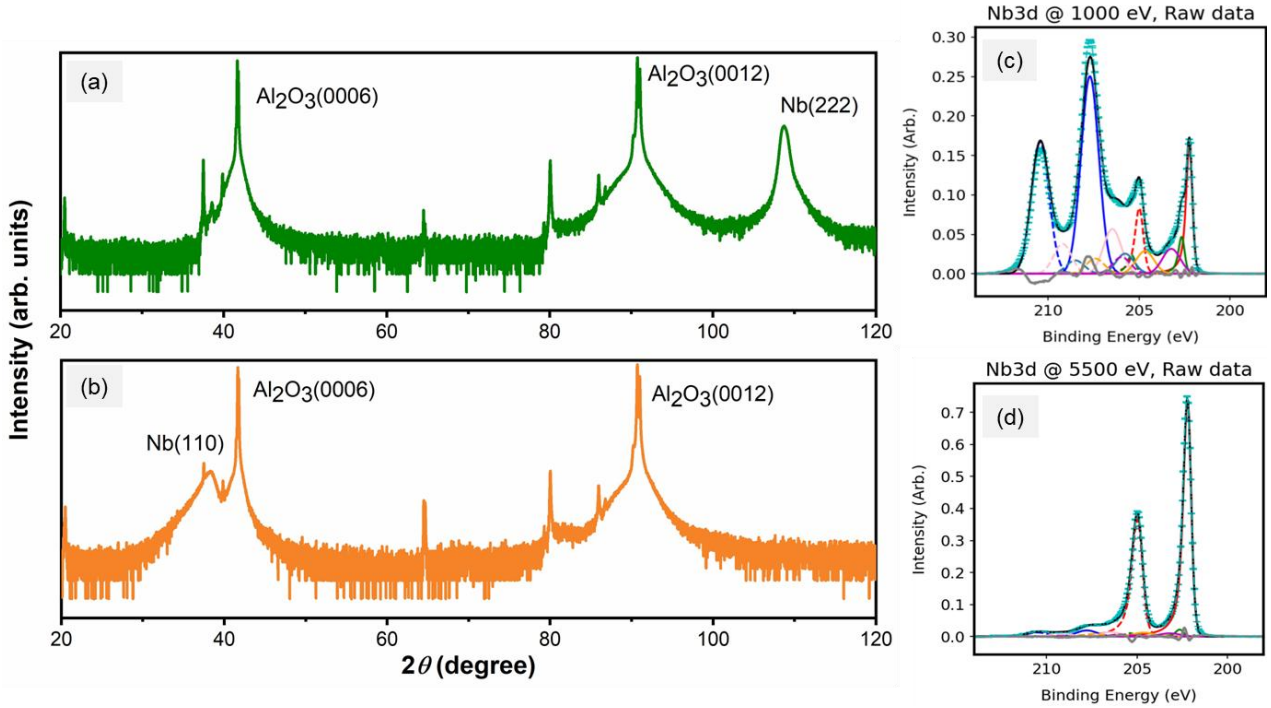

Figure S1. Structural and spectroscopic characterization of sputtered Nb thin films.

(a–b) X-ray diffraction (XRD) θ–2θ scans of Nb films grown on Al_2O_3(0001), showing the substrate peaks at Al_2O_3(0006) and Al_2O_3(0012). Sample (a) exhibits a dominant Nb(222) reflection, while sample (b) shows a preferential Nb(110) orientation. (c–d) Raw Nb 3d core-level spectra acquired using variable-photon-energy Hard X-ray Photoelectron Spectroscopy (HAXPES) at 1000 eV (c) and 5500 eV (d). The spectra are shown with corresponding multi-component fits illustrating contributions from metallic Nb and suboxide species (Nb_2O_5, NbO_2, and NbO_x). Increased photon energy enhances bulk sensitivity, leading to a relative increase in the metallic Nb signal compared to surface oxides.