Growth of Native Oxides of Niobium Thin Films for Superconducting Qubits with Etching Chemistry Zhicheng(Jason) Lei, Maithlee Shinde, Adam Clairmont, Jaeyel Lee, Akshay Murthy; SQMS center, Fermilab, Batavia, IL

Introduction

Niobium (Nb) has been a promising material for quantum systems. But scaling from superconducting qubits to energy-sensitive quantum systems requires mitigating the losses from Two Level Systems (TLSs), which is mainly contributed by Nb2O5 and other oxides from Nb–Air interfaces. Study of the growth of these oxides helps finding mitigation strategies efficiently.

Method

Native oxides growth is investigated across samples that are with Nb thin films on Sapphire (Al2O3) as comparative studies. Samples' exposure time are controlled by high vacuum prior to and after the etching process. Instruments involved are Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) and SPECS Custom-built XPS. They are complementary to each other to establish a depth and chemical profile for oxides of the samples.







XPS: Quantification for chemical composition

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Result







FIG. 3. High resolution XPS spectra and peak fitting for Nb 3d of sample W114 over exposure time (a) 2 hrs and 16 mins, (b) 8 hrs, (c) Reference of over 3 months.

Data background is bounded by Shirley method. Fit peak indicates the presence of Nb metal and oxides. Nb metal doublet peaks are fitted using line shape LA(1.2, 5, 12) and GL(30) for Nb oxides doublet peaks. Binding Energy spectra are calibrated based on Nb Metal binding energy at 202.2 eV. Doublet separations are set to be 2.72 eV. Calibration and Fitting are implemented with CasaXPS.

FIG. 1. Depth Profile for sample W25 and W114. **Approximate depth is** calculated by sputter time provided by ToF-SIMS, and sputter rate. Sputter rate for W25 is 0.032 nm/s and 0.035 nm/s for W114. Signals below 10 are considered noise.

FIG. 2. Oxide thickness over exposure time after etching for sample W25, W114 and W118.

Oxide thickness is derived from sample depth profile based on Nb2O5 signal. Data points before t = **Ohr represent thickness** before etching. Oxide thickness of all samples are assumed to be 0 nm immediately after etching. **Error bar indicates standard** deviation across different spots on samples.

Time	Nb 3d	NbO 3d	NbO2 3d	Nb2O5 3d	NbO ratio	NbO2 ratio	Nb2O5 ratio
2 hrs 16 min	69.165%	2.78%	4.9%	22.5%	9.21%	16.2%	74.6%
8 hrs	60.61%	2.61%	5.535%	29.335%	6.96%	14.8%	78.3%
3 months	22.925%	2.305%	10.535%	60.605%	3.14%	14.3%	82.5%

Table 1. Nb Oxide Atomic Percentage Concentration(%At conc) and Oxides ratio of Sample 114 before etching.

Atomic percentage concentration is quantified using the Scofield Sensitivity Factor at excitation energy of 1487 eV for XPS source Aluminum 400 W. Oxide ratios are calculated by oxide %At conc over total oxide %At conc.



Discussion

Both XPS and ToF-SIMS data and analysis suggest that Nb oxides grow rapidly and overwhelm Nb metal within the first 24 hours following a logarithmic growth. Nb2O5 growth is dominant out of all types of Nb oxide with reaching 80% At conc within 80 days. NbO2 is quickly saturated, maintaining 10% At conc over time with a logarithmic growth. NbO on the opposite follows an exponential decay. Oxide thickness growth also implies sample preparation techniques impact oxide saturation and growth rate.

Future Work

More data can be collected to clarify and establish stronger correlation. Comparison with other promising materials such as Tantalum which has thinner oxides thickness and less loss are worth investigation.





FIG. 4. Nb oxide %At conc growth of Sample 114 before etching. Graph is derived from
Table 1. Error bar
indicates standard deviation across different spots on samples.

