Quantum Science and Technology
Room 304 - Session QS2-MoA

Surfaces, Interfaces, Defects, and Microwave Loss in Superconducting Devices

Moderators: Dr. Suman Bhaumik, TEL Technology Center, America, LLC, **Dr. Drew Rebar**, Pacific Northwest National Laboratory, **Dr. Preetha Sarkar**, Brookhaven National Laboratory

4:00pm **QS2-MoA-11 Control of Defects and Interfaces for High–Coherence Superconducting Qubits**, ***Peter Sushko***, Pacific Northwest National Laboratory **INVITED**

Superconducting qubits have advanced rapidly, yet coherence and device-to-device reproducibility remain limited by material imperfections concentrated at surfaces, buried interfaces, and ultrathin native surface oxides. These regions occupy a small fraction of the device volume, yet can dominate loss via two-level systems associated with defects located there. I will highlight materials science challenges that must be addressed to enable scalable superconducting quantum processors, emphasizing the need for precise synthesis and tightly controlled processing of films and interfaces that form qubits and their circuit elements.

We will cover a few examples of how the combined input from high-resolution microscopic and spectroscopic techniques, together with ab initio simulations, has provided mechanistic, atomic-level insights into the processes leading to the formation of these interfaces and their properties. First, we discuss an atomistic picture of Ta surface oxidation and the formation of a semi-ordered TaO_{1-x} suboxide at the boundary between the amorphous Ta_2O_5 and metallic Ta. Building on this mechanistic understanding, we demonstrate a materials-by-design strategy to suppress Ta oxidation using a reactive Mg and noble-metal capping layers. Beyond free surfaces, we discuss the Ta/sapphire interfacial layer and show that sapphire surface termination prior to Ta deposition controls the heterojunction structure, Ta film orientation, and likely the density of grain boundaries and defect traps in the Ta film. Extending these concepts to Nb, we show how controllable processing can deliberately re-engineer oxides, producing thinner, smoother Nb oxides and improving resistance to oxygen exchange/diffusion. Experiments and simulations together indicate that hydrogen segregates to the oxide/metal interface and can migrate during oxide evolution. Finally, we present a scalable passivation strategy for qubit-grade Nb that uses encapsulation and show how structural characterization and ab initio simulations elucidate the mechanisms of atomic rearrangement and stabilization that suppress oxide formation.

Overall, improving coherence and yield requires atomic-level insight to enable predictive control of oxidation, intermixing, and impurity-induced effects, thereby transforming native interfaces into engineered, reproducible materials systems.

4:30pm **QS2-MoA-13 Microscopic Impact of Sapphire Preparation on Losses in Superconducting Tantalum Thin Films**, ***Aswin Kumar Anbalagan***, *Hyeongjun Koh,* Brookhaven National Laboratory*; Suhas Ganjam,* Yale University*; Ruoshui Li, Daniel Olds,* Brookhaven National Laboratory*; Vesna Stanic,* IBM T. J. Watson Research Center*; Jean-Jordan Sweet,* IBM TJ Watson Research Center*; ChenYu Zhao, Shuoyuan Huang,* Brookhaven National Laboratory*; Jinhyun Cho,* Stony Brook University/Brookhaven National Laboratory*; Ananya Chattaraj, Kim Kisslinger, Sooyeon Hwang, Steven L. Hulbert,* Brookhaven National Laboratory*; Luigi Frunzio, Robert J. Schoelkopf,* Yale University*; Mingzhao Liu, Judith Yang, Andrew L. Walter, Andi M. Barbour,* Brookhaven National Laboratory

Understanding the microscopic origins of dielectric loss in superconducting quantum devices is essential for improving qubit coherence and scalable production. Here, we investigate the relationship between crystalline ordering, interfacial structure, and superconducting loss in tantalum (Ta) thin films deposited on c-plane sapphire substrates prepared using edge-fed film growth (EFG) and heat exchange method (HEM) sapphire. HEM sapphire substrates were chemically cleaned and selectively annealed at 1200 °C in an oxygen-rich environment prior to high-temperature Ta deposition by DC magnetron sputtering. Superconducting measurements reveal that Ta films grown on non-annealed EFG sapphire exhibit lower surface loss factors, higher residual resistivity ratio (RRR), and sharper superconducting transitions compared to annealed HEM sapphire, despite the care taken to fabricate HEM samples with stronger epitaxial ordering that may be conventionally anticipated to improve superconducting performance. Synchrotron X-ray diffraction (XRD) and X-ray reflectivity (XRR) measurements reveal differences in epitaxial ordering, rotational disorder, and interfacial oxide layers. Using four-dimensional scanning transmission electron microscopy (4D-STEM), Ta grown on both EFG- and HEM-samples were found to exhibit single crystallinity with (111)Ta || (0001) sapphire orientation. However, the HEM-annealed sample contains ~100 nm-wide secondary grains associated with local epitaxial breakdown driven by elastic strain relaxation, whereas the EFG-non-annealed sample shows gradual in-plane lattice rotation without secondary grain formation, suggesting strain accommodation through lattice curvature. Altogether, these results suggest that sapphire surface preparation, substrate homogeneity, and interface chemistry strongly influence microwave loss in superconducting Ta devices and highlight the need for further optimization of sapphire processing and early-stage film growth conditions.

4:45pm **QS2-MoA-14 Engineering the α-Ta/Sapphire Heterostructure: Phase Diagrams, Single-Crystal Growth, and Interface-to-Oxide Characterization for Next-Generation Quantum Devices**, ***Joseph Perry Corbett***, Miami University Ohio

Superconducting qubits are one of the leading candidates for quantum computers capable of surpassing modern supercomputers on specific problems, with steady progress over the last 20 years increasing both quantum state lifetimes and qubit counts. The recent demonstration of α-Ta thin film qubits with coherence times of 0.5 ms, alongside the well-recognized impetus in the QISE community for fundamental materials science on the insulator/superconductor heterostructure, motivates the work presented here. We perform a comprehensive multi-faceted investigation of sputter-grown Ta thin films on sapphire, integrating studies of phase selectivity, single-crystal epitaxy, and thickness-dependent microstructure alongside first-principles calculations of interfacial energetics and surface oxidation. Phase diagrams constructed for DC magnetron sputtering on c-plane Al_2O_3 (with oxygen partial pressure spanning 5.5×10^{-11} to 2.23×10^{-4} Torr and substrate temperatures from 300 to 900 °C) demonstrate that elevated temperatures exclusively stabilize α-Ta while increased oxygen at low temperatures drives single-phase β-Ta formation, with mixed α/β coexistence at intermediate conditions; complementary measurements resolve phase-dependent surface morphologies and work function values relevant to superconducting performance. Sputter epitaxy at 650 °C followed by UHV annealing at 1000 °C yields single-crystal α-Ta in multiple orientations on c- and a-plane sapphire, as confirmed by XRD pole figures, rocking curves, asymmetric scans, and XRR modeling. Thickness-resolved characterization from 2 to 250 nm identifies three structurally distinct regions (a 0.88 nm pseudomorphic interface, a bulk α-Ta(111) film with terrace widths saturating near 150 nm, and a self-limiting 2.25 nm amorphous oxide), and Van der Pauw transport reveals a superconducting Tc that increases smoothly from 2.9 K at 7.5 nm to 4.2 K at 269 nm, consistent with universal thickness scaling. Complementary DFT calculations rationalize the Ta-rich thermodynamic stability of α-Ta/Al_2O_3 interfaces (with mixed ionic/covalent Ta–O bonding and no oxygen interdiffusion into the film) and the emergence of amorphous TaO once the Ta:O ratio exceeds 1:1. Together, these results provide a quantitative roadmap for phase-selective, orientation-controlled, thickness-tuned α-Ta growth on sapphire for next-generation superconducting qubit platforms.

5:00pm **QS2-MoA-15 Mitigating Vortex Losses in Tantalum Superconducting Resonators Through Defect Landscape Engineering**, ***Rohin Tangirala***, *Chaman Gupta,* University of Washington*; Benjamin Palmer,* Laboratory for Physical Sciences, University of Maryland*; Yongqiang Wang,* Los Alamos National Laboratory*; Serena Eley,* University of Washington

Tantalum (Ta) has recently emerged as a low-loss material for superconducting circuits, due to its stable native oxide with fewer two-level system (TLS) defects that may cause dissipation and decoherence. Stray and applied magnetic fields can introduce additional energy losses due to the motion of Abrikosov vortices, especially in clean-limit tantalum films. To mitigate this loss channel, we intentionally introduce defects through proton irradiation and lithographically-defined antidots into tantalum superconducting resonators to engineer the vortex pinning landscape and control vortex dynamics. We characterize device performance across a range of applied magnetic fields and conditions relevant to superconducting qubit operation, including single-photon power levels and millikelvin temperatures, in order to quantify losses arising from vortices and explore design considerations for increasing the performance of tantalum resonators under magnetic fields. This may enable the integration of magnetic-field-resilient tantalum resonators into superconducting and hybrid quantum systems.

5:15pm **QS2-MoA-16 A Comparative Study of Niobium Superconducting Resonators on Silicon and 4H-Silicon Carbide Substrates***, **Marcelo Velasco Forest**, Joseph Falvo,* Quantum Collaborative Research Corps & Department of Physics, University of Maryland, College Park*; Kiana Reed,* Department of Physics and Astronomy, University of California, Irvine*; Ivan Lainez, Kasra Sardashti,* Quantum Collaborative Research Corps & Department of Physics, University of Maryland, College Park

Energy loss from two-level systems (TLS) at metal–dielectric and substrate interfaces continues to limit coherence in superconducting quantum circuits. We investigate whether substrate selection and surface preparation can suppress TLS-related loss by comparing niobium (Nb) coplanar-waveguide resonators fabricated on silicon (Si) and 4H-silicon carbide (SiC). Nb films (~150 nm) are deposited by DC magnetron sputtering using a standardized baseline process. Substrate preparation spans a controlled matrix of ex-situ and in-situ treatments, including solvent sonication, O_2 plasma, piranha clean, and HF clean by dip and vapor methods.

TLS-related losses and the effects of different preparation methods were determined from fitting resonator complex transmission, S_{21}, to well-tested theoretical models. We will report a comparison of Si and SiC under identical deposition conditions, as well as the surface preparation procedure that yields the lowest losses for each substrate. The primary outcome is a ranked set of substrate/preparation combinations that maximize single-photon internal quality factor and minimize inferred TLS-related loss.

5:30pm **QS2-MoA-17 Spectroscopy of Two-Level-System Defects via Multilevel Relaxation in a Fixed-Frequency Transmon***, **Tanay Roy**, Xinyuan You, David van Zanten, Francesco Crisa, Sabrina Garattoni, Shaojiang Zhu, Anna Grassellino, Alexander Romanenko,* Fermi Lab

Temporal fluctuations in the coherence of superconducting transmon qubits are widely believed to originate from two-level system (TLS) defects coupled to the qubit. Existing TLS spectroscopy techniques typically rely on qubit frequency tunability or AC-Stark-based approaches, which can introduce additional complexity and offer limited bandwidth. Here, we demonstrate an alternative method for TLS spectroscopy based on monitoring the relaxation dynamics of multiple excited states in a fixed-frequency transmon [1]. By analyzing temporal correlations between multilevel decay processes, we identify signatures of TLS defects that are detuned by more than 100 MHz from the qubit transition yet still significantly impact coherence. Our results establish multilevel relaxation spectroscopy as a simple and broadly applicable technique for probing defect-induced noise in superconducting qubits without requiring flux tunability[1] https://arxiv.org/abs/2602.11127This work was supported by the U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Superconducting Quantum Materials and Systems Center (SQMS), under Contract No. 89243024CSC000002. Fermilab is operated by Fermi Forward Discovery Group, LLC under Contract No. 89243024CSC000002 with the U.S. Department of Energy, Office of Science, Office of High Energy Physics.

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