Quantum Materials Fabrication and Analysis at BNL User Facilities

Mingzhao Liu
Co-design Center for Quantum Advantage (C²QA)
Center for Functional Nanomaterials

Workshop on DOE User Facilities for Quantum Information Science
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BNL team for QIS user support

**NSLS II**


**CFN**

One of 5 DOE Nanoscience Research Centers (NSRCs)
Understand and mitigate superconducting qubits loss

- $T_1$ for 2D transmon qubits had been limited to $\sim 0.1$ ms due to TLS loss at capacitor/resonator surface
Correlate material properties with qubit performance

- Identify key material proxies to infer qubit coherence at low T
- Build stronger synergy between BNL and C²QA device efforts

Synchrotron X-ray spectr.
TEM; X-ray diffraction
Magnetron sputtering
PPMS

Surface Proxies
Structural Proxies
Synthesis & Processing
DC Transport Proxies
Resonator Proxies

Post-fab survey
Device Fabrication
T₁/T₂
RF Low T Measurement

Cleanroom facilities
Dilution refrigerator (Princeton, Yale)
Niobium-based qubits

Deposition

- Sputtering
- HiPIMS Optimized
- HiPIMS Normal

$T_1$ dependence on Nb deposition technique

- HiPIMS = High-power impulse magnetron sputtering

Qubit device with Nb capacitor/resonator and AlO$_x$/Al/AlO$_x$ JJs

$T_1$ dependence on Nb deposition technique

Oxidation at surface and grain boundaries

- HiPIMS Normal (worst) film has smallest grains
- Native oxide and oxygen diffusion along grain boundaries
Nb surface chemistry studied by XPS depth profiling

- XPS profiling with 7 different incident energies
- Native oxide on Nb is about 10 nm thick
- Nb forms suboxides beyond Nb\(_2\)O\(_5\)
- Worst film forms most diffusive oxide layer with high fraction of suboxides
Replacing Nb with bcc-Ta ($T_c = 4.3$ K) brings 3x longer $T_1$

- Ta can grow epitaxially over sapphire
- Native oxide on Ta is thin and simple ($\text{Ta}^{5+}$ dominated), but still an oxide (likely amorphous)
Ta still oxidizes

- Forming native oxide of 2-3 nm thick, universal across all sources
- Amorphous, host of TLS
- Surface treatment may lower loss
- Resonator $Q$ as proxy for qubit lifetime
In-situ/ex-situ XPS depth profiling

- XPS profiling w/ 17 incident energies
- Study of oxide variation by wet/dry chemical treatments
- In situ study of oxide removal/regrowth during annealing

Princeton-BNL team

- 7-ID-1
  - HAXPES
  - 0.15– 2.2 keV

- 7-ID-2
  - HAXPES
  - 1.5– 7.5 keV

- 23-ID-2
  - In situ and operando XPS
  - 0.25 - 2 keV
Polymorphism of tantalum

- Sputter deposition of Ta easily leads to a metal stable $\beta$–phase
- A superconductor with $T_c \sim 0.8$ K
- Undesired due to more quasiparticle contribution

Two Ta films deposited at similar conditions

- $\alpha$-Ta (bcc)
- $\beta$-Ta (tetragonal)
Robust fabrication of crystalline, bcc-Ta film

- Yale-Princeton-BNL team
- Film growth + XRD survey
- High sensitivity to substrate temperature
Electron microscopy

- Fully epitaxial growth of Ta on a-plane sapphire (CFN) -- most previous studies was on c-plane sapphire
Synchrotron X-ray diffraction

- X-ray powder diffraction (XPD) & pair-distribution function (PDF)
- Film ordering & homogeneity w/ 500 μm spot
- Both in-plane and out-of-plane ordering
- High-throughput screening
Low temperature transport properties

- New facility at CFN: Quantum Design DynaCool PPMS with 12 T magnet
- $^3$He sub-Kelvin insert (~350 mK base)
- Multi-function probe for custom experiments
Resonator device fabrication

- Hanger type Ta CPW (coplanar waveguide) resonator fabricated in CFN Cleanroom
- Using Princeton patterns
- Reactive ion etching gives sharp, straight edge profile
LEEM/XPEEM on qubit device

XPEEM/LEEM:
- Surface potential mapping
- Local work function
- Surface chemical composition mapping
- Local chemistry (μXPS)
TM silicides for superconducting qubits

- Superconducting qubits on silicon substrate
- Silicides form on silicon-metal interface
- Superconducting TM silicides -- compatible with CMOS
- Use superconducting silicides as for silicon-compatible Josephson junctions and resonators

<table>
<thead>
<tr>
<th>Silicide</th>
<th>$T_c$ (K)</th>
<th>Silicide</th>
<th>$T_c$ (K)</th>
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<tr>
<td>Nb$_3$Si*</td>
<td>19</td>
<td>Sc$_5$Ir$<em>4$Si$</em>{10}$</td>
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<td>PtSi</td>
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<td>LaIr$_2$Si$_2$</td>
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CoSi$_2$-based Josephson junction

- CoSi$_2$-Si-CoSi$_2$ coplanar Josephson junctions
- On p$^{++}$ Si wafer (no carrier freeze out) for S-N-S junction
- Junction width $W$ below 100 nm

- CoSi$_2$ constriction for S-c-S type junctions
- On intrinsic Si wafer
CFN quantum material press (QPress)

- **Automate study of 2D heterostructures**
  - 3-year DOE QIS project (since FY 2019)
  - Reliably fabricate complex stacks of atomically-thin (2D) materials
  - Understand physics of exfoliation
  - Study QIS materials
  - Non-expert access to frontier synthesis

- **Partnerships**
  - P. Kim, A. Yacoby (Harvard)
  - D. Shahrjerdi (NYU)
  - Broader user community
QPress modules

**Exfoliator**
- CFN custom roll-to-roll design
- Reproducible control of exfoliation process
- Enables rapid generation of exfoliated substrates

**Cataloger**
- Optical microscope with integrated Raman imaging/AFM
- Machine-vision identifies/classifies flakes
- Generate “flake libraries”

**Stacker**
- Robotic control of stamp and sample
- Build heterostructure stacks, such as graphene/hBN

**Cluster tool**
- Custom design from Lesker
- Installed and operating in CFN
- Robotic transfer between stations
  - Through vacuum/inert atmosphere (glovebox)
  - Thermal/plasma processing
  - E-beam deposition (multiple targets)
QPress science progress

- **Bound States in Graphene Heterostructure**
  - Identify new quantum confinement resonance in twisted graphene bilayers
  - Developed special TiO\(_x\)-coated SiO\(_x\) substrates


- **Build heterostructures**
  - Generate graphene library using QPress exfoliator
  - Built hBN/graphene/hBN heterostructures using QPress stacker (~6× faster fabrication)
  - Demonstrated high-performance FETs from heterostructures
Future QPress

- **Complete commissioning/integration**
  - Continue to refine modules
  - Integrate into single software framework
  - Deploy data tools for automated experiments

- **Facility expansion**
  - Integrated Multimodal Characterization and Processing (QM-IMCP;$6.9M, 3 years since FY ’22)
  - Processing heterostructure materials with atomic level precision at a new atomic layer etching tool
  - Characterization of electronic states, magnetic imaging, and chemical analysis at the upgraded synchrotron-based microscope
  - Analysis of carrier dynamics at an upgraded optical ultrafast-microscope
  - Mapping the electrostatic potential of atomic defects and single spin detection at the new scanning probe microscope (SPM) with quantum sensors, making direct connection with C2QA efforts

QM-IMCP

**Low-Temperature Multimodal Characterization**

- Synchrotron spectro-microscopy
- Ultrafast magneto-optical microscopy
- SPM with quantum sensor

**Material Synthesis**

**Precise Processing**

- Plasma Treatment
- Atomic layer etching