Structure and Dynamics of Interfacial Water near CuO Nanostructures

A Neutron Scattering Study

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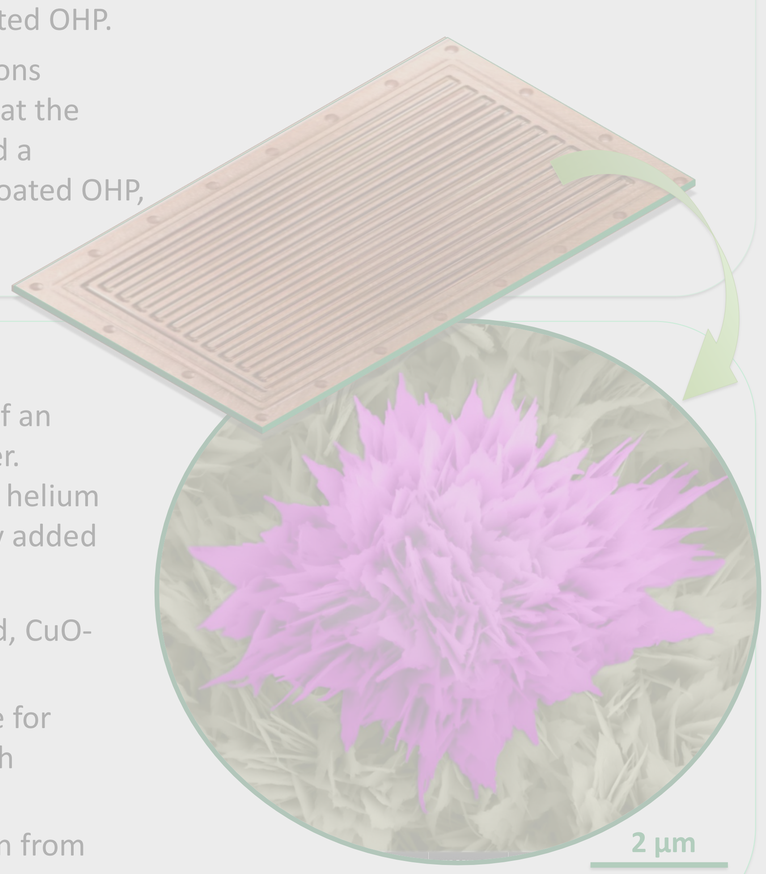

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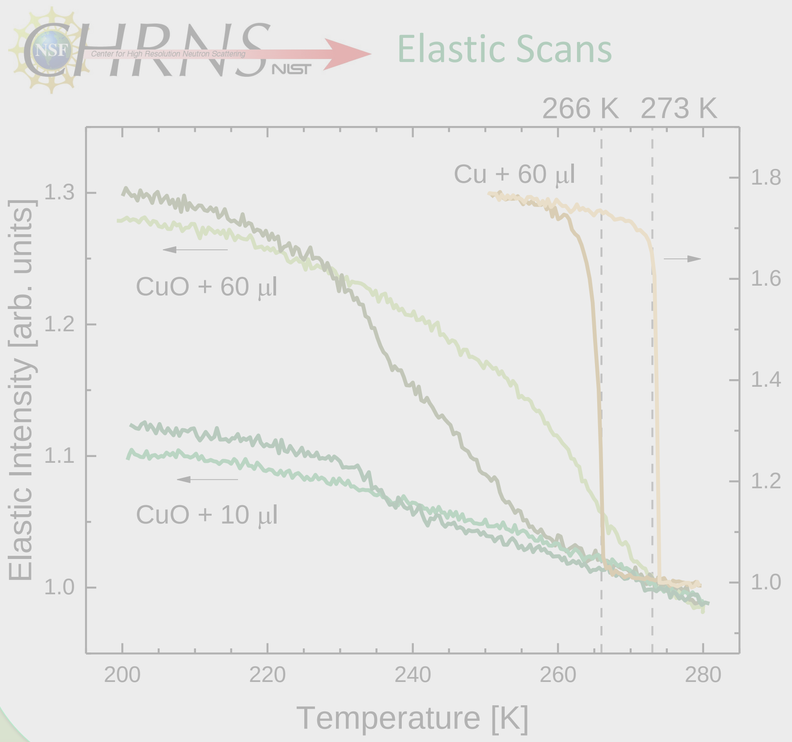

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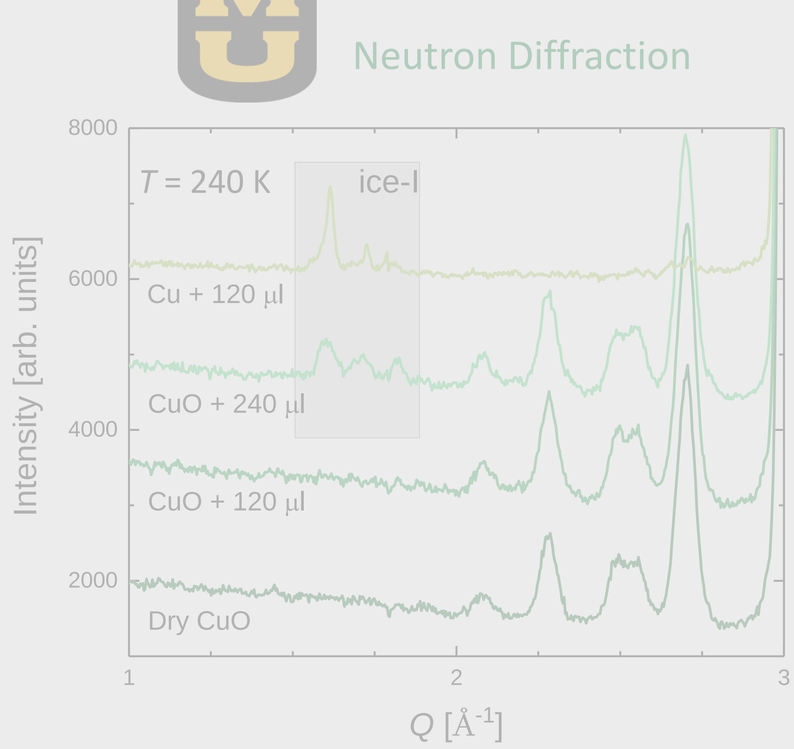

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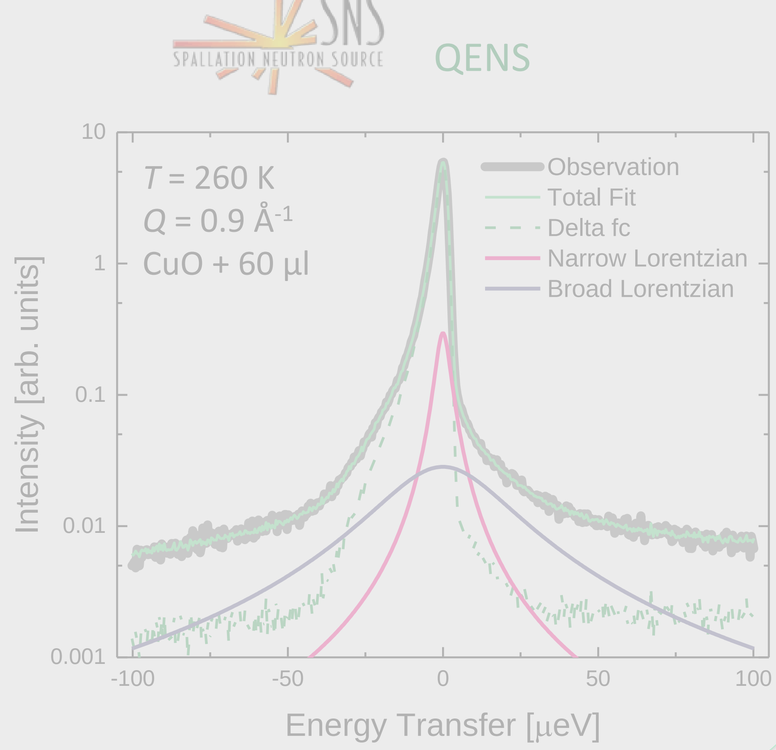

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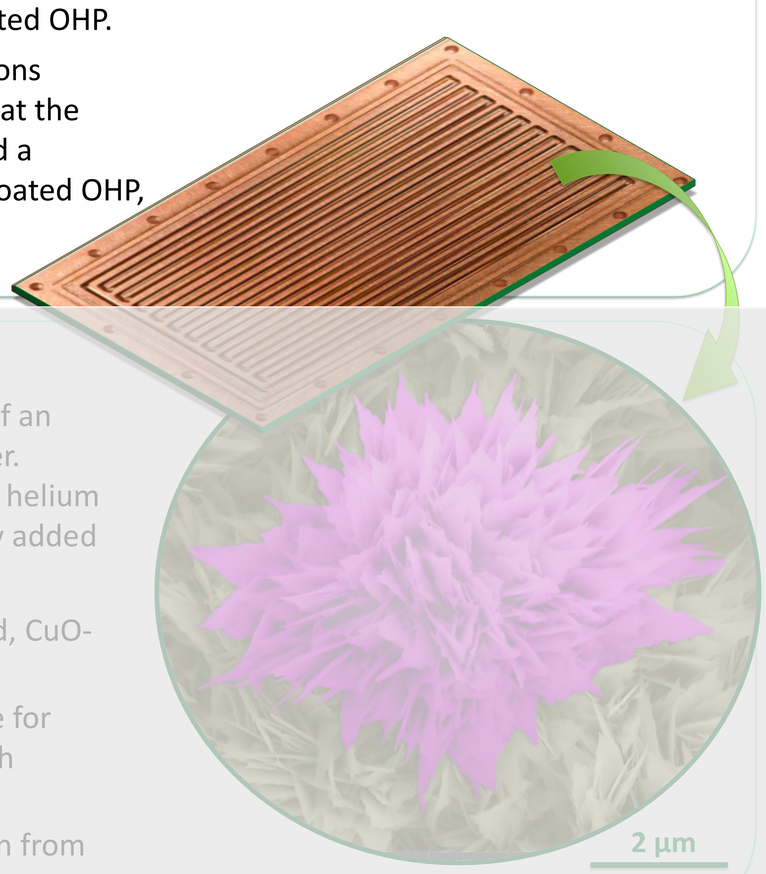

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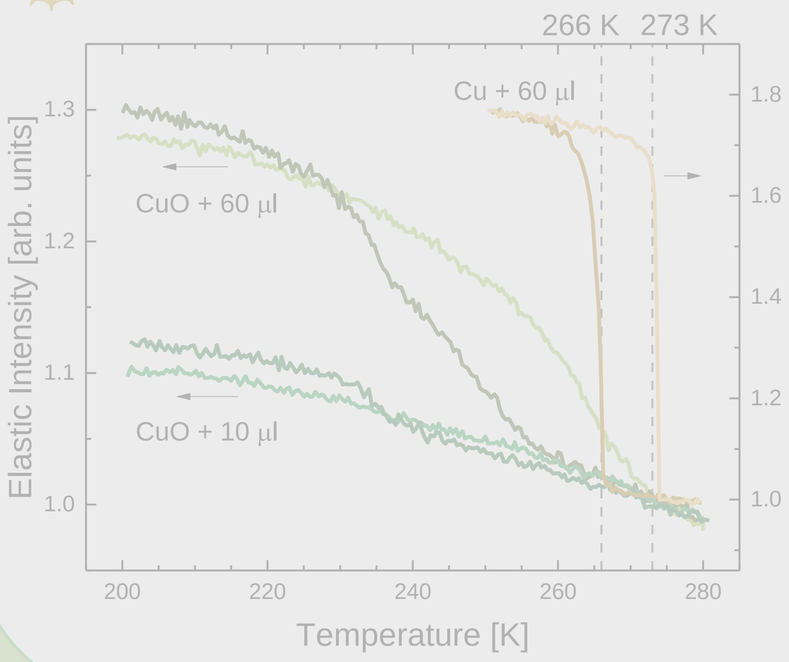

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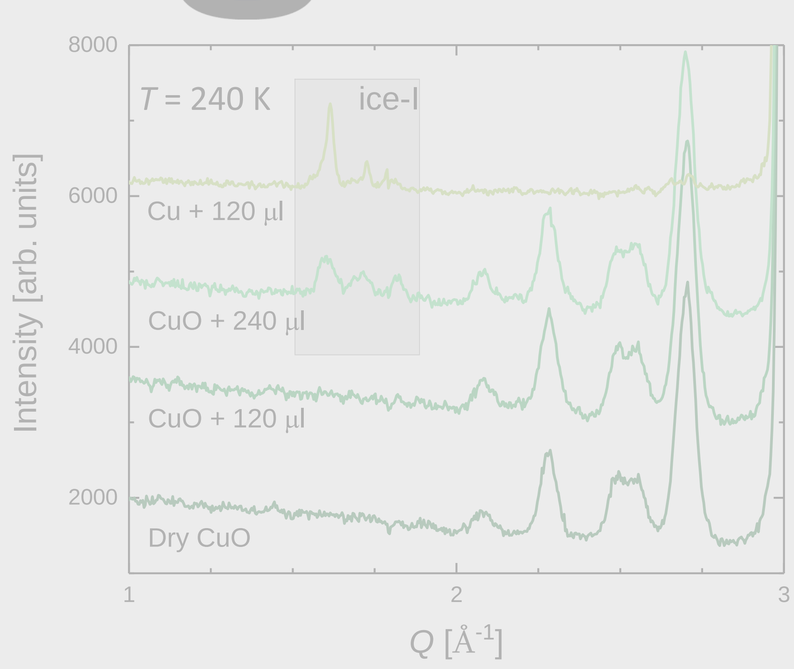

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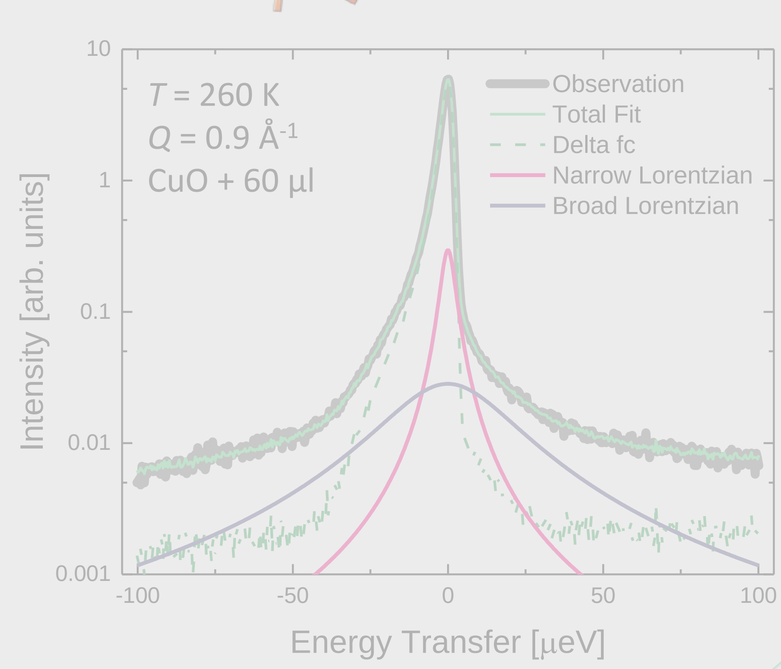

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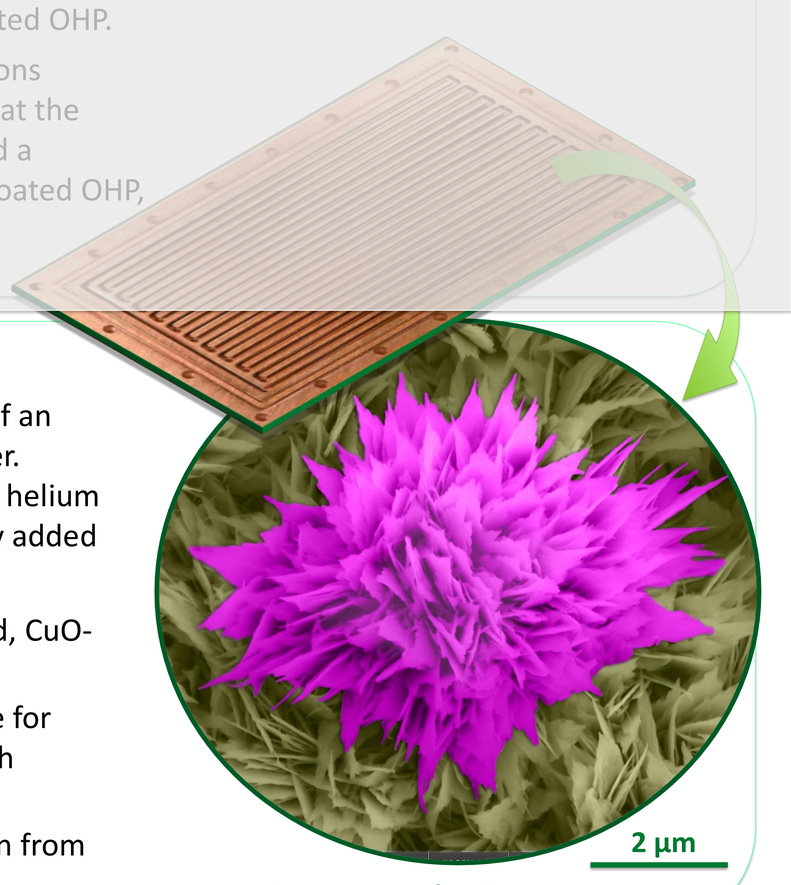

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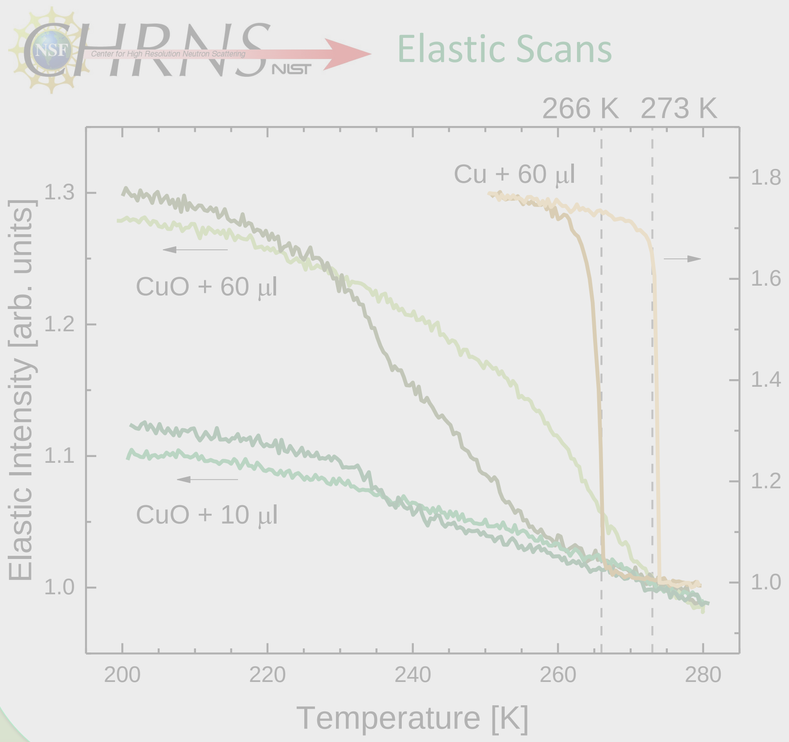

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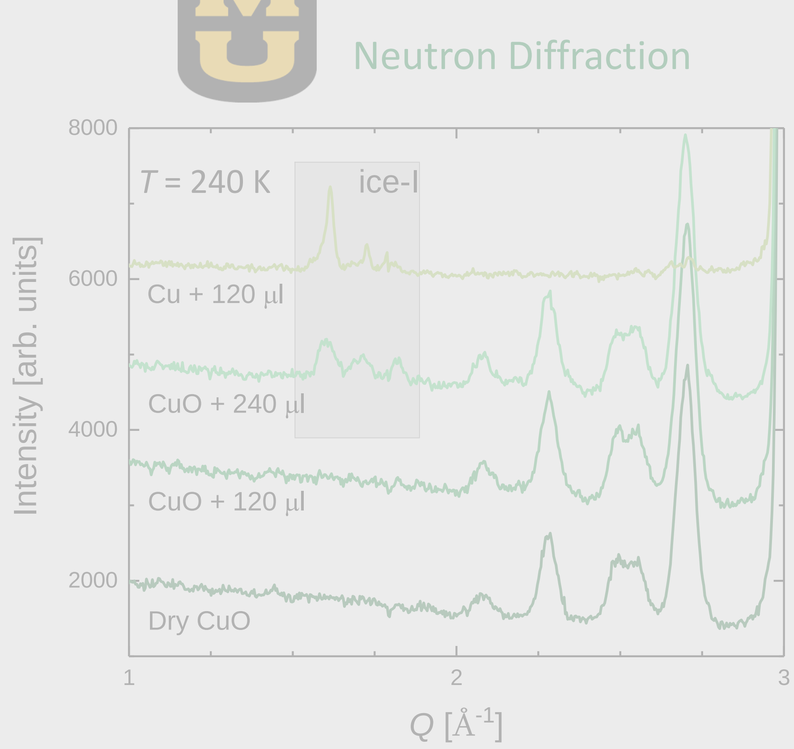

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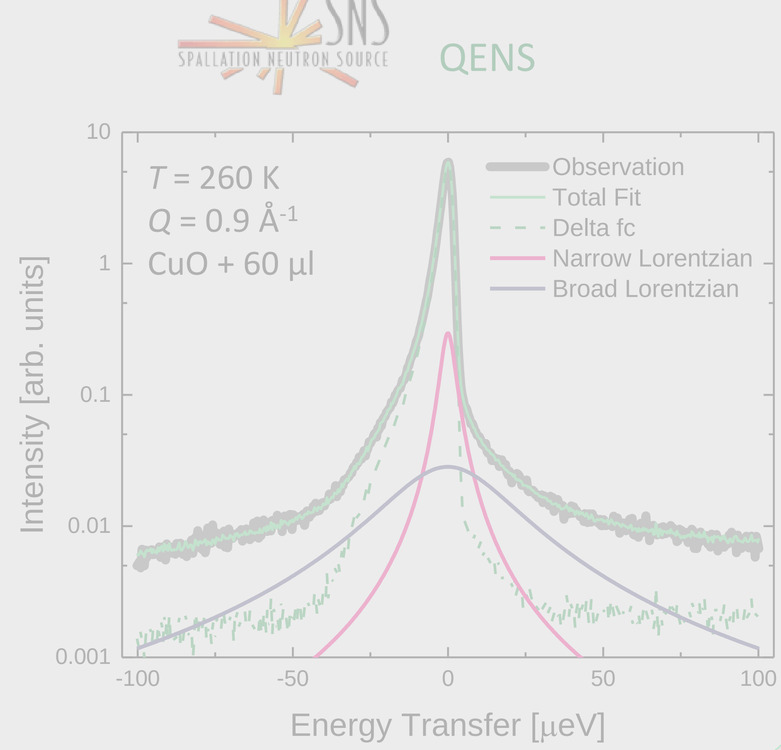

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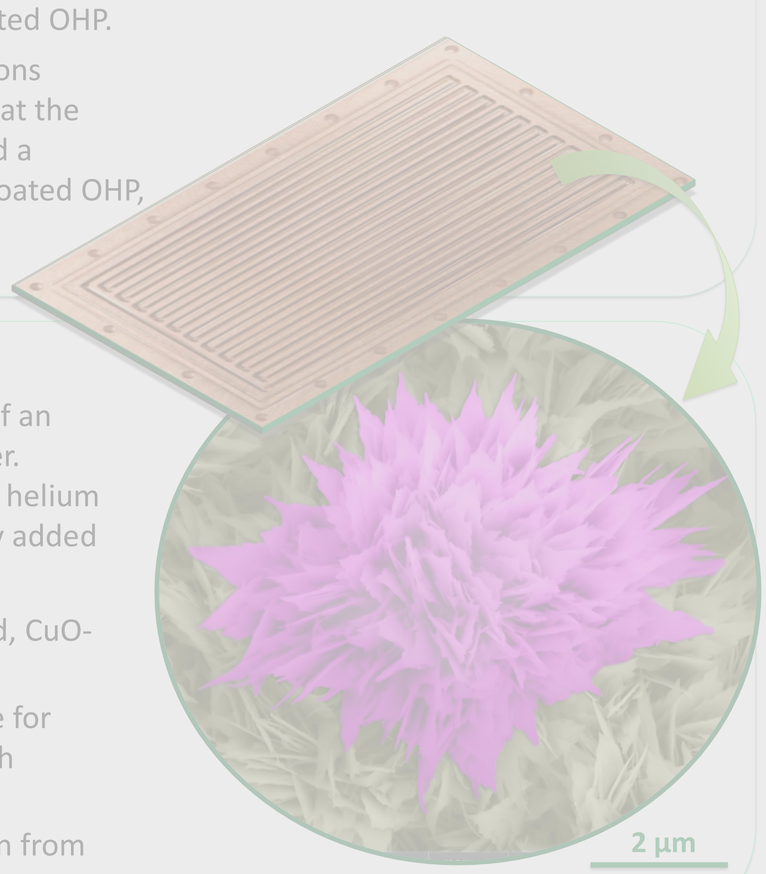

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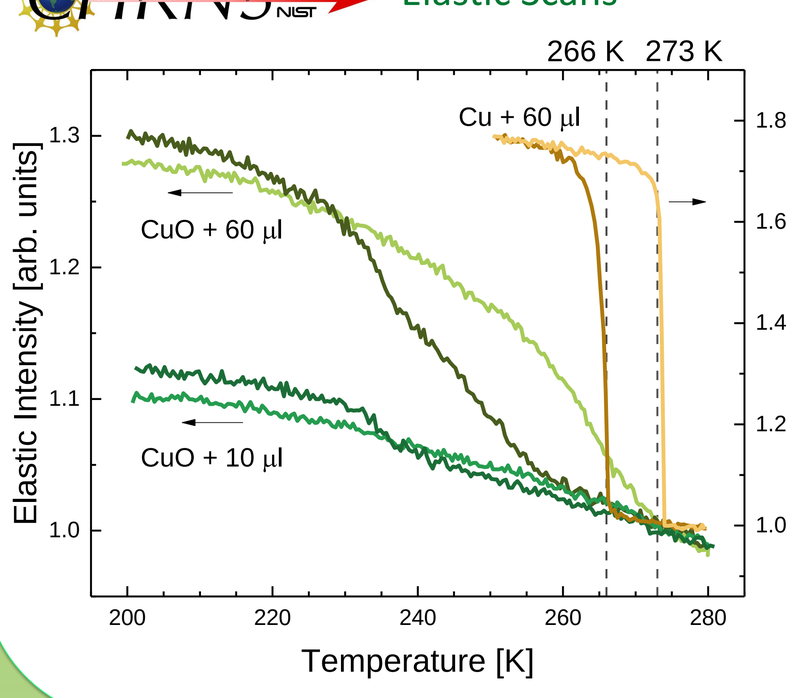

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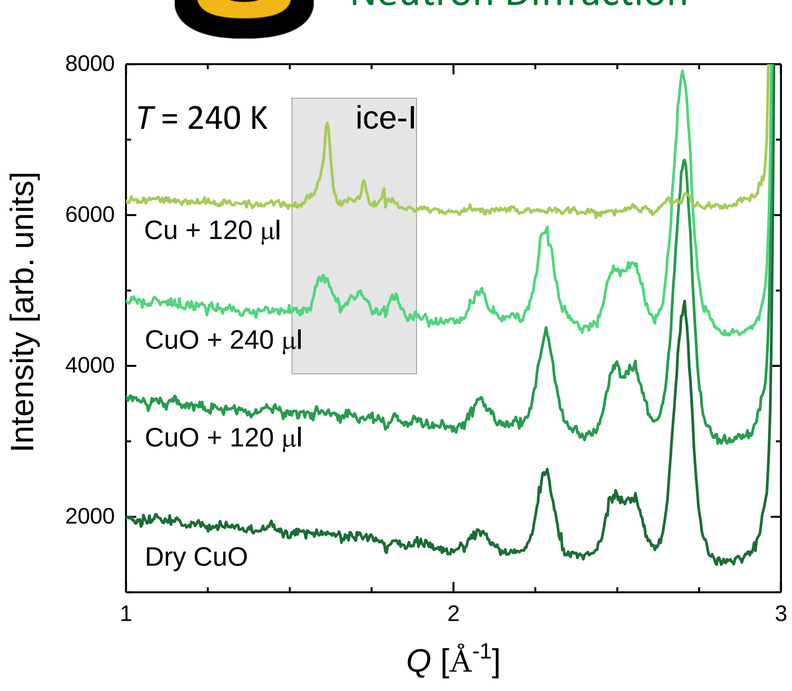

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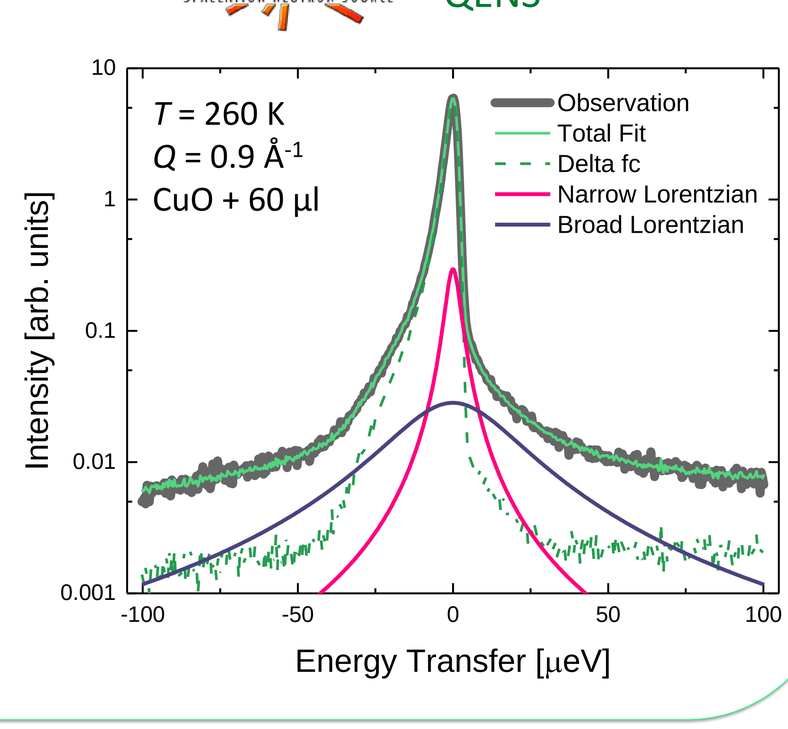

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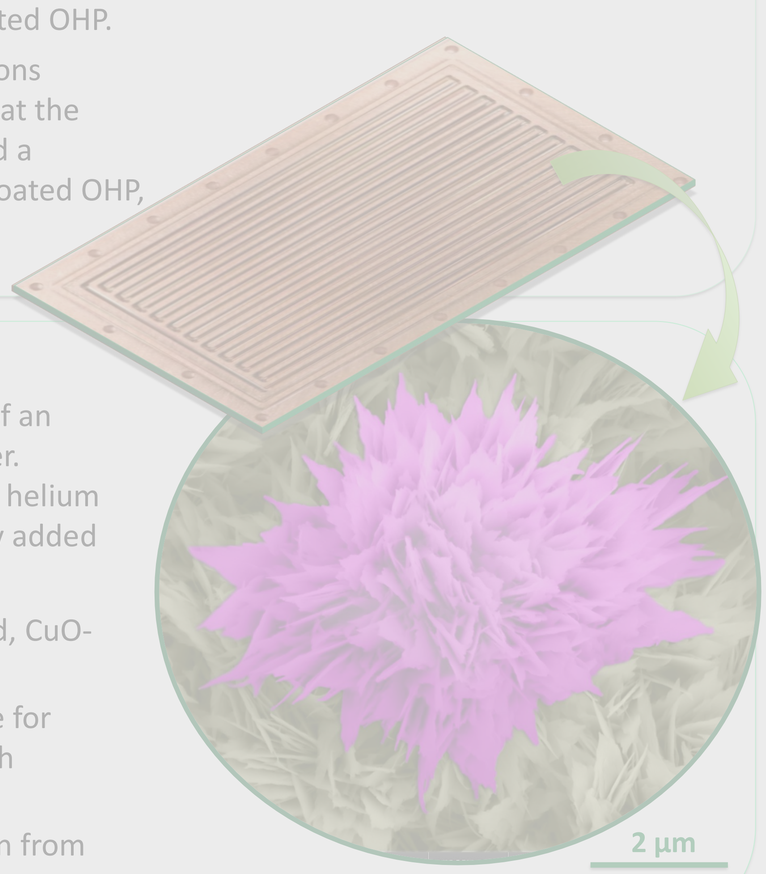

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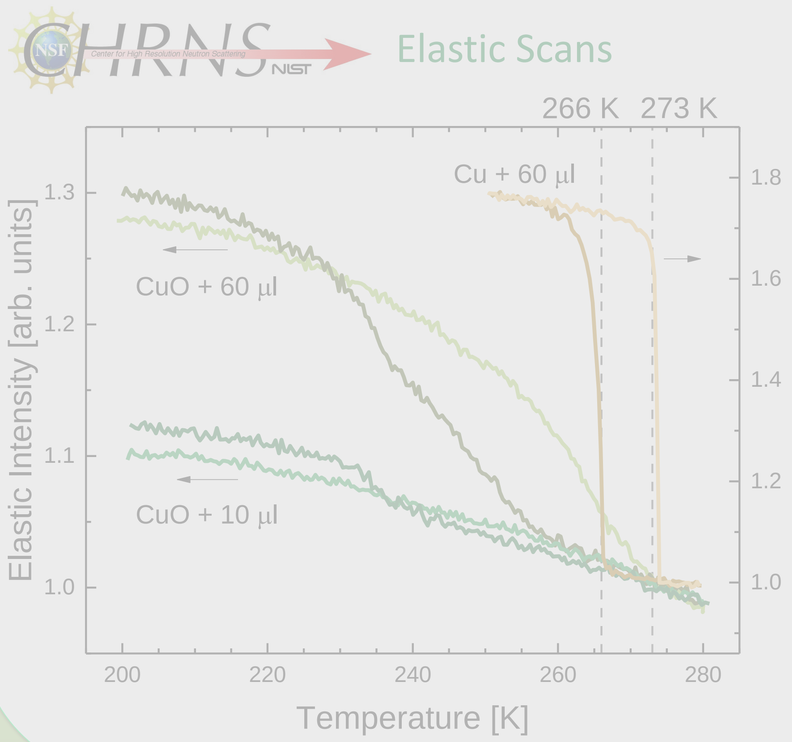
Methods

Neutrons are highly sensitive to incoherent scattering from hydrogen nuclei, more so than the other elements of an OHP. Therefore, we employ several neutron scattering techniques to elucidate the structure and dynamics of interfacial water. Samples consist of one hundred, 5 cm diameter copper foil disks (13 μm thick) stacked in aluminum cans and sealed under a helium atmosphere. CuO nanostructures were grown on copper foil via a wet chemical method [3]. Hydration level is determined by added water droplet (H_2O/D_2O) placed outside of the neutron beam.

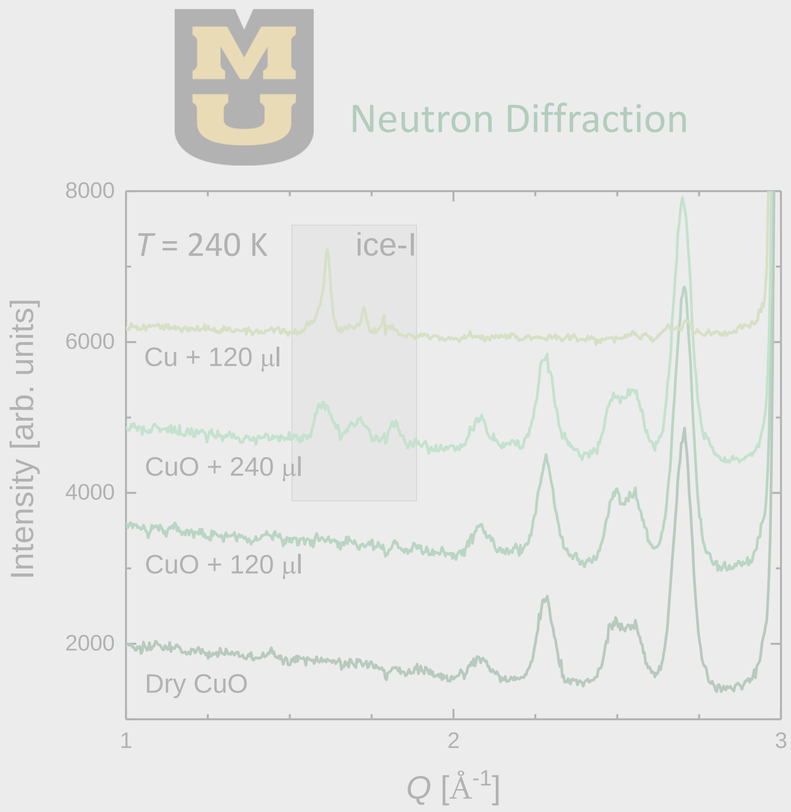
- Freezing and melting behavior of interfacial water: Scans of elastic neutron intensity versus temperature for H_2O-hydrated, CuO-coated copper foils were performed on the HFBS at the NIST Center for Neutron Research.
- Structure of "frozen" interfacial water: Neutron powder diffraction scans as a function of hydration level and temperature for D_2O-hydrated, CuO-coated copper foils were recorded using the PSD-diffractometer at the University of Missouri Research Reactor.
- Dynamics of interfacial water: Quasielastic neutron scattering (QENS) scans at various temperatures below 280 K – chosen from our HFBS elastic scans – were recorded from the BaSiS at ORNL-SNS (IPTS-18634).

Results

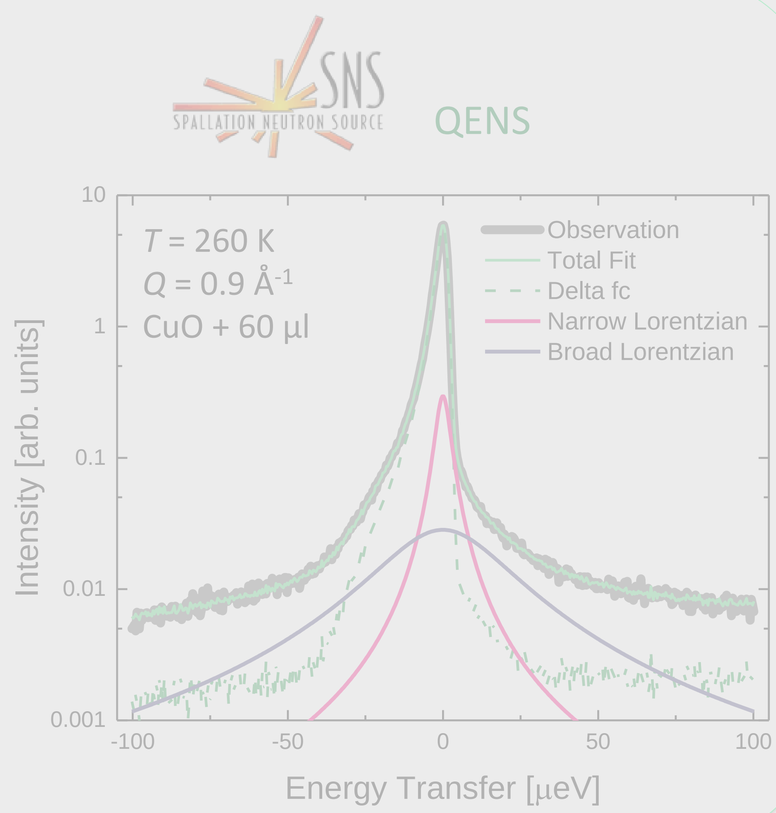
Elastic Scans



Neutron Diffraction



QENS



Discussion

Elastic Scans

Our temperature-dependent HFBS elastic scans indicate that CuO interfacial water continuously freezes and melts over a broad temperature range. In contrast, water near untreated copper freezes and melts within a narrow temperature range.

Neutron Diffraction

Neutron diffraction at the MU Research Reactor for D_2O-hydrated CuO shows that hexagonal ice (ice-I) forms at a hydration level that is a factor of two lower on untreated-Cu (at ~272 K) than on the CuO coating (at ~260 K). Is there a critical hydration level needed to form ice-I? This possibility will be explored in our Future Work.

QENS

QENS directly probes interfacial-water dynamics at the molecular scale. We have identified two populations of water based on their dynamics: a "fast" motion whose dynamics appear similar to bulk supercooled water; and, a "slow" component that we have interpreted as water which interacts directly with the hydrophilic nanostructures.

Future Work and References

- Calorimetric response of interfacial water: Differential scanning calorimetry (DSC) at the ORNL-CNMS will be used in search for an endo-/exothermic response characteristic of bulk (non-interfacial) water as function of hydration level (CNMS2018-108). In this way, we can determine a critical hydration-level threshold needed to form ice-I.
- Vibrational modes of interfacial water: Our comprehensive view of interfacial water dynamics will include an investigation of water's vibrational modes using inelastic neutron scattering on the VISION instrument at ORNL-SNS, to be scheduled later this year (IPTS-20466).

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3. Y. Nam and Y. S. Ju, *Journal of Adhesion Science and Technology* **27**, no. 20, 2163-2176 (2013)

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