

Machine learning enhanced microscopy identification of defects

Nicole Bishop^{1,2}, K.S. Mao^{2,3}

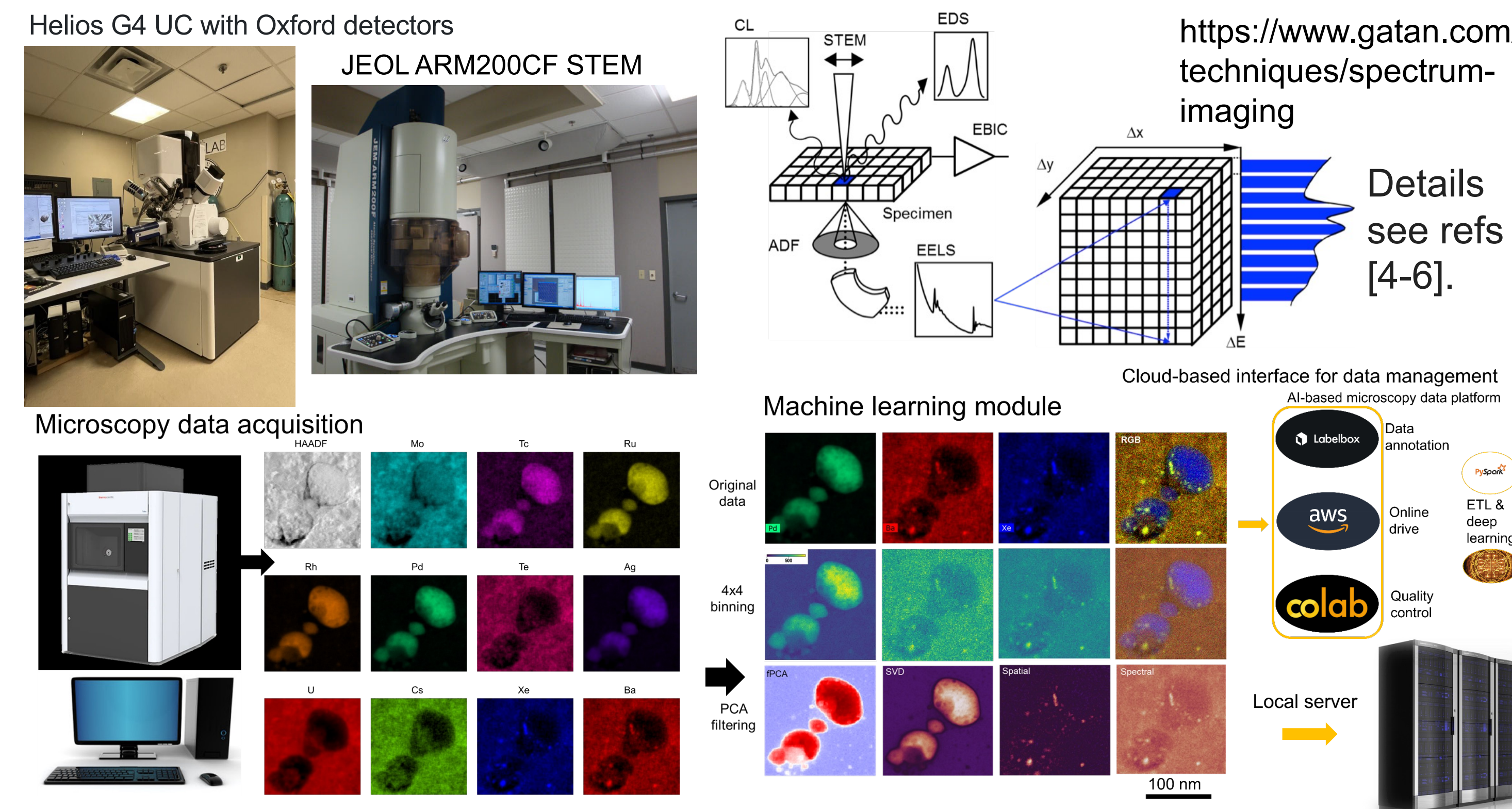
1. Florida State University College of Medicine, Tallahassee, FL 32306, USA.
2. National High Magnetic Field Laboratory, 1800 East Paul Dirac Drive, Tallahassee, FL 32310, USA.
3. Department of Industrial and Manufacturing Engineering, FAMU-FSU College of Engineering, Florida State University, Tallahassee, FL, 32310, USA



Why Machine Learning?

- This study focuses on the identification of defects in compounds for extreme applications: Nb₃Sn used in superconducting radio frequency cavities and SiC for fusion reactors.
- Machine learning algorithms have been applied to process atomistic structure images of interfaces of Cu/Nb₃Sn and defect evolution with an increase in irradiation dose in SiC.
- Advanced technology has facilitated the emergence of cutting-edge medical technologies, such as compact superconducting cyclotrons for external beam therapy with protons and ions.
- Thermo Fisher Scientific Talos F200X FEG-STEM and JEOL ARM200CF S/TEM were used for analytical microscopy for chemical composition using scanning transmission electron microscopy-energy dispersive X-ray spectroscopy (STEM-EDS) [1,2]. The process culminated with taking images of SiC defects that were analyzed through unsupervised machine learning algorithms.
- The results from the analysis provide insights into defect behavior to create strategies for maximizing the life and strength of materials [1,3]. The broader impact of this work would also result in cost and size reduction advantages in isotope production.
- We found defects with better resolution and confidence in the microstructure of these materials for extreme conditions.

Methods on characterization and data processing

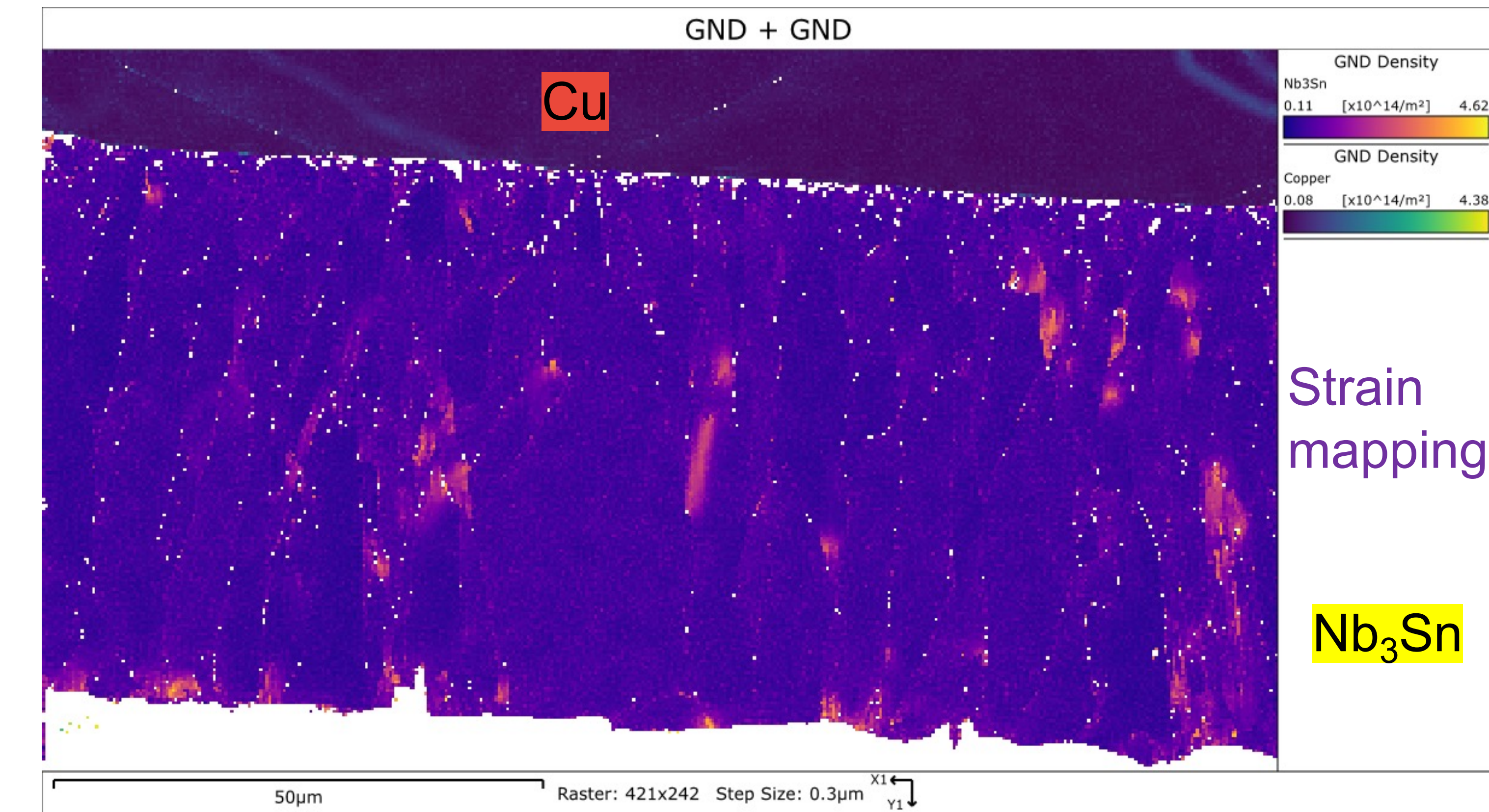


General application and coding

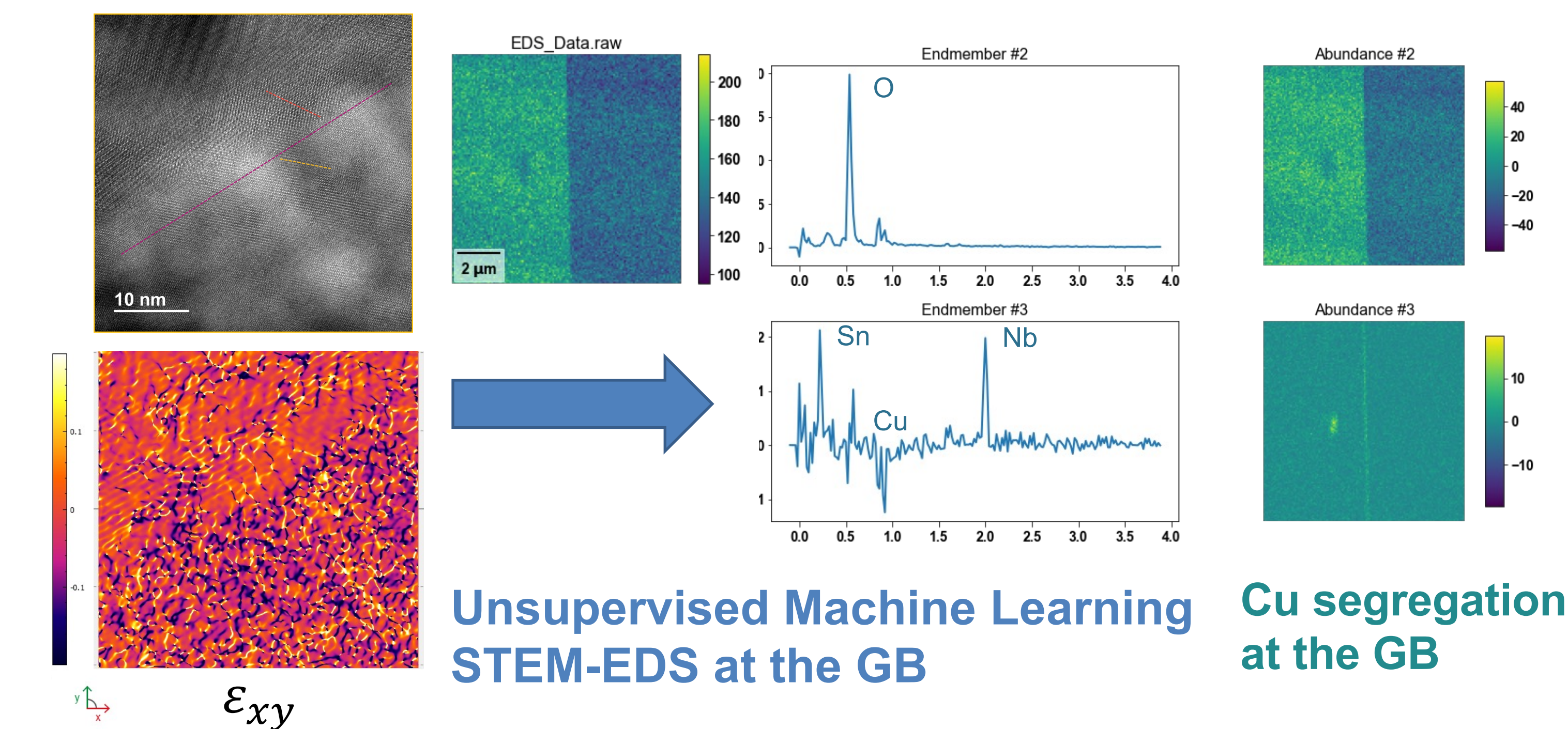
- SiC is a wide gap semiconductor with decent radiation tolerance leads it to serve in extreme environments (space exploration, fusion reactors).
- The microstructural evolution of SiC under these conditions needs to be examined with modern electron microscopy.
- Establishing a machine learning (ML) platform using existing Python-based data science/ML libraries and data visualization tools to exhibit the defect evolution of SiC composite fiber with the increase of irradiation dose.
- An ML-enhanced approach helps better understand the defect behavior and proposes mitigation strategies to reduce their negative implications on structural materials.



Thin-film Nb₃Sn-on-Cu ILC cavities interface



Looking at the Nb₃Sn Grain Boundary



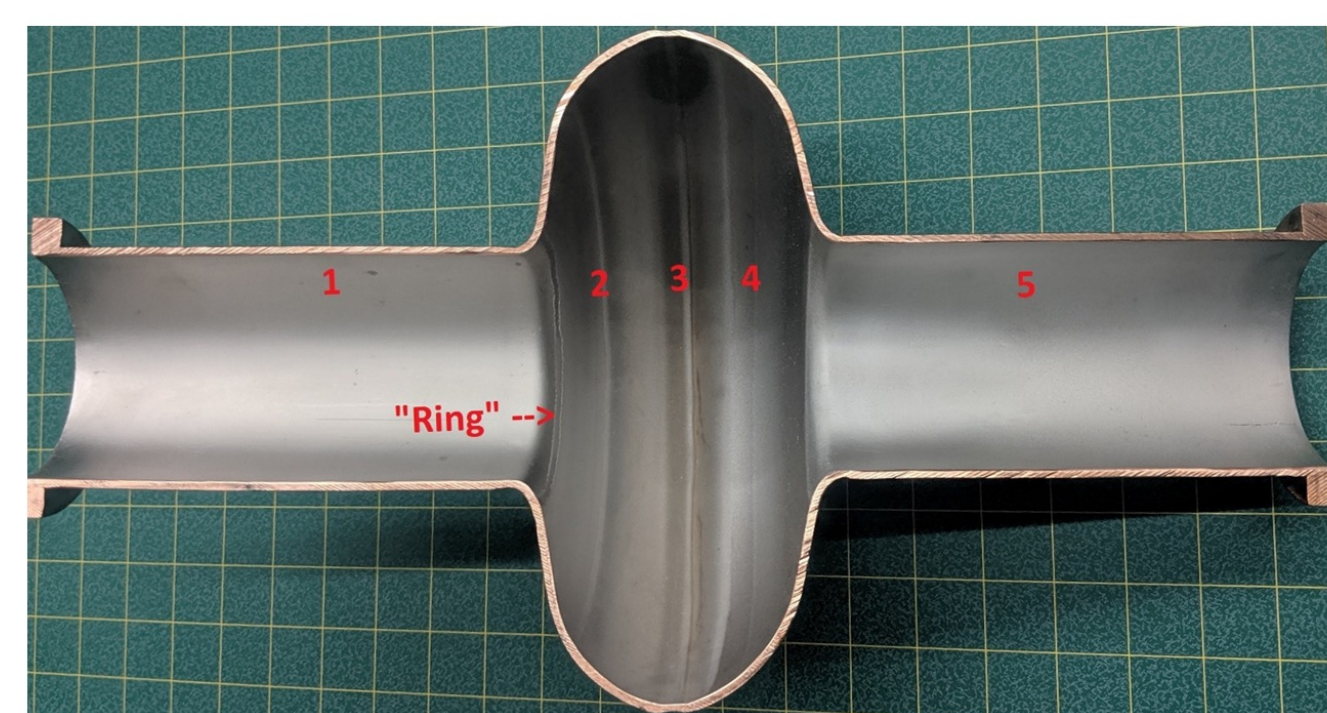
Background on materials and processing

Chemical Vapor Deposition (CVD)

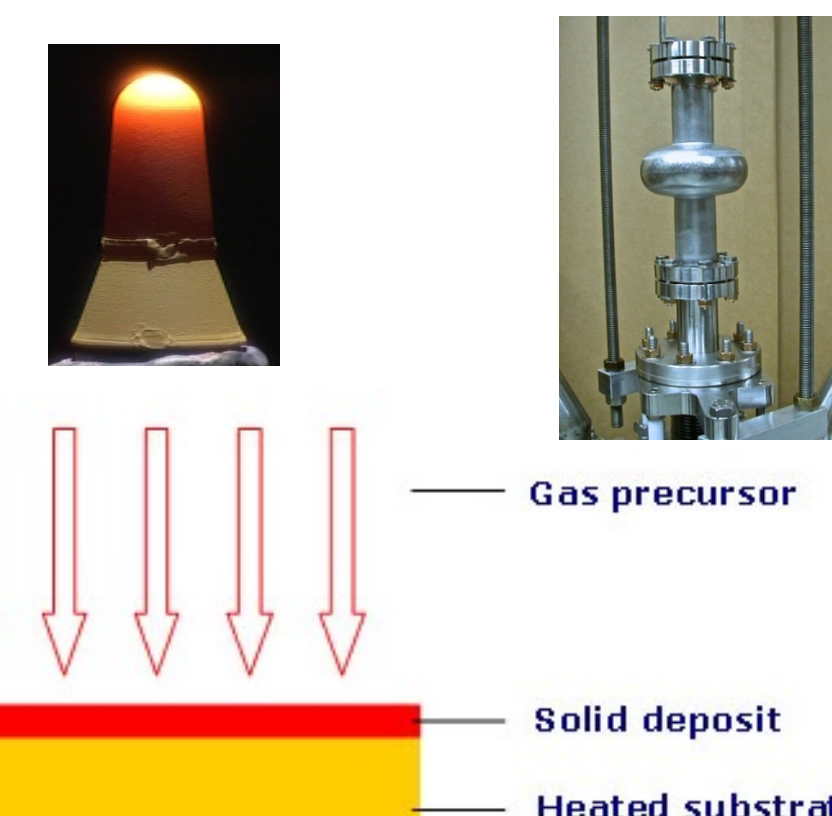
Thin-film CVD Nb₃Sn-on-Cu via pre-alloyed precursors



Bailey Tool seamless cavities

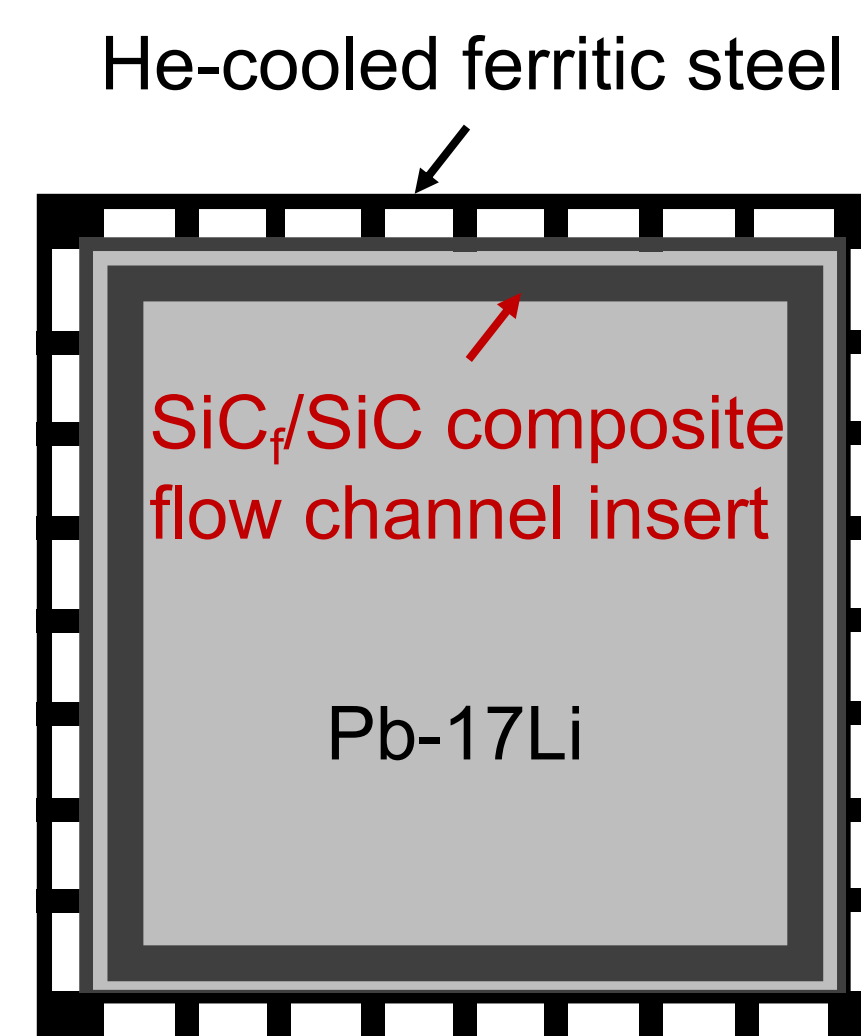


Ultramet CVD Nb₃Sn on bare Niowave welded copper cavity (SN43-45) using FSU A-Nb₃Sn-1 precursor



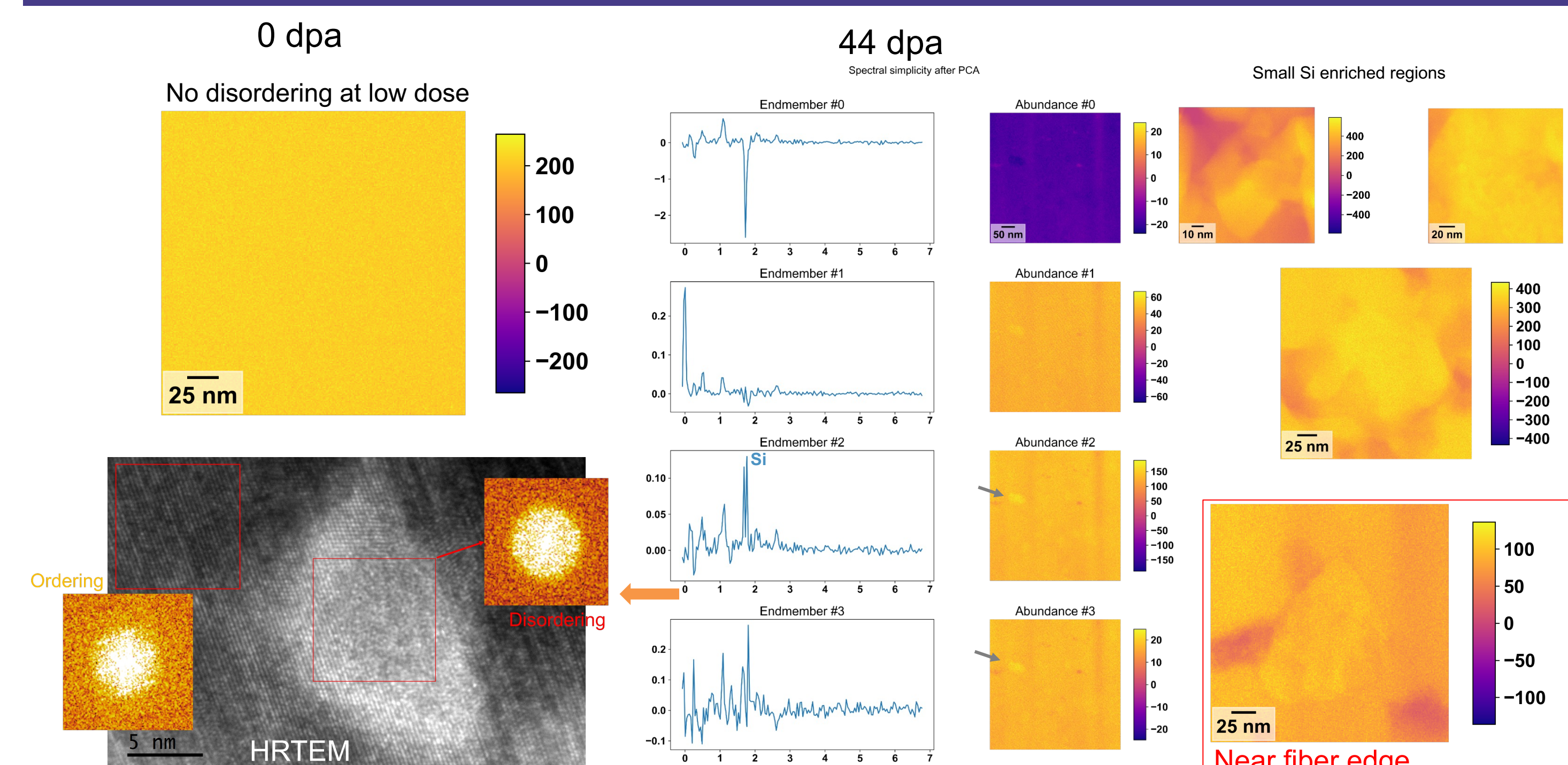
The dual-coolant helium/lead-lithium (DCLL) blanket is a candidate for a fusion DEMO reactor. DCLL uses SiC as the flow channel insert (FCI) in the coolant ducts to provide electrical and thermal insulation.

SiC for fusion



Cross section of the Pb-Li breeder unit cell of DCLL blanket [7].

Si Map in the irradiated SiC using Machine Learning



STEM-EDS maps on Si inside random single grains denoised the artifacts and low-counting background signals.

Summary

- The defect evolution was experimentally investigated through the construction of atomistic-level microscopy characterization enhanced by machine learning.
- We found a detailed analysis of cavities and elemental distribution that is helpful to understand the effects of radiation of SiC and heterogeneity in Nb₃Sn thin films.

References

1. Mao, K. S., Gerczak, T. J., Harp, J. M., McKinney, C. S., Lach, T. G., Karakoc, O., ... & Edmondson, P. D. (2022). Identifying chemically similar multiphase nanoprecipitates in compositionally complex non-equilibrium oxides via machine learning. *Communications Materials*, 3(1), 21.
2. Mao, K. S., Koyanagi, T., Nozawa, T., & Katoh, Y. (2022). Identifying Chemical Disorder in Irradiated SiC Fiber-Reinforced SiC Matrix Composites with High-Throughput Correlative Microscopy. *Microscopy and Microanalysis*, 28(S1), 2060-2061.
3. Balachandran, S., Polyanski, A., Chetri, S., Dhakal, P., Su, Y. F., Sung, Z. H., & Lee, P. J. (2021). Direct evidence of microstructure dependence of magnetic flux trapping in niobium. *Scientific reports*, 11(1), 5364.
4. Keenan, M. R. (2007). Multivariate analysis of spectral images composed of count data. *Techniques and applications of hyperspectral image analysis*, 89-126.
5. Stewart, G. W. (1993). On the early history of the singular value decomposition. *SIAM review*, 35(4), 551-566.
6. Keenan, M. R., & Kotula, P. G. (2004). Optimal scaling of TOF-SIMS spectrum-images prior to multivariate statistical analysis. *Applied Surface Science*, 231, 240-244.
7. Sharafat, S., Aoyama, A., Morley, N., Smolentsev, S., Katoh, Y., Williams, B., & Ghoniem, N. (2009). Development status of a SiC-foam based flow channel insert for a US-ITER DCLL TBM. *Fusion science and technology*, 56(2), 883-891.

CONTACT INFORMATION: nsb21b@fsu.edu

This work was supported by The National High Magnetic Field Laboratory, the National Science Foundation under NSF/DMR-1644779 and NSF/DMR-2128556, the State of Florida Research, and the U.S. Department of Energy, Offices of Nuclear Energy and Fusion Energy Sciences, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

