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Local User Project - 2024

Harnessing Machine Learning to Visualize and Understand the Role of Defects in a Metal-to-Insulator Transition in a Charge Density Wave Material

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Quantum materials are of fundamental and technological interest, with potential applications ranging from quantum computers to next-generation microelectronics. An exciting property of layered quantum materials like tantalum sulfide (TaS_2) are charge density waves (CDW)—emergent periodic modulations of the electron density. TaS_2 hosts several CDW states that spontaneously break crystal symmetries, mediate metal-insulator transitions, and compete with superconductivity, but are also challenging to visualize on the nanoscale. Quantum materials are commonly studied with bulk averaging probes and thus their nanoscale properties are poorly understood.

Here, **PARADIM**'s development of real-time temperature control during **cryogenic** scanning transmission electron microscopy has enabled its users to image the CDW transition while altering temperature and electric field. Unsupervised machine learning is applied to cluster the five-dimensional, terabyte scale microscopy datasets, and demonstrates a one-to-one correlation between device resistance, CDW phase, and the material microstructure. The team shows that basal dislocations—which are ubiquitous in 2D materials—both nucleate and pin the CDW transition and locally alter the transition temperature (T_c) by nearly ~75 K. Further, the team shows that the dislocation density can be used to engineer device properties.

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Data: https://doi.org/10.34863/0k5x-w691.

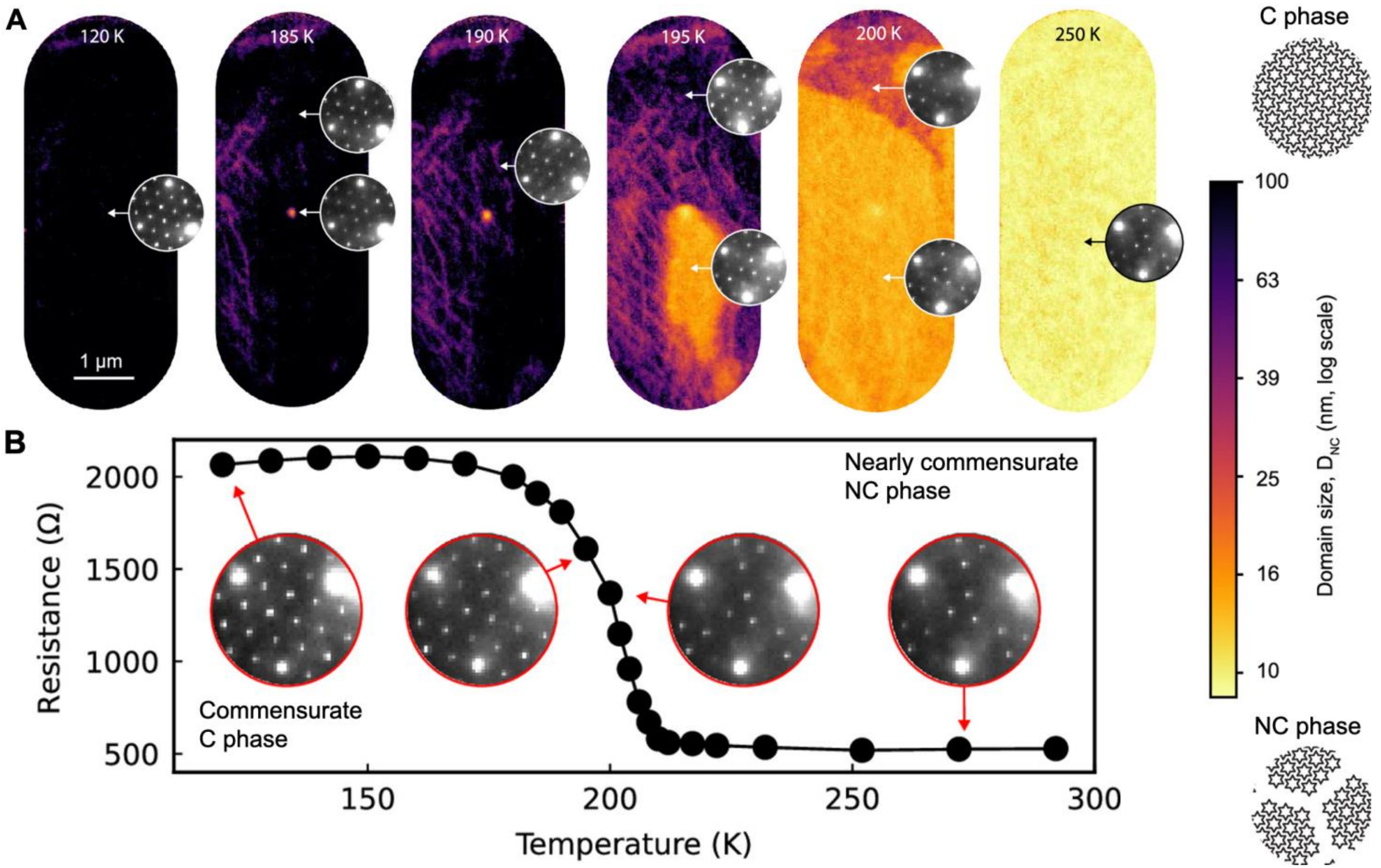

Figure: CDW phase transition during warming experiment. (**A**) 4D-STEM derived maps, color-coded for the domain size D_{NC} for select temperatures. Insets show extracted diffraction data. (**B**) The electrical resistance measured during the *in situ* 4D-STEM experiment upon warming.