Investigation of $NbTe_2$ Charge Density Wave Domain Boundaries

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Motivation

Niobium Ditelluride is a quantum material which is being studied for its potential use in computing, optoelectronic, and biomedical applications. Understanding the structural, chemical, and electronic properties of materials is essential to determining their technological potential.

One of the applications of these materials is in computing, where we look for features that can act as a bit. On a nano-scale, this could be achieved by measuring whether an isolated electronic state is empty or filled.

Transition Metal Dichalcogenides

Transition metal dichalcogenides (TMDCs) are a class of layered materials, some of which exhibit the quantum properties of charge density waves (CDWs) and superconductivity. CDWs are a macroscopic quantum state consisting of a periodic modulation of charge in conjunction with a periodic distortion of the crystal lattice.

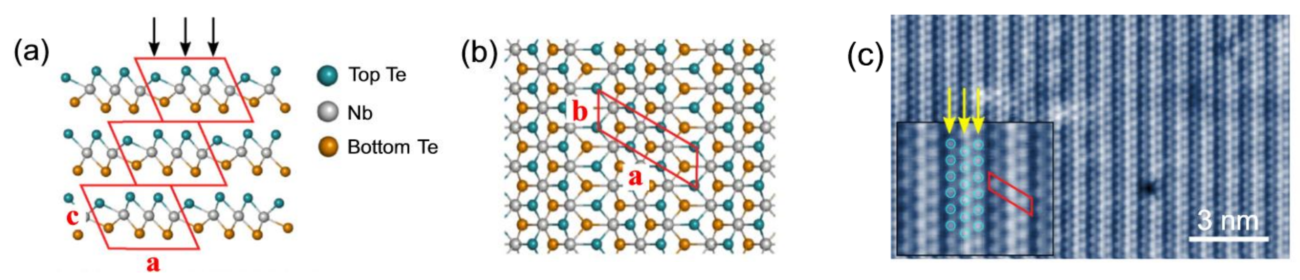

Figure 1: (a) Side view of the crystal structure depicting three $NbTe_2$ layers. (b) top view of the crystal with the conventional unit cell outlined in red (c) STM topography image with the inset showing the unit cell and cyan circles showing the location of the top Te atoms. The yellow arrows in (c) correspond to the arrows in (a) and point to top layer Te atoms [1]

In the same way that a crystal can have differentially oriented atomic domains, we observe multiple CDW domains. We call the intersection between two adjacent domains the domain boundary. Because the CDW is a charge modulation, CDW domain boundaries can have interesting electronic features. One example of this is in another TMDC, TaS_2, where at specific energies researches have observed conducting channels, essentially electron highways, on or adjacent to the domain boundaries.

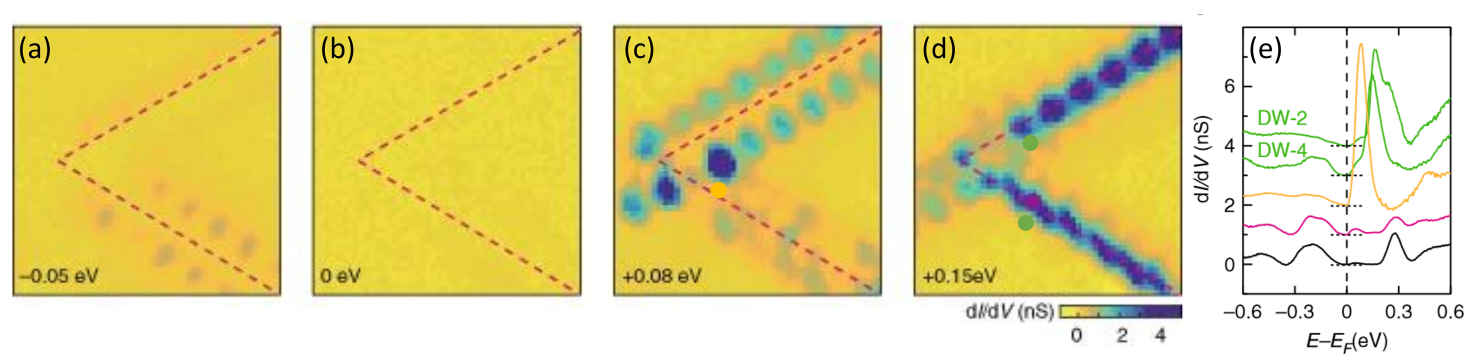

Fig 2: (a-d) Spectroscopy maps at varying energies of a CDW domain boundary. (e) Point spectra, the green and yellow correspond to points in (d) and (c) respectively [2]

STM Data

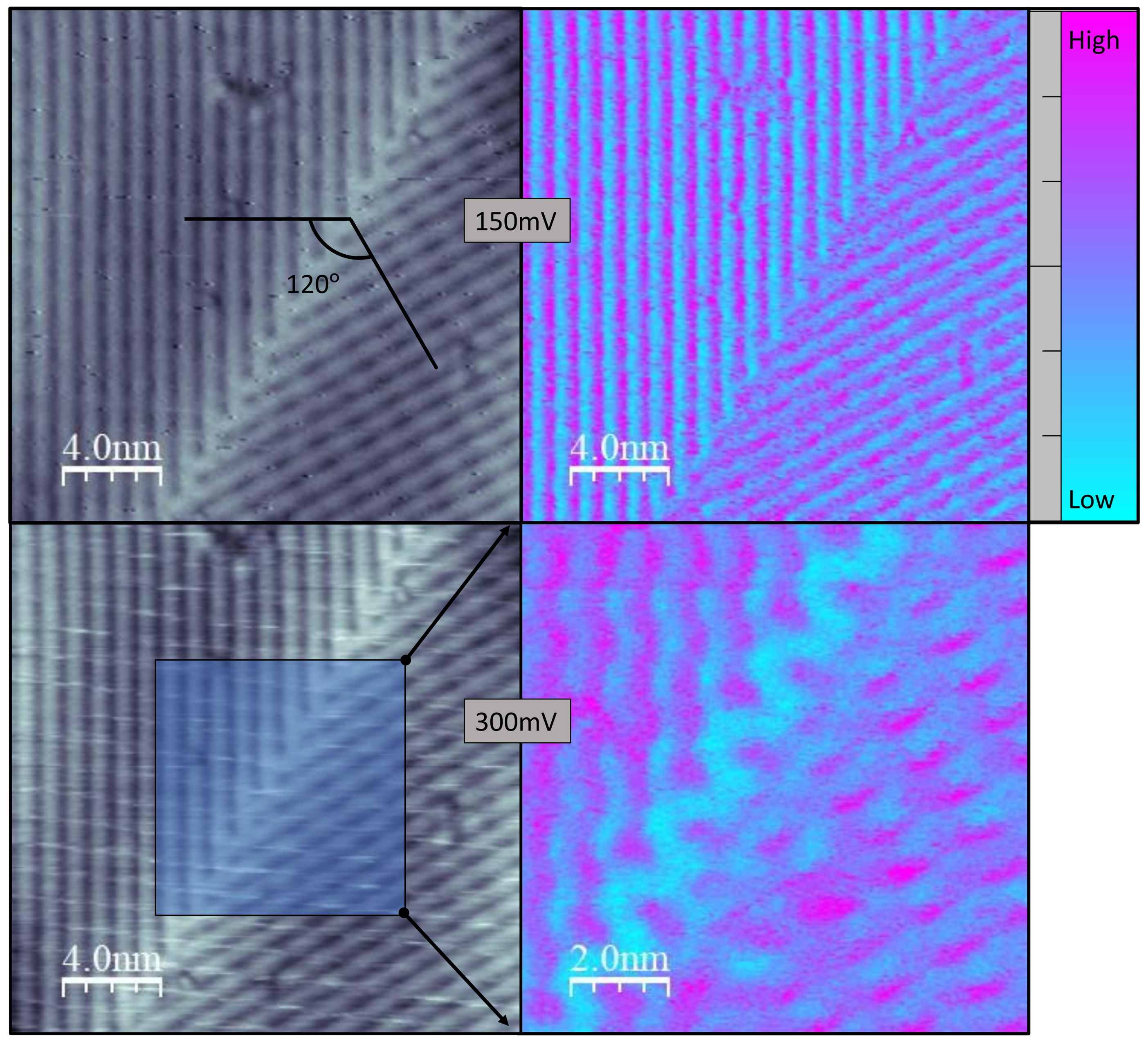

Fig 4: STM images (topography left column, dI/dV map right column) showing 120° charge density wave domain wall in our NbTe2 sample. On the right we see that at a bias of 300 mV we observe a zig-zag distortion which represents a lack of electronic states at the CDW domain wall

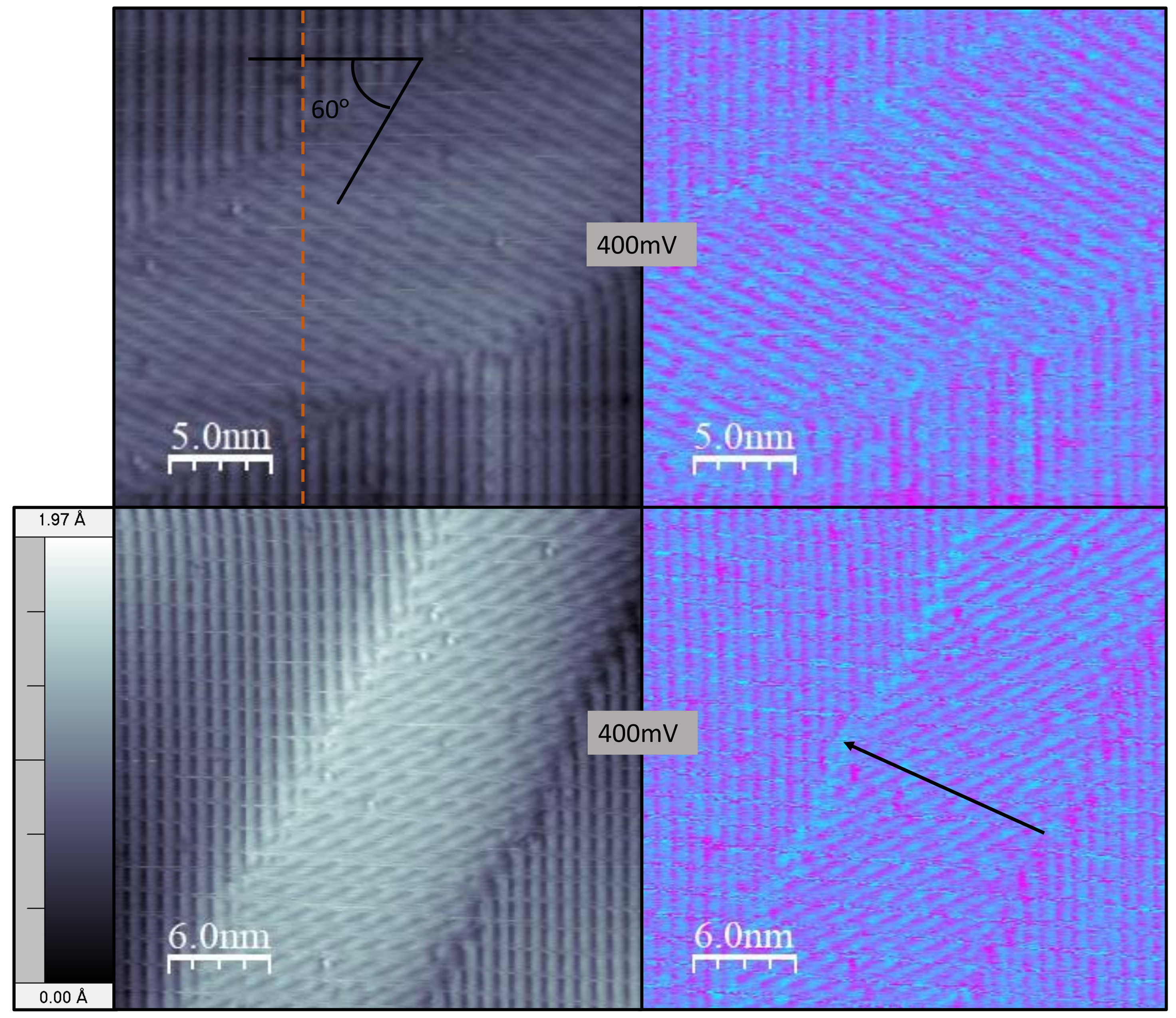

Fig 5: Top row: CDW stripe with 60° (ortho) boundaries. Bottom row: CDW stripe separated by 120° (meta) boundaries. Along the top boundary we see a lack of states (more blue) which is not observed along the bottom boundary.

Our Instrument

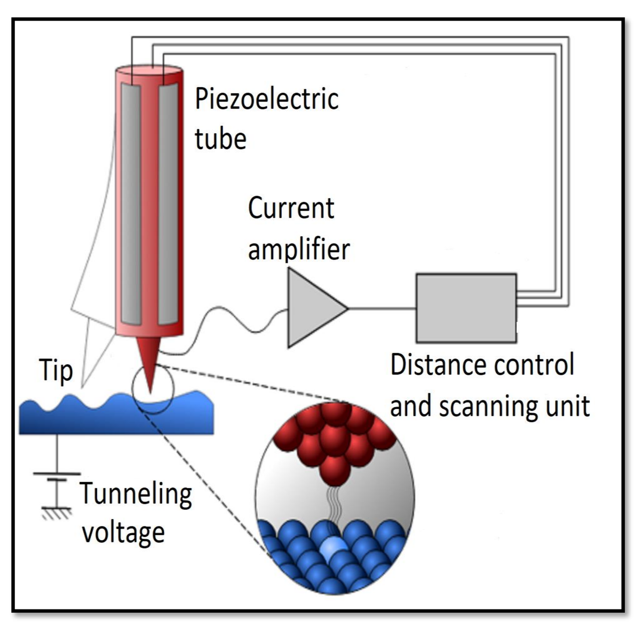

Fig 3: Left: Diagram of a STM, depicting atoms in the material and an atomically sharp metallic tip [3] Right: Image of the Hollen Lab STM showing our sample in the vacuum chamber

Scanning tunneling microscopes (STM) use the quantum mechanical phenomena of electron tunneling. When we position a sharp tip very close (<1nm) to a surface and apply a bias we can induce a tunneling current. To do this we must operate in an ultra-high vacuum, and often at ultra-low temperatures. For this project we collected all our data at 11K.

Results

We observed several domain boundaries and collected data on both their spatial and electronic features. On certain meta-boundaries we observed a zig-zag distortion representing a low number of electronic states which was absent from all observed ortho-boundaries. For the meta-boundary stripe, the upper boundary exhibits a lower density of electronic states compared to the lower boundary, resulting in the formation of a dipole-like feature at certain energies.

In this quantum material, topographically identical features show different electronic structure.

This result suggests that contributions from subsurface layers are controlling the electronic structure of these states.

References

1. Jang, W.-J. *et al. Phys. Rev. B,* 2022
2. Cho, D, et al., *Nat Commun*, 2017
3. "File:Scanning Tunneling Microscope schematic.svg" by Michael Schmid and Grzegorz Pietrzak is licensed under CC BY-SA 2.0.

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