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Atomic-Scale Visualizations of Low-Temperature Phase Transitions

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Probing the structure of layered materials offers a gateway to better understand and potentially manipulate

their electronic properties. While interactions within the individual layers are dominant, the proximity of neighboring layers significantly impacts the properties of such quasi-2D systems. Transition-metal dichalcogenides containing tellurium are especially noteworthy for their modulated structures and prominent interlayer contributions.

Here, members of PARADIM's in-house research team combine cryogenic scanning transmission electron microscopy (cryo-STEM) with theoretical modeling to visualize and understand complex patterns of displacements of atoms in the layered material TaTe₂. At room temperature, Ta atoms form small clusters in a staggered three-layer stacking. At low temperatures, the Ta clusters become even more distorted, creating a superstructure that includes subtle displacement of the Te atoms. Snapshots of the structure showed faint contrast modulations which could only be quantified by pushing the resolution and stability of a cryogenic sample holder available to all users of PARADIM. Theoretical calculations revealed a connection between the contrast modulations and the pattern of atomic displacements, which opens the door for visualizing a range of new materials with complex structural arrangements.

I. El Baggari et al., Phys. Rev. Lett. 125, 165302 (2020)





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