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Emergence of CDW and a Psuedogap in Single-Layer 1T-$TiTe_2$

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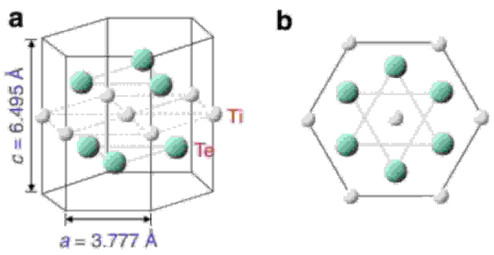
Introduction

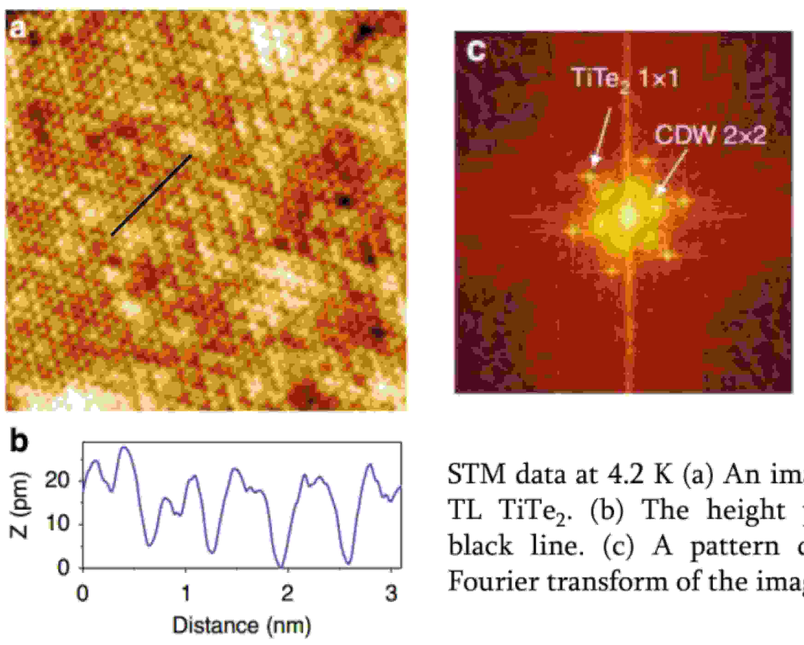
- 1T-$TiTe_2$ is a type of layered transition metal dichalcogenide (TMD) material of the form MX_2 (M for metal and X for chalcogenide).
- Bulk $TiTe_2$ is metal/semimetal with a negative band gap and shows no CDW phase transition.
- In our studies of $TiTe_2$ monolayer and multilayers we observed a surprisingly (2x2) CDW transition in monolayer but not in bilayer and multi-layer $TiTe_2$.



(a) Atomic Structure of a single layer of $TiTe_2$. The quantities a and c are the lattice constants of bulk $TiTe_2$.
(b) Same structure projected onto the (0001) plane.

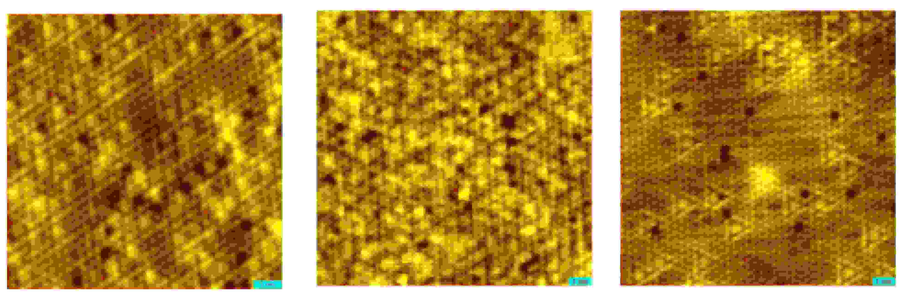
CDW Order

- STM
  - The triangular lattice is associated with the top Te atoms
  - The 2x2 height modulation is 5pm illustrated from the line profile
  - Fourier transform shows sharp (1x1) lattice peaks and comparatively weak and broad (2x2) spots.



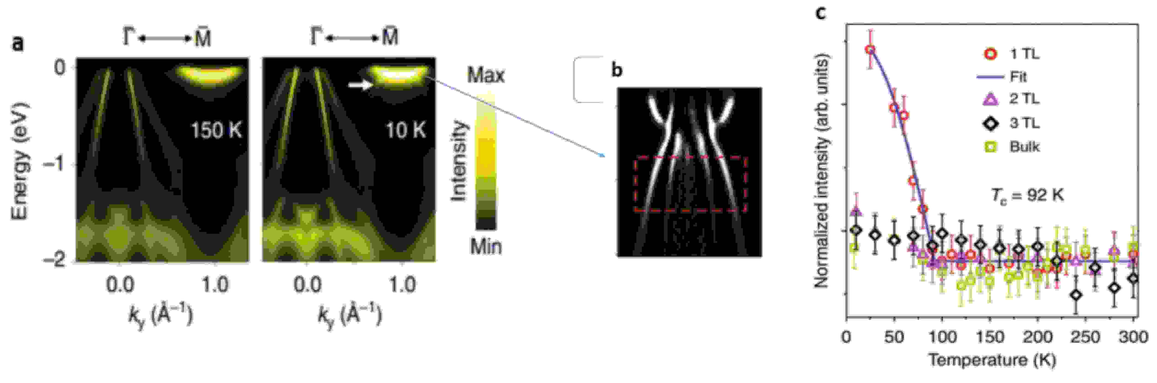
STM data at 4.2 K (a) An image taken from 1-TL $TiTe_2$. (b) The height profile along the black line. (c) A pattern derived from the Fourier transform of the image.

- Presence of different domains at different locations at 4.2 K



Band Structure

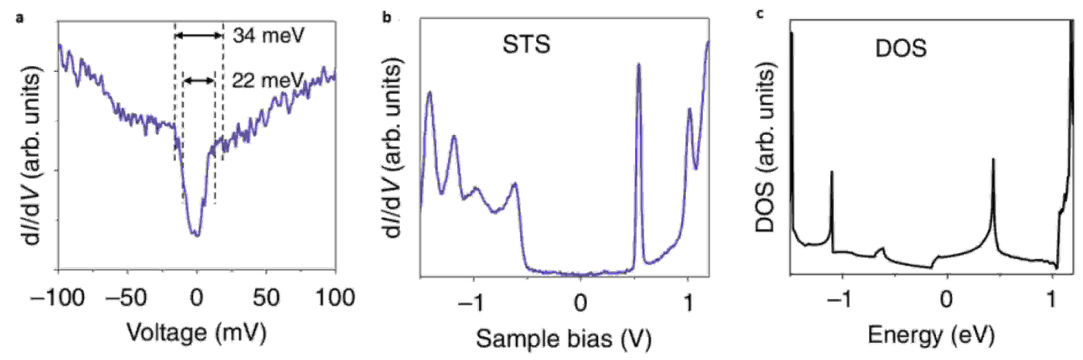
- ARPES
  - The semimetal negative bandgap is of about 0.5 eV.
  - Bulk $TiTe_2$ shows additional dispersion in the layer-stacking direction
  - 10K data shows weak replica of the valence band
  - Transition temperature of $T_c = 92 \pm 3$ K was obtained



(a) ARPES spectra taken from a one trilayer (1-TL) $TiTe_2$ along the Γ -M direction at 150 K and at 10 K. (b) ARPES map around M
(c) Integrated ARPES intensities as a function of temperature for the 1-TL, 2-TL, and 3-TL

Pseuedogap

- STS
  - A STS reveal 60% conductance dip at the fermi level hence it is not true but a pseudogap.
  - The pseudogap size is about 28 meV, equals 3.5 $K_B T_c$ where T_c= 92K
  - A wide energy range STS agrees closely with the computed density of states of a 1-TL $TiTe_2$.



STS data at 4.2 K (a) A STS differential conductance curve (b) STS data over a wide energy range. (c) Computed density of states (DOS) for 1-TL $TiTe_2$.

Conclusion

- The Excitonic mechanism and John-Teller mechanism does not fit into CDW seen in single layer $TiTe_2$
- Bilayer and multi-layer $TiTe_2$ shows no related CDW transitions.
- Issues: the origin of the pseudogap at the Fermi level

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