



# Chemical Vapor Transport growth and characterization of $WTe_2$

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# Tungsten ditelluride $WTe_2$ : unique member of 2D TMDCs

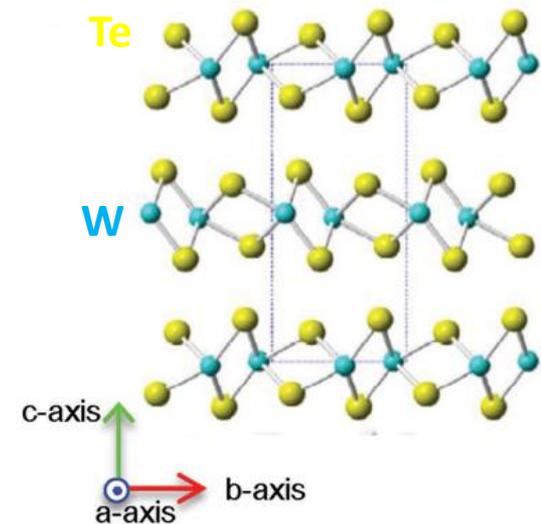
$WTe_2$  - a type-II Weyl semimetal material with extremely large magnetoresistance

Unique among TMDs as it crystallizes in a distorted  $1T'$  phase (also known as Td phase).  $WTe_2$  has orthorhombic crystal structure in contrast to the commonly observed 2H and  $1T$  structures.

In Td phase, the W-atoms are octahedrally coordinated by Te-atoms and the successive layers in between are rotated by  $180^\circ$ .

The unique electronic nature leads to:

- strong anisotropic electrostatics,
- extremely large, non-saturated magnetoresistance,
- “negative” magnetoresistivity,
- room temperature ferroelectric semimetal, superconductivity and plasmon polariton activity



small 2016, 12, No. 42, 5802–5808

Numerous perspectives for topological, spintronic and opto-electronic applications.

# Growth of WTe<sub>2</sub> single crystals: Challenges

Due to low chemical reaction activity of Te with W, WTe<sub>2</sub> is very challenging **chemically**, especially for various synthesis techniques as Chemical Vapor Deposition (CVD) and Molecular Beam Epitaxy (MBE).

The majority of contemporary WTe<sub>2</sub> studies aiming in 2D limit relied on mechanically-exfoliated samples from single crystals.

Necessity for an improvement of the synthesis and growth techniques for preparation of high quality crystals closer to the structural perfection.

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# Growth of $WTe_2$ single crystals by Chemical Vapor Transport (CVT)

- A mixture containing stoichiometric amounts of W and Te powder was slowly heated from RT to 920°C for 12 h, and held at 920°C for 3 days in a sealed evacuated quartz ampoule.
- $WTe_2$  single crystals were grown from the synthesized powder by CVT with  $Br_2$  as transport agent for 14-21 days in a sealed evacuated quartz ampoule with source and growth zones kept at 895°C and 715°C, respectively.
- The obtained bulk crystals were pumped under dynamic vacuum at RT for 1 day to remove any residual Br.

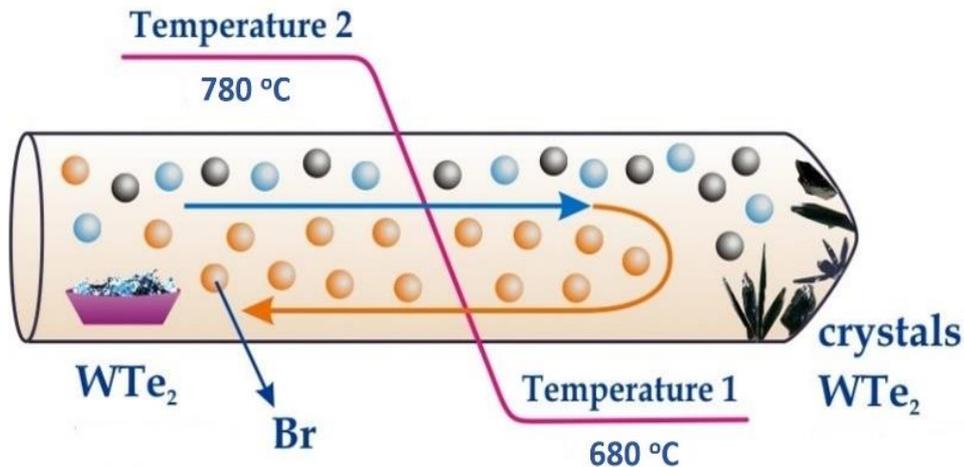


Fig. Schematics of  $WTe_2$  single crystals growth process by CVT method



Fig. Photograph of  $WTe_2$  single crystals

# XRD and Raman analysis

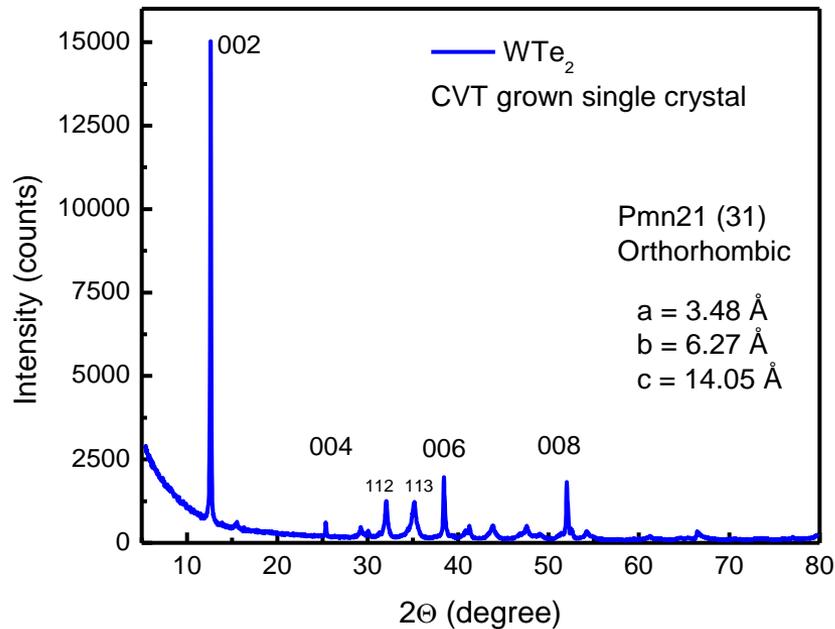


Fig. XRD analysis of WTe<sub>2</sub> single crystals

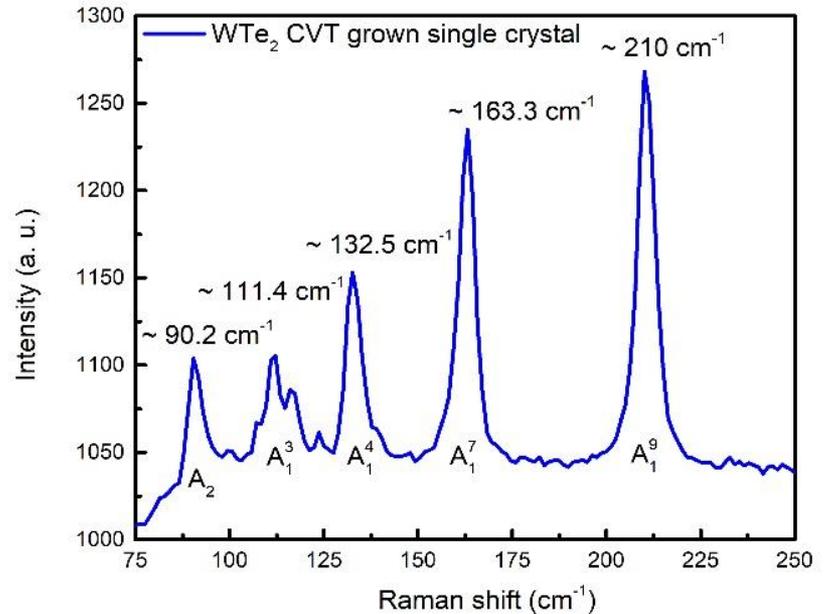


Fig. Raman spectra and characteristic vibration modes for WTe<sub>2</sub> single crystal

- X-ray powder diffraction (XRD) patterns confirms that WTe<sub>2</sub> crystallizes in space group P<sub>mn</sub>21 in orthorhombic Td structure.
- Raman shows typical vibrational modes for WTe<sub>2</sub> detected at: A<sub>1</sub><sup>9</sup> ~ 210 cm<sup>-1</sup>, A<sub>1</sub><sup>7</sup> ~ 163 cm<sup>-1</sup>, A<sub>1</sub><sup>4</sup> ~ 132 cm<sup>-1</sup>, A<sub>1</sub><sup>3</sup> ~ 111 cm<sup>-1</sup> and A<sub>2</sub> ~ 90 cm<sup>-1</sup> confirming the desired chemical composition.

# AFM analysis

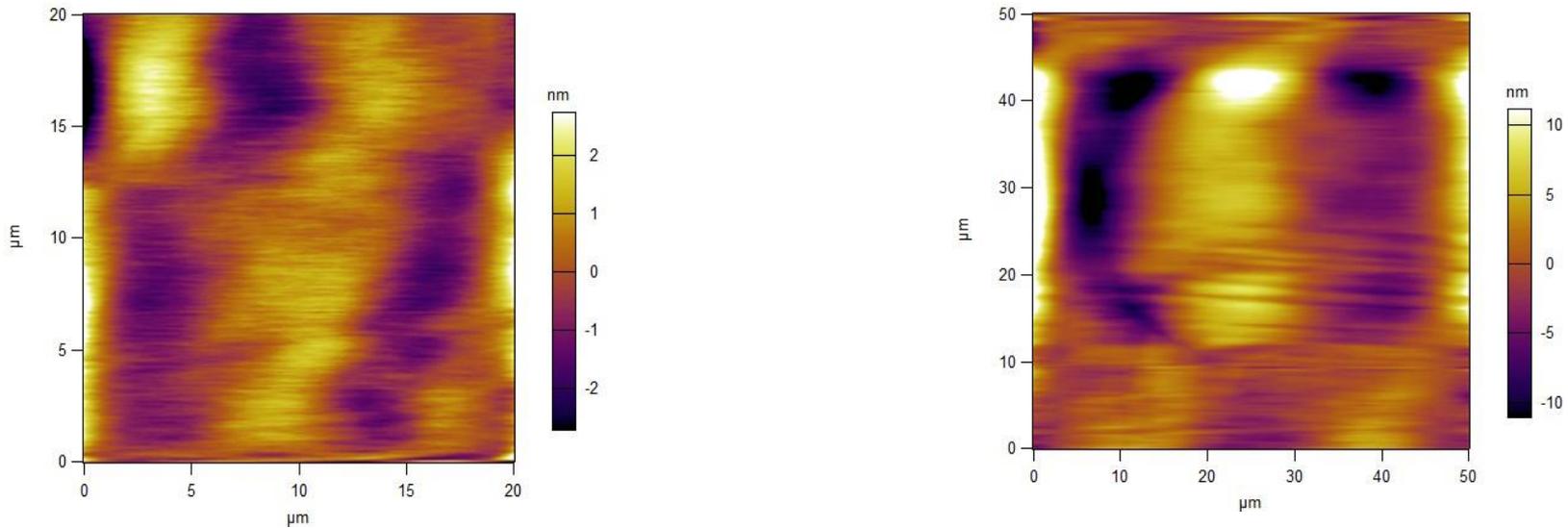


Fig. AFM analysis of two separate sectors from  $WTe_2$  single crystal surface topology.

- AFM data revealed that the surface topology is close to the structural perfection even on a nanoscale level (RMS roughness relief varies within 1 nm to 4 nm).
- This is a fine verification of the quality of the crystal which will be suitable for further alterations as mechanical exfoliation for instance.

## Conclusion

Detailed description of the preparation stages, technical considerations and growth procedure of  $WTe_2$  by means of Chemical Vapor Transport method are presented.

Performed XRD and Raman spectroscopy analysis verified excellent crystallinity of  $WTe_2$

The surface topology via AFM analysis with construction of topography 2D map revealing a few nanometers variation of the morphology features.

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