Sub-nanometer control of low-dimensional tantalum tellurides via encapsulation within carbon nanotubes

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Abstract: Transition metal trichalcogenides $TaTe_3$ and transition metal dichalcogenides $TaTe_2$ are under-studied materials due to their instability in air and difficulty in separating the two products from one another. Both the issue of instability and isolation can be resolved by encapsulating the reaction within carbon nanotubes. There are two main factors, carbon nanotube width and reaction temperature, which can affect the overall structure encapsulated. Here, we show how temperature shows the most control over the targeted synthesis of a preferred species.

Ta-Te system structures

- For the Ta-Te system, there exists two distinct, low-dimensional van der Waals (vdW) structures: $TaTe_2$ and $TaTe_3$
- Transition metal dichalcogenide (TMD), $TaTe_2$: atom-thick nanosheet (Fig. 1 and 2) and the transition metal trichalcogenide (TMT), $TaTe_3$: quasi 1-dimensional chain (Fig. 3 and 4)
- Weak vdW forces allows us to strip down crystals into their low dimensional counterparts via carbon nanotube (CNT) encapsulation

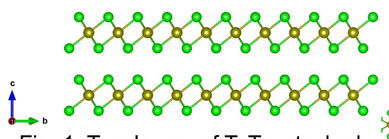

Fig. 1: Two layers of $TaTe_2$ stacked on top of each other

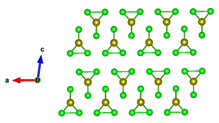

Fig. 3: Frontal view of nanochains

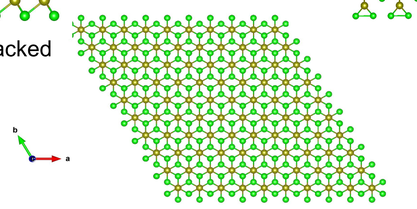

Fig. 2:Bird's-eye view of $TaTe_2$ nanoribbon

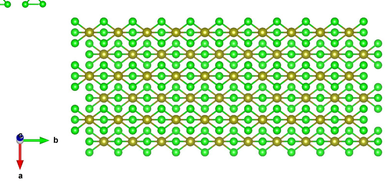

Fig. 4: Brid's-eye view of $TaTe_3$ nanochains

Material Synthesis and Characterization

- Chemical Vapor Transport
- Stoichiometric amounts of powdered Tantalum (Ta) and Telluride (Te), with (CNT) are sealed under a vacuum in a quartz ampoule

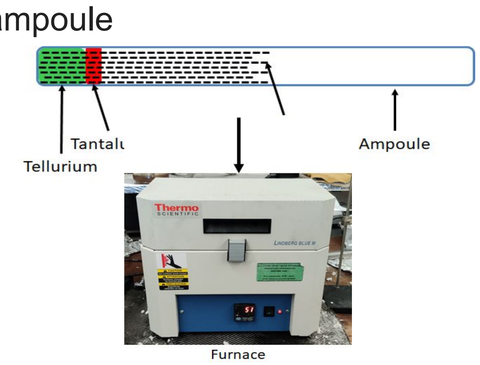

Fig. 5: Diagram of how tantalum telluride crystals are synthesized.

- Scanning transmission electron microscopy (STEM) imaging of these crystals done at NCEM
- Java-based image analysis program (FIJI) used to observe structural differences between samples

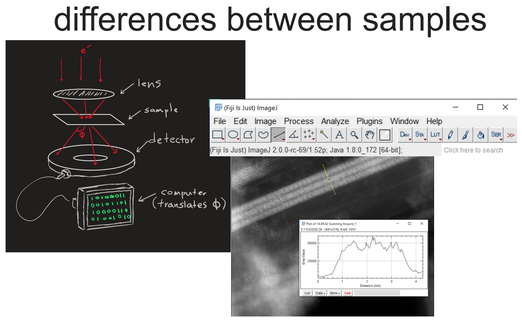

Fig. 6: Brief overview of how STEM imaging and analysis is done.

Structural Variations in Encapsulated $TaTe_2$

- One group of structures observed matches that of $TaTe_2$, where the encapsulated structure reveals a sheet-like appearance that has been confined into a nanoribbon (NR)
- Some of the observed $TaTe_2$ structures have a standard NR form (Fig. 4)
- Another commonly observed $TaTe_2$ structure appears to consist of 2 NRs overlapping within the CNT, but a potential misalignment (~38°) of the layers creates a moiré pattern (Fig. 5)

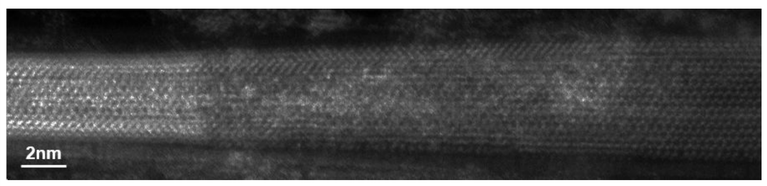

Fig.7: STEM image of an encapsulated $TaTe_2$ nanoribbon

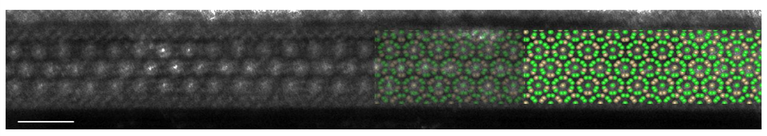

Fig. 8: STEM image of a $TaTe_2$ nanoribbon exhibiting a larger, periodic pattern. Atomic model overlay of proposed mis-aligned nanoribbons.

Structural Variations in Encapsulated $TaTe_3$

- The other group of structures observed matches that of $TaTe_3$, where the encapsulated structure reveals a chain-like appearance
- Some of the observed structures have a standard nanochain form (Fig. 6)
- A special case of $TaTe_3$ occurs when the number chains is smaller than 4, where the chains begin to wrap around each other in a spiraling manner

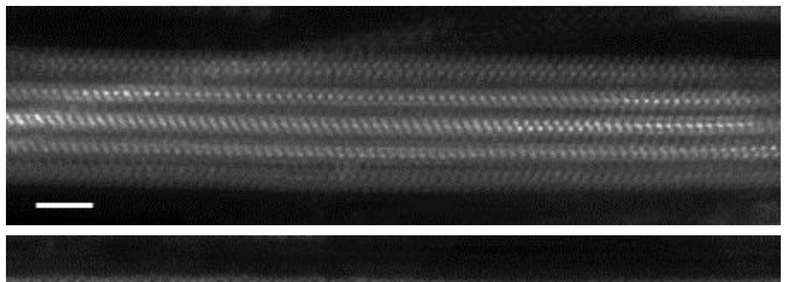

Fig. 9: STEM image of encapsulated $TaTe_3$ nanochains

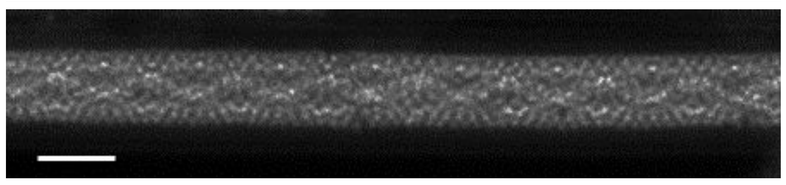

Fig. 10: STEM image of $TaTe_3$ chains wrapping around each other in a helical fashion

Results and Discussion

- The box plot t demonstrates that the system's structural preference between nanoribbons and nanochains isn't greatly dependent on CNT width
- Temperature is a factor that affects preference. Typically, neither are preferred at temperatures <600°C. Nanochains are favorable at lower temperatures (600°C-700° C) and nanoribbons have a larger frequency at higher temperatures (Temperatures >700°C).
- This suggests a gap in their activation energies as well as a variation in structural stability.

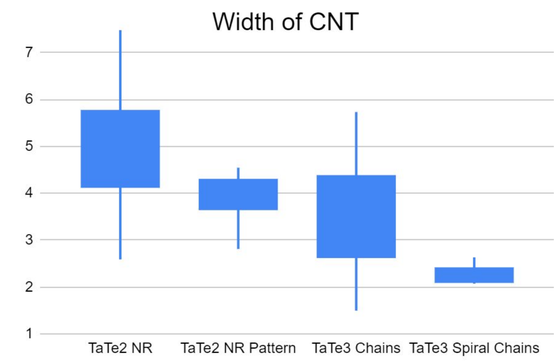

Fig. 11: Box plot of the ranges of carbon nanotube widths each structure was found in

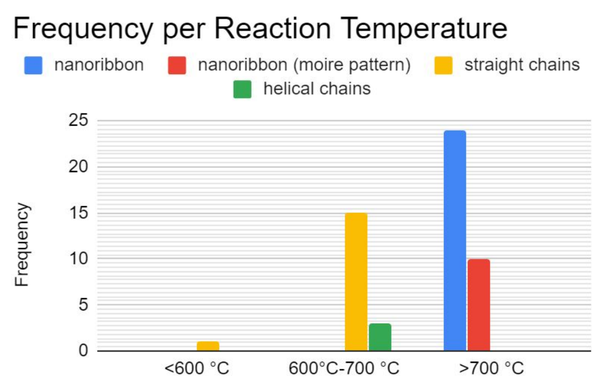

Fig. 12: Bar graph of frequency of each structure for ech reaction temperature.

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