







P-45

# IMEC18

## Structural investigation of the MoTe<sub>2</sub> phases

Sir Oshry, Gil Yaari, Sergey Krybak, Albert V. Jaryvd, Viktor Zenoar, David Fuks, Louisa Meshi  
Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva 84105 POB 653, Israel  
Materials Measurement Laboratory, National Institute of Standards and Technology, Maryland, 20899, USA  
Nuclear Research Center Negev, Israel

### Literature Survey

MoTe<sub>2</sub> belongs to the class of the 2D transition metal dichalcogenides (TMDCs). Structural properties of the MoTe<sub>2</sub> change as a function of the transition element. The phase for the transition element is 2H (hexagonal) or 1T (trigonal) or 2T (orthorhombic) structure. The 2H structure is the most stable structure in the 2D TMDCs. The 1T structure is the most stable structure in the 3D TMDCs. The 2T structure is the most stable structure in the 3D TMDCs. The 2H structure is the most stable structure in the 2D TMDCs. The 1T structure is the most stable structure in the 3D TMDCs. The 2T structure is the most stable structure in the 3D TMDCs.

### Experimental

MoTe<sub>2</sub> crystals were grown using CVT method with iodine. The growth was optimized by reaction between stoichiometric amounts of Mo (99.999%) and Te (99.999%) powders at 750 °C for 72 h in vacuum sealed quartz ampoules. In order to retain the 1T and 2H phases, the ampoules were quenched in low-water or cooled to room temperature at 20 °C/h, respectively, after 7 days of growth. **EXEDS characterization** samples were etched using 1-methyl-2-pyrrolidone in an ultrasonic bath and placed on lacy Cu grid. **Theoretical calculations** were performed by Density Functional Theory (DFT) applying the Full Potential method with Linearized Augmented Plane Waves (FP-LAPW), as implemented in the WIEN2K code (ver. 3.8.2).

### Results

#### Structure Relationship

In this research group, the relationship between the 2H and 1T structures were found and the relationship between the 2H and 1T structures were found and the relationship between the 2H and 1T structures were found.

#### Second Intermediate structure

Second intermediate structure has same lattice parameters as 1T, but by 1T, which structure of 1T was found, it was found that the space group of this structure might be either P6<sub>3</sub>/m or P6<sub>3</sub>/m. Later we found that in transition to the 2H structure.

#### Comparison between the second through group structure and conventional 1T structure

Comparison between the second through group structure and conventional 1T structure, showing the difference between the two structures.

### Carbon Nanotubes

#### Rubber by

##### scopy

Yona Lachman-Semesh  
Ben-Gurion University

### EXPERIMENTAL

EXPERIMENTAL

### IR AND RAMAN BAND SHIFTS DESCRIPTION

IR AND RAMAN BAND SHIFTS DESCRIPTION

























