Investigation of Structural Rearrangement of Twisted WS_2 In Atomic Substitution Nitridation Reaction

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Introduction

Background

- Two-dimensional (2D) materials such as graphene, WS_2, and MoS_2 are made up of atomically thin flakes held together by weak van der Waals (vdW) forces
- Stacked and twisted 2D materials can form Moiré superlattices

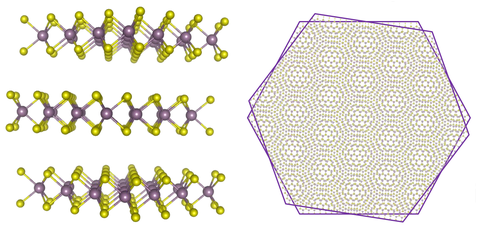

Fig 1. Crystal structure of WS_2 and Moiré pattern in twisted WS_2

- 2D Moiré superlattices induce many intriguing physical and chemical properties while creating a unique platform for manipulating chemical reactions at the atomic scale[1][2]

Objective

- This study aims to use the nitridation of WS_2 as a model system to investigate structural changes in Moiré chemistry

Methods

Sample Fabrication

- Gold-assisted mechanical exfoliation of WS_2 onto SiO_2/Si substrate
- Dry transfer process using transfer stage with adhesive poly(bisphenol A carbonate) (PC)

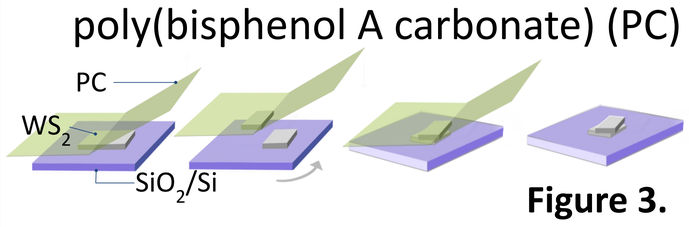

Figure 3. Diagram of dry transfer process

Nitridation Conditions

- Nitridation of WS_2 was carried out in a quartz tube furnace with ammonia gas carried by argon with a flow rate of 100 sccm. The reaction was performed at 850°C for 10 min with a ramping rate of 45°C / min.

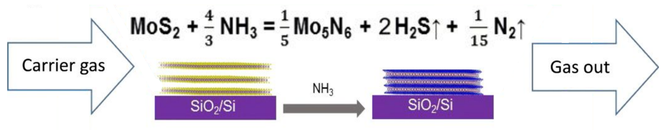

Figure 4. Nitridation reaction schematic and equation[2]

Raman Spectroscopy

- Renishaw inVia Raman Microscope
- 532 nm, 2.5 mW

Results

Preliminary Results

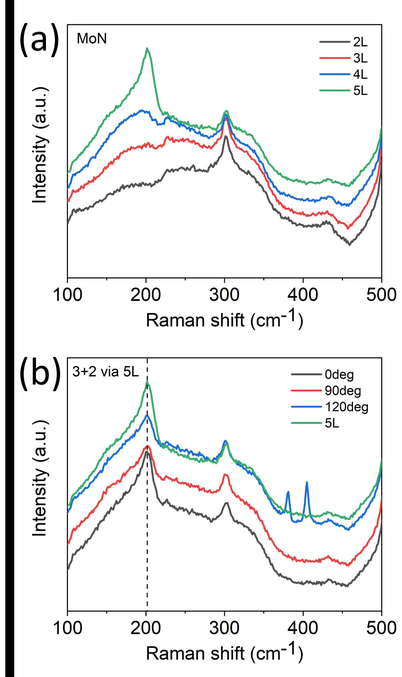

Figure 5. Raman spectra of non-stacked (a) and stacked (b) MoS_2 conversion product and SAED pattern before (c) and after (d) the reaction, revealing lattice domain shifting as part of the mechanism of the nitridation reaction.

Thickness Dependent Raman Characteristics of WN

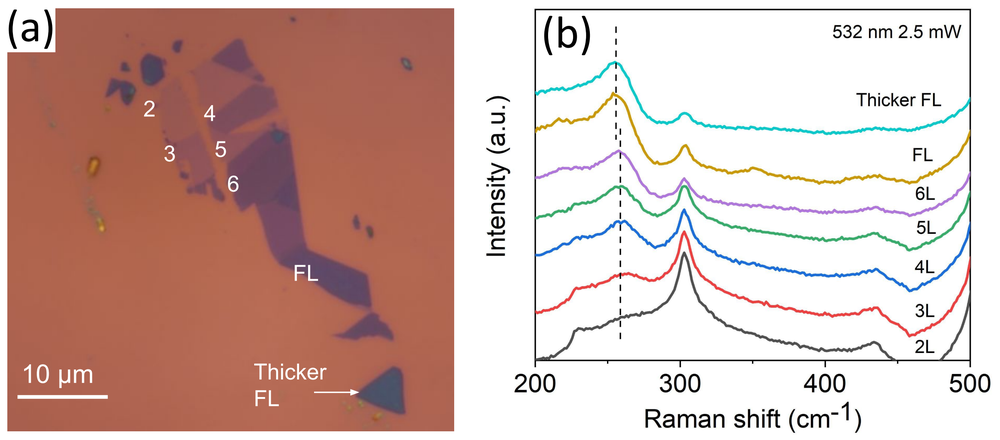

Figure 6. Optical image (a) of a WN flake converted from WS_2 and Raman spectra (b) acquired at different locations. The Raman spectra of WN exhibit thickness dependence in both peak shape and position.

Nitridation of t-WS_2 and Raman Characterization

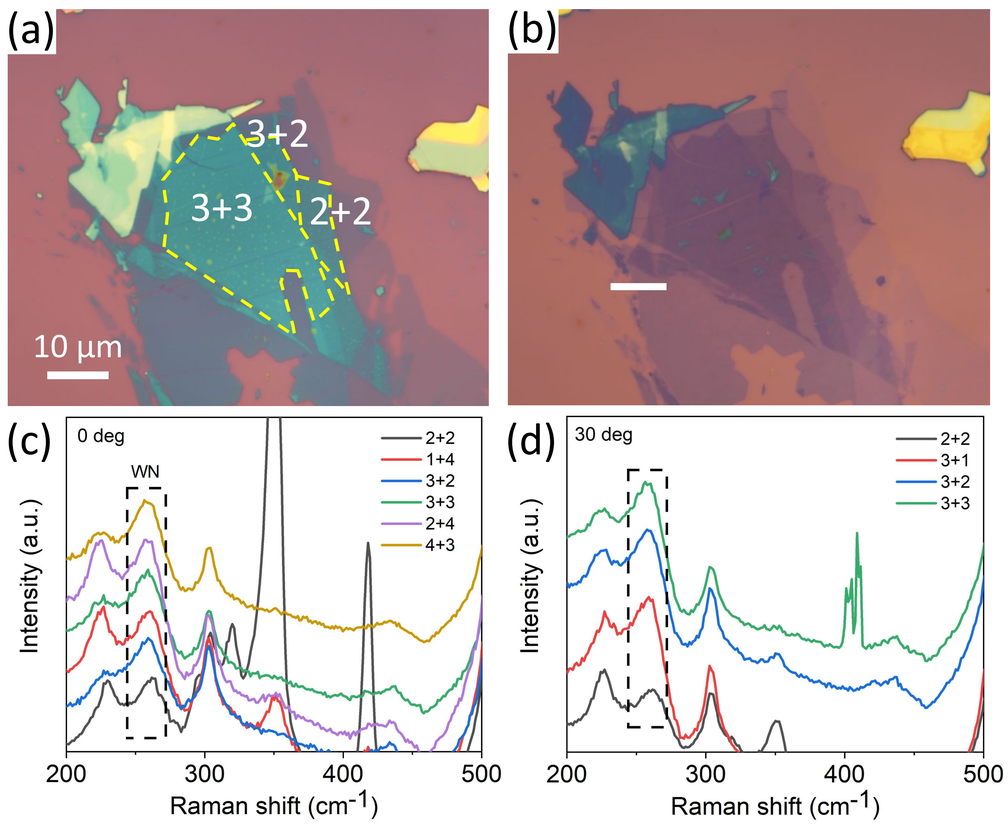

Figure 7. WS_2 sample with a 0° twist angle before (a) and after (b) the nitridation reaction. Raman spectra for WS_2 samples with 0° (c) and 30° (d) twists exhibit peaks characteristic of layers of combined thickness across all angles and stacking configurations.

Discussion

Summary

- Raman spectroscopy was carried out on WN converted from WS_2 with differing layer counts. Results show that WN has a thickness-dependent Raman signal in both peak shape and peak position.
- Twist WS_2 samples with various stacking configurations were prepared via a dry transfer process and converted into WN through an atomic substitution nitridation reaction.
- WN Raman signals from combined layer thicknesses were also observed on converted t-WS_2, revealing that the crystal structure of WS_2 changes in a manner similar to MoS_2.

Future Plans

- Perform TEM characterization on twist WS_2 and MoS_2 samples with different stacking configurations before and after the reaction, to further investigate the structure rearrangement mechanism
- Perform computational studies to simulate the lattice structure rearrangement

References

[1] Cao, Y., Fatemi, V., Fang, S. *et al.*, Unconventional superconductivity in magic-angle graphene superlattices. *Nature* **556**, 43–50 (2018).

[2] Cao, J. *et al.*, Realization of 2D crystalline metal nitrides via selective atomic substitution. *Sci. Adv.* **6** (2020).

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