Transfer Process with 2-Dimensional Transitional Metal Dichalcogenides Materials

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Outline

• Transitional Metal Dichalcogenides (TMD)
• Project Objective
• Vienna Ab-initio Simulation Package
• Experimental Procedures
• Process
• Raman Spectroscopy Results
• Conclusion
• Future Work
• Acknowledgments
Transitional Metal Dichalcogenides (TMD)

• Currently in research stage

• Flexible and printable that has a great potential replacing organic semiconductors and graphene

  • Graphene – poor semiconductor device material

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Objective

• To expand RIT’s knowledge on non-traditional 2D materials
• Tape transfer monolayer MoS$_2$ material from a substrate containing bulk MoS$_2$ to a blank substrate
• Able to differentiate different layers of MoS$_2$ with Raman Spectrometer
• Electrically test and characterize behavior of mono and bulk MoS$_2$ material
• To obtain a working method to extract band-gap from electrical testing
Vienna Ab-initio Simulation Package

• One of the software that uses Density Function Theory (DFT) to compute quantum problem for materials

• K-points in Brillouin zone
  • Affects with the accuracy of simulation

Vienna Ab-initio Simulation Package
MoS\textsubscript{2} Monolayer

MoS\textsubscript{2} Monolayer
van der Waal DFT
12x12x1, 400 eV cutoff

Energy (eV)

M \quad \Gamma \quad K
MoS$_2$ Bilayer

van der Waal DFT
12x12x1, 400 eV cutoff
MoS$_2$ Bandgap Comparison

MoS$_2$ Monolayer
van der Waal DFT
12x12x1, 400 eV cutoff

MoS$_2$ Bilayer
van der Waal DFT
12x12x1, 400 eV cutoff
Experimental Procedures

• A various sizes of mask designs that will be able to fit tape transferred materials
  • Smaller grid size may cause transfer materials laying on the grid pattern causing the material to warp due to the step height of silicon for level 0 marking

• An efficient way to determine mono and bulk layer material under microscope for Raman Spectrometer inspection

• Observe the different behavior properties between mono and bulk layer material after being fabricated into resistors
Process Flow

- Grow 3000Å Oxide on second substrate

1. Substrate 1
   - MoS₂
   - Kapton Tape

2. Substrate 2
   - MoS₂
   - Tape
   - MoS₂
   - Kapton Tape

3. Substrate 2
   - Oxide

4. Substrate 2
   - Tape
   - Oxide

5. Substrate 2
   - MoS₂
   - Aluminum Oxide

6. Substrate 2
   - MoS₂
   - Aluminum Oxide

7. Substrate 2
   - Oxide
Tape Transfer Process
Raman Spectrometer

• Provide molecular vibrations and crystal structures
• Laser wavelength used for Raman Spectroscopy is 633nm
• Each material has its own unique fingerprint pattern that serves as its identification
Visual Inspection
Raman Spectroscopy – Raman Inspection Setup

40.38µm

55.92µm
Raman Spectroscopy – Raman Inspection Setup

12.22µm

20.38µm

12.22µm
Raman Spectroscopy – Sample Data Collection
Raman Spectroscopy – Sample Data Collection
Conclusion

• The tape transfer result were proved to be promising. Achieving for a bi-layer transfer is possible and a mono-layer exfoliation is also feasible but with restriction on the inspection tool, a mono-layer transfer can only be assumed by visual inspection.

• Simulation result agrees with theoretical understanding on the material

• Expecting high peaks for Raman Spectroscopy results ranging between 383 and 404 cm\(^{-1}\) for monolayer MoS\(_2\)

• Expecting bandgap result to be between 1.2eV to 1.9eV depends on how many atomic layers
Future Work

• A method that can confirm the mono-layer MoS2 transfer
• To build a mono layer MoS$_2$ device at RIT
  • Conduct electrical testing for its material and electrical properties to confirm and further improve simulation results
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