Exploration and Improvement of Material Analysis Technique Using Auger Electron Diffraction (AED)

Team members: Eve Wang, Daniel Lee, Hiro Chou, Wei-wei Yang

Research Motivation

- In freshman year, we learned about the concept of **wave–particle duality**, which describes how electrons are not only particles but can also behave like waves, producing interference and diffraction. We wondered: *Is it possible to directly observe the wave nature of electrons?*

- We discovered that **electron diffraction techniques** are used in material analysis to observe this phenomenon. Our goal was to perform an experiment to see whether we could detect electron wave behavior ourselves.

- To observe diffraction patterns, we first needed a material thin enough for electrons to penetrate. We chose a widely used **two-dimensional material—molybdenum disulfide (MoS_2)**—and began by studying how to prepare high-quality samples.

Research Objectives

1. Prepare two-dimensional material samples suitable for analysis.
2. Conduct complete material analysis using **AED (Auger Electron Diffraction)**.
3. Build a **Python simulation model**.
4. Compare the simulated results with experimental data to verify the wave nature of electrons.

Research Methods

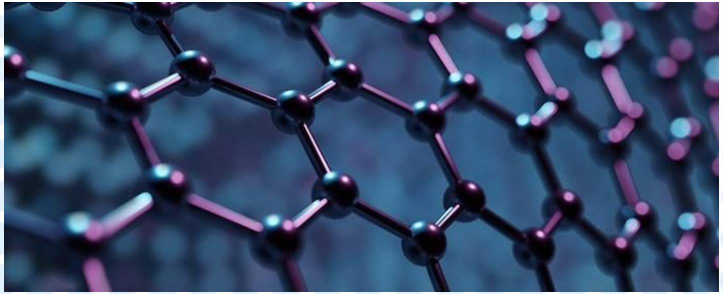
1. **Sample Preparation** – MoS_2 layers were exfoliated using **UV tape**.

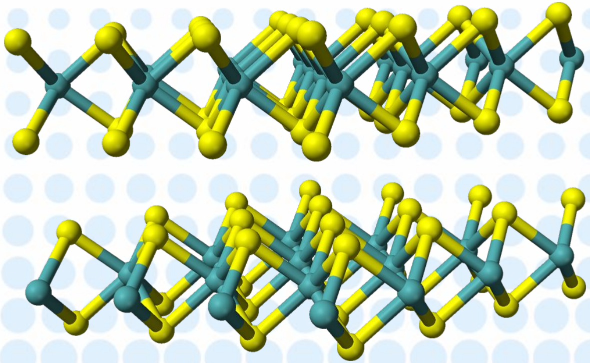
2. **Experimental Analysis** – We conducted **AES/AED** experiments for energy spectrum and diffraction analysis.

3. **Computational Simulation** – A **Python program** was developed to simulate interference and diffraction patterns.

材料準備
UV-Tape → 儀器操作
AES/AED → 數據分析
能譜圖+圖像 → 程式模擬
Python模擬干涉 → 比對驗證

Choice of Two-Dimensional Materials



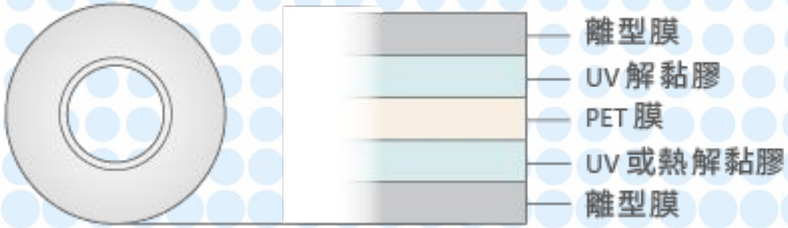


Graphene

Molybdenum Disulfide(MoS_2)

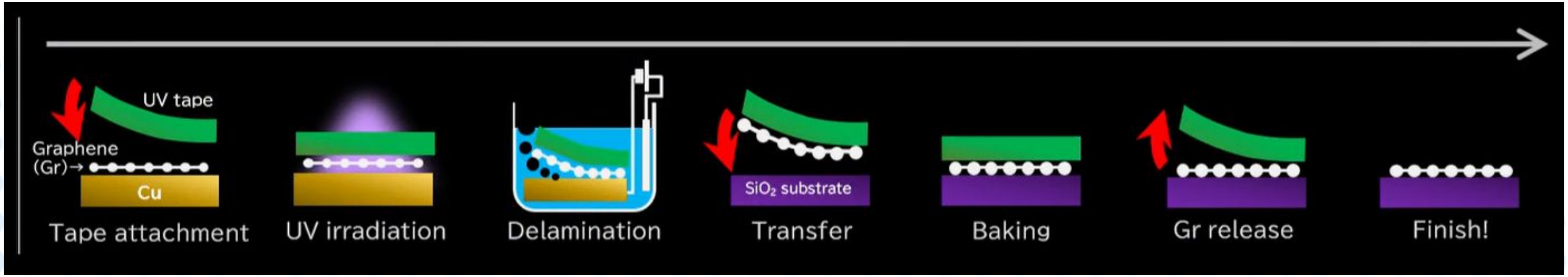
How to Obtain Monolayer MoS_2?

Regular tape

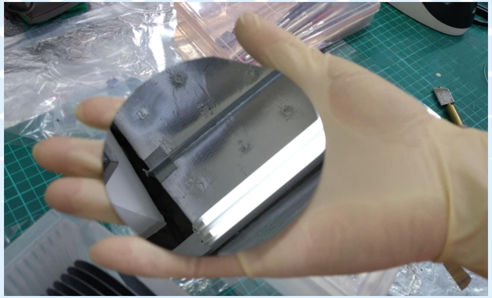


UV Tape Detackified tape

MoS_2 Sample Preparation



Monolayer MoS_2 Exfoliation Process (Using UV Tape)

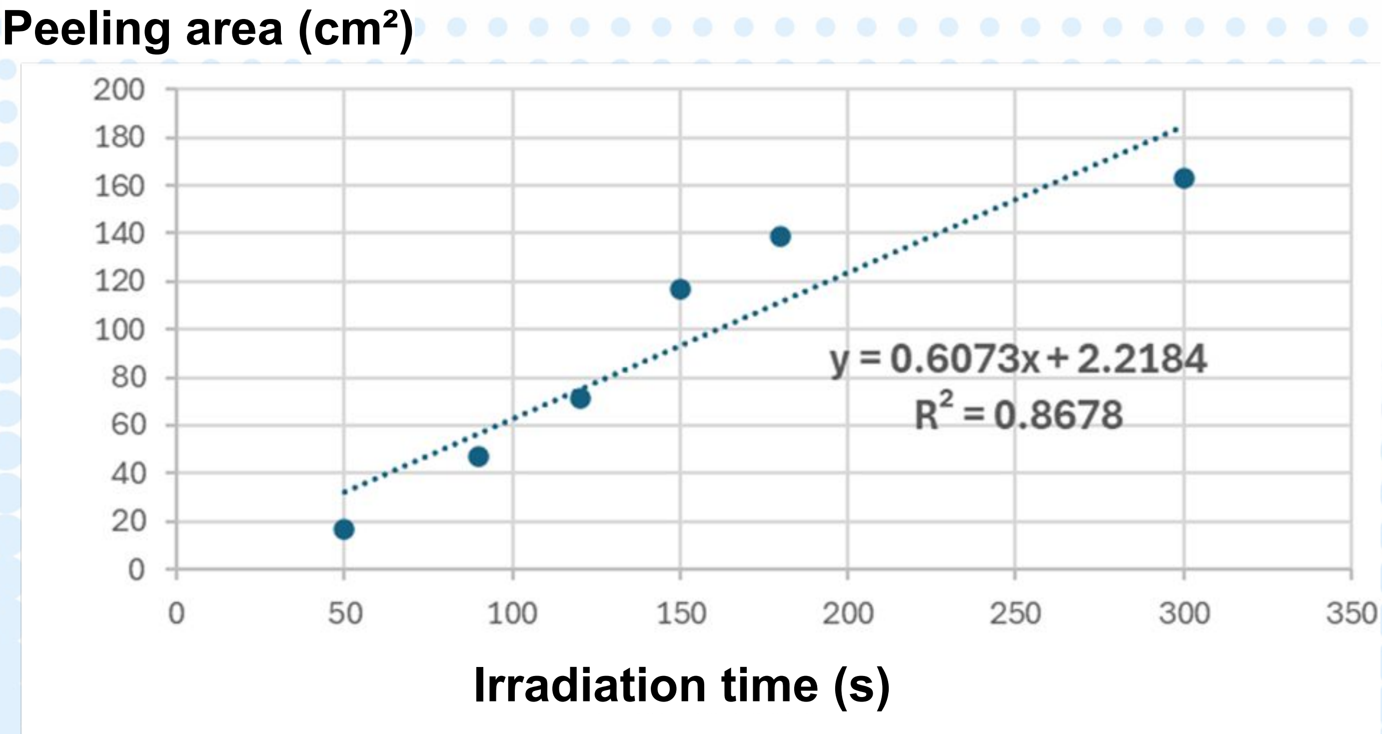


Base substrate: SiO_2 wafer

MoS_2 flakes

UV light

Experimental variables



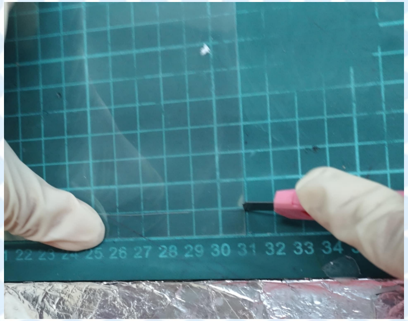
Process of exfoliating MoS_2 using UV tape

Cutting Silicon

Washing Silicon

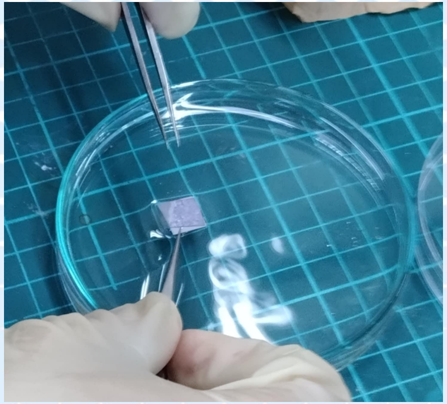
Repeat Taping MoS_2

Counter-Sticking



Taping with UV-Tape

Process of exfoliating MoS_2 using UV tape



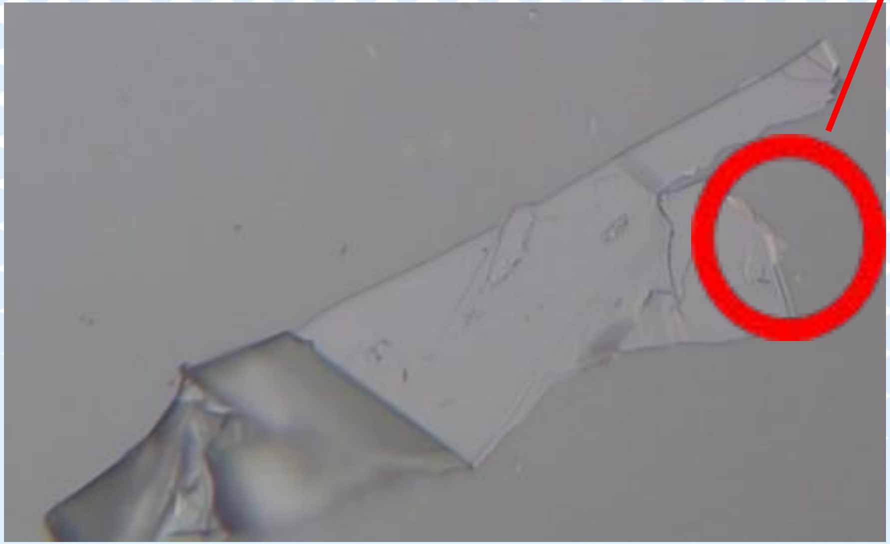
Transfer to Silicon

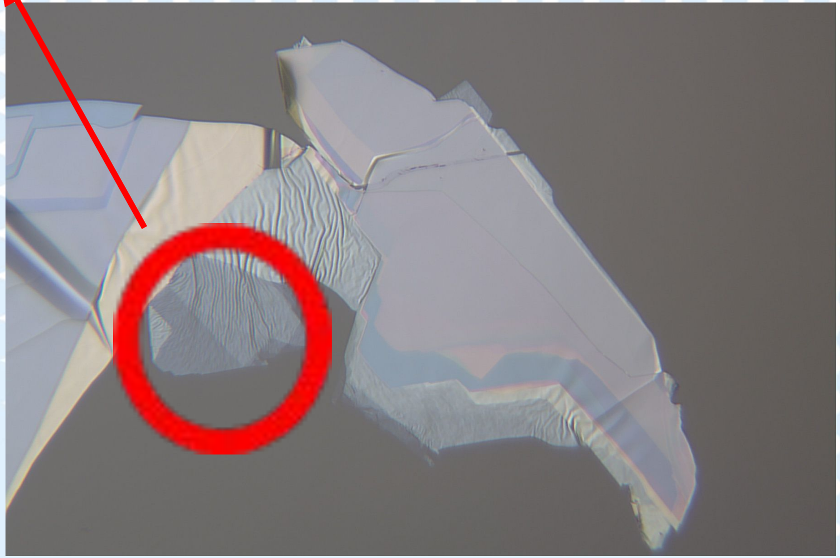
Irradiate with UV-Light

Observing with OM

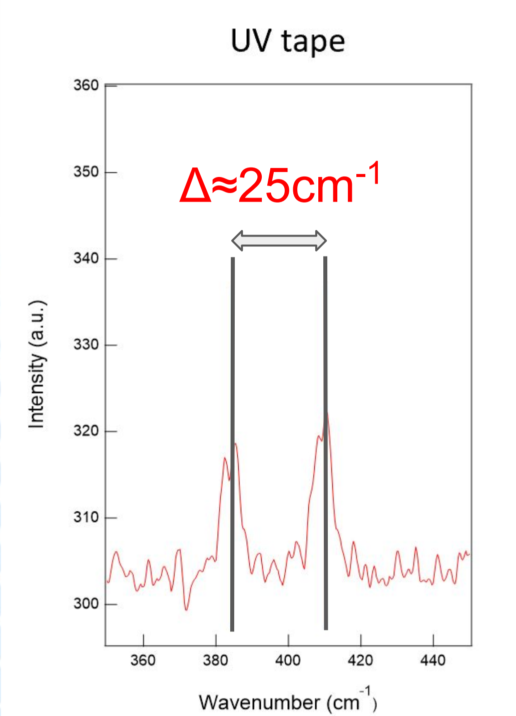
Experimental Result

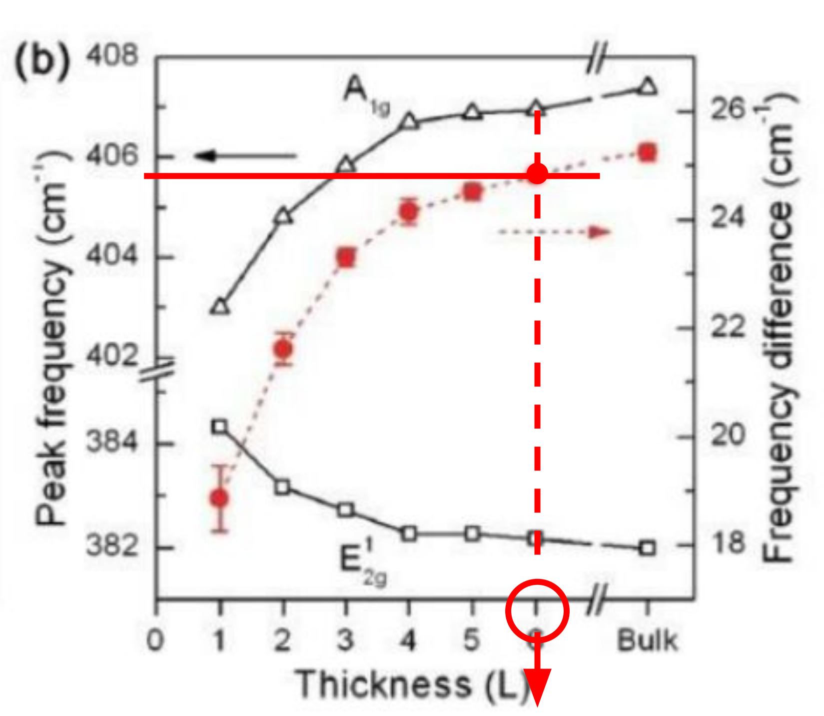
Monolayer MoS_2





How to confirm a monolayer?



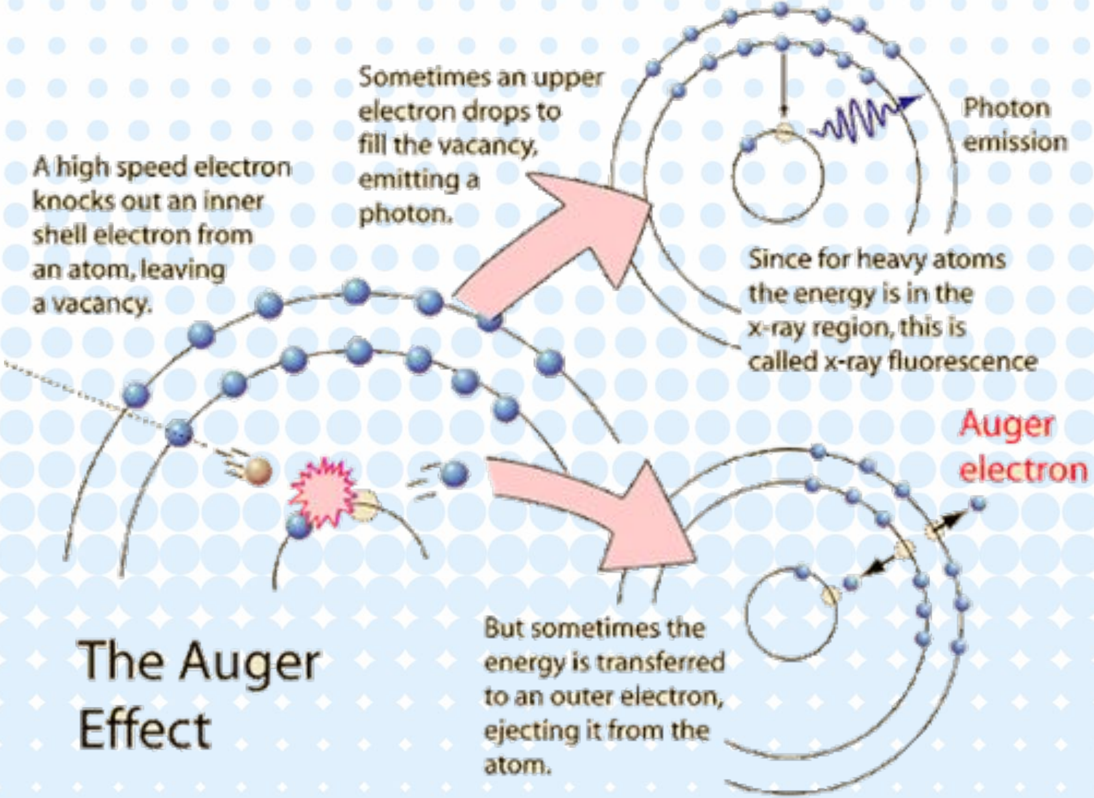


Raman spectroscopy data

Multilayer

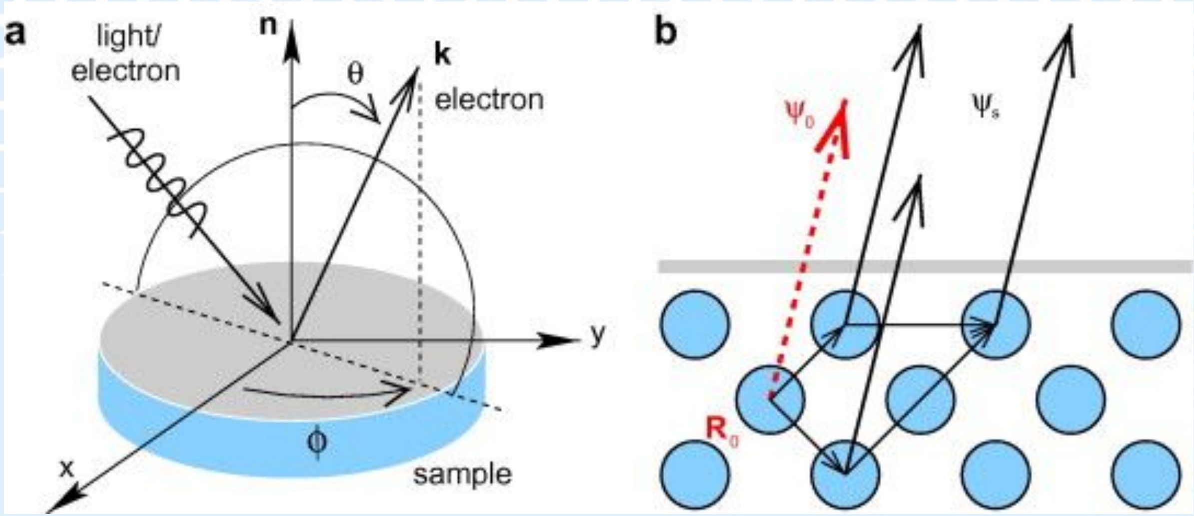
What is AES? Auger Electron Spectroscopy

- **Auger Effect**
- By measuring the energy distribution of Auger electrons, one can determine the elements and their quantities present on the surface of a sample.



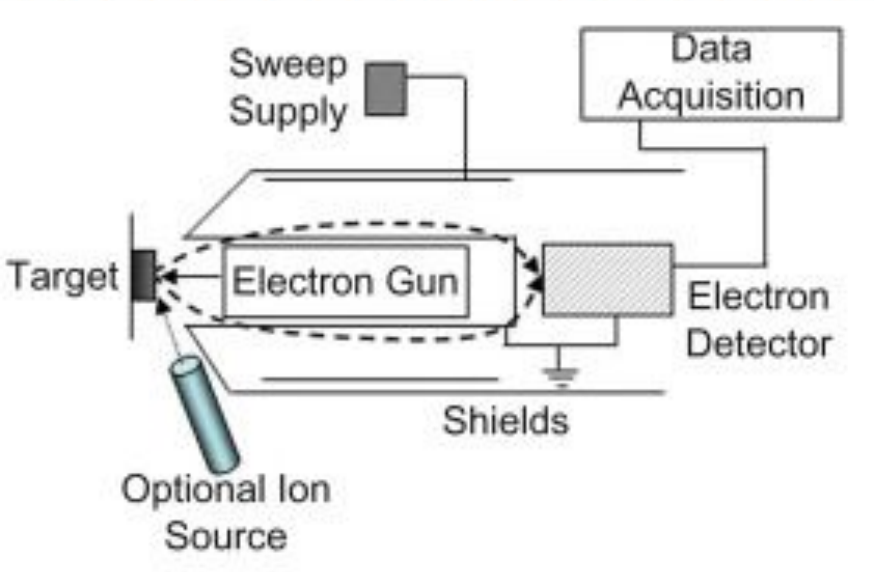
What is AED? Auger Electron Diffraction

- In addition to measuring the energy distribution of Auger electrons, AED observes the interference and diffraction patterns produced by these electrons.
- Since Auger electrons emitted in different directions generate different patterns, AED can be used to determine the atomic arrangement on a material's surface.



Structure of the AES

- Electron gun
- Vacuum system
- Energy analyzer
- Detector (DLD + MCP)
- Ion sputtering gun

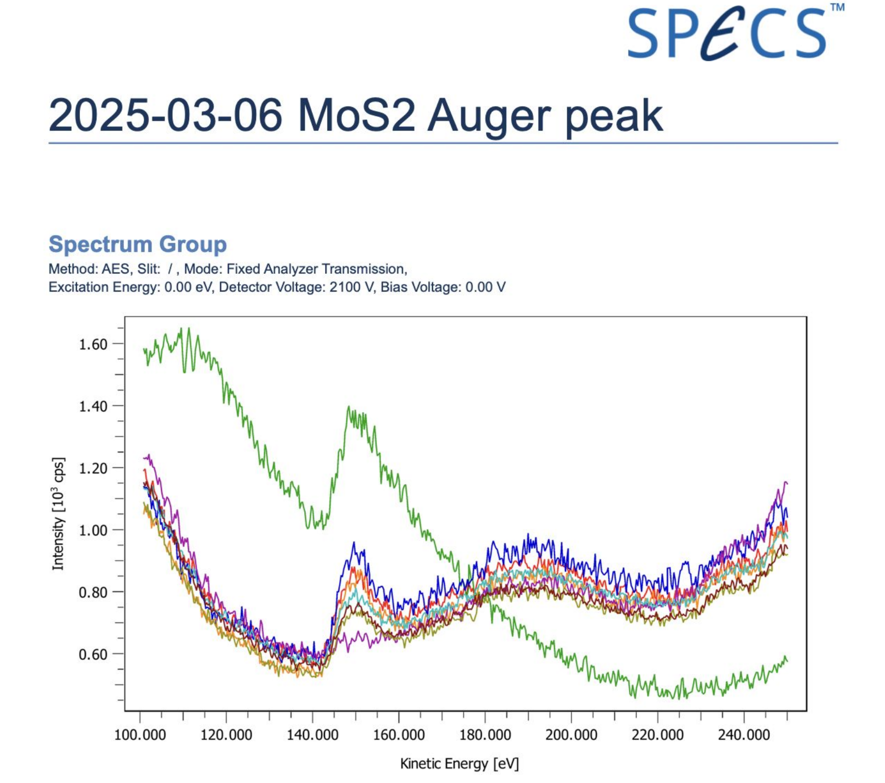


Introduction to AED/AES Material Analysis Techniques

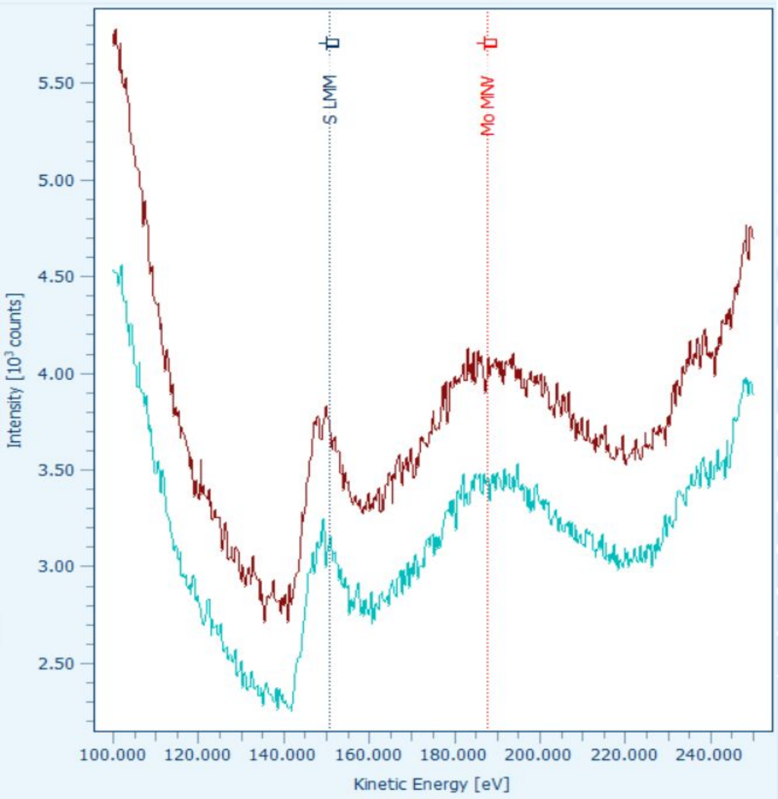
Spectrum:

(1) The x-axis represents **kinetic energy**, and the y-axis represents **intensity**.

(2) Each Auger peak corresponds to the **Auger electron energy** of a different element.

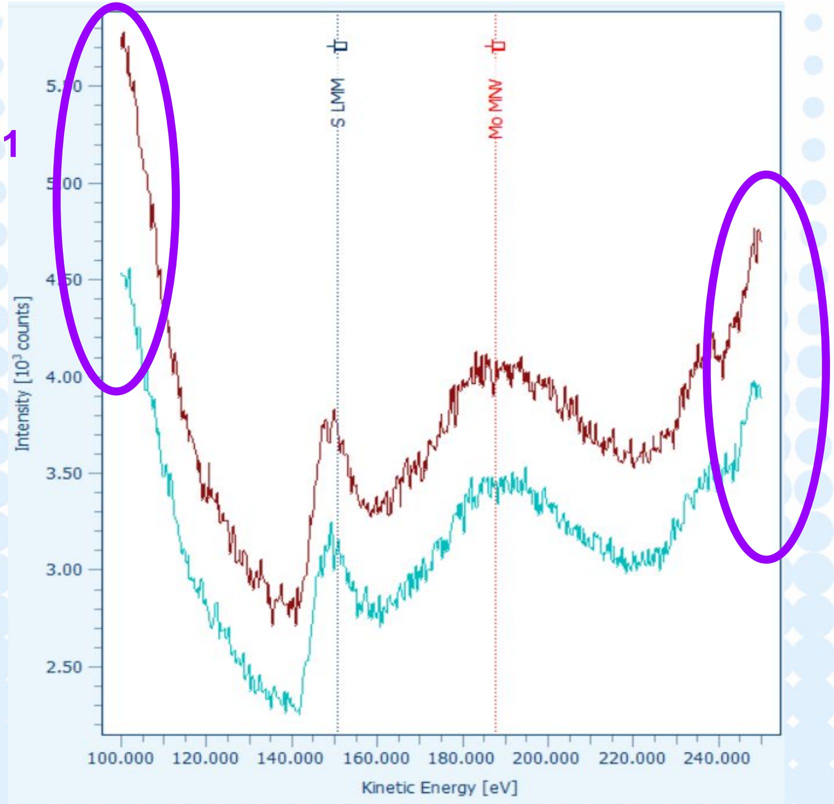


Introduction to AED/AES Material Analysis Techniques



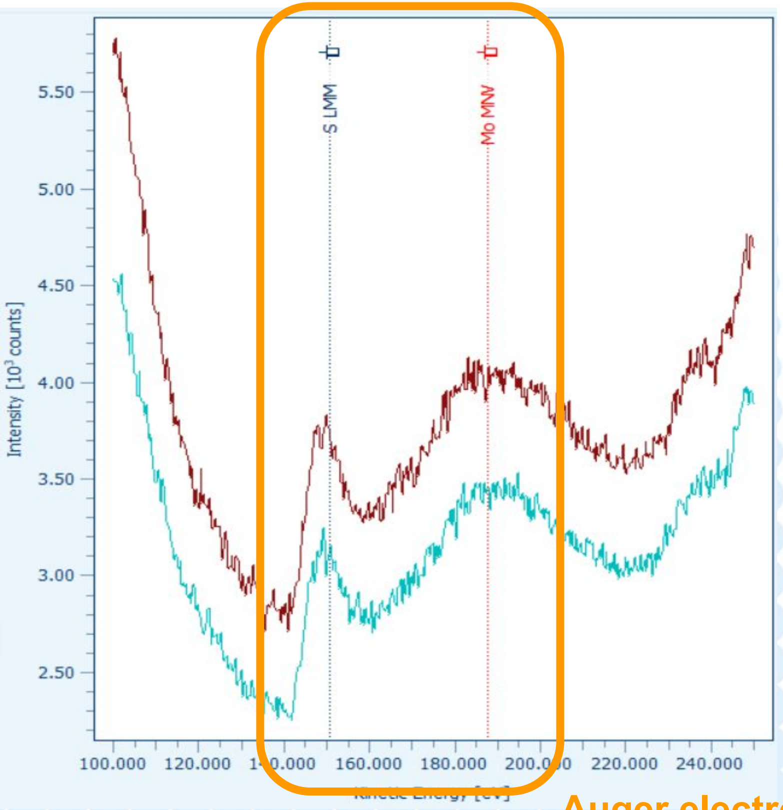
Introduction to AED/AES Material Analysis Techniques

Photoelectron energy — Shell 1



Photoelectron energy — Shell 2

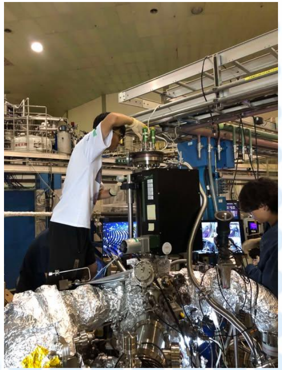
Introduction to AED/AES Material Analysis Techniques

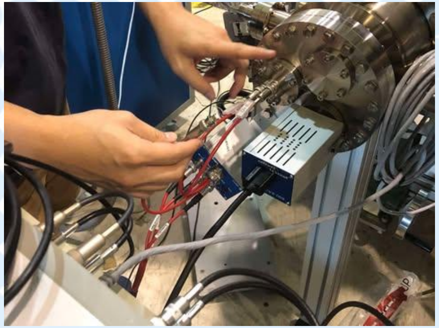


Auger electron energy

Challenges: Instrument Malfunction and Repair

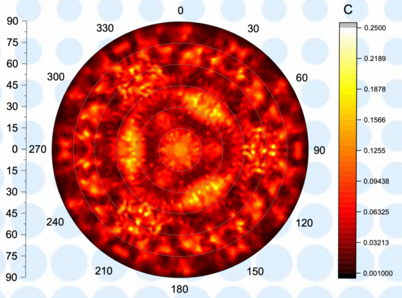
- *Time-of-flight* function failure
- Checked control panel and reconnected circuits
- Replaced damaged copper sample tube
- Restored the instrument to a vacuum environment (repeated nitrogen purging and pumping)



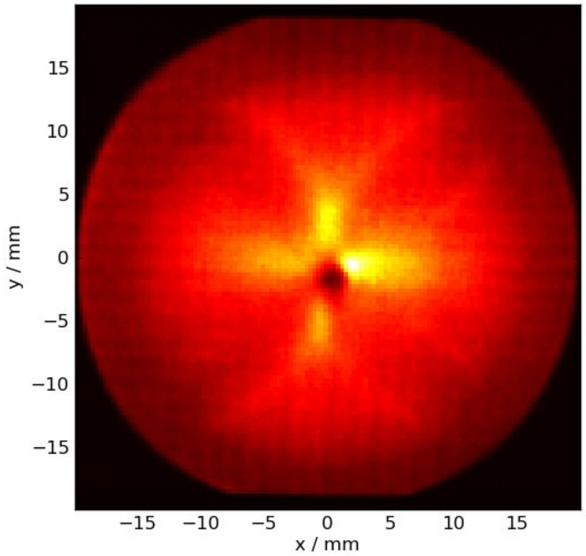


AED Diffraction Patterns Obtained from Experiment

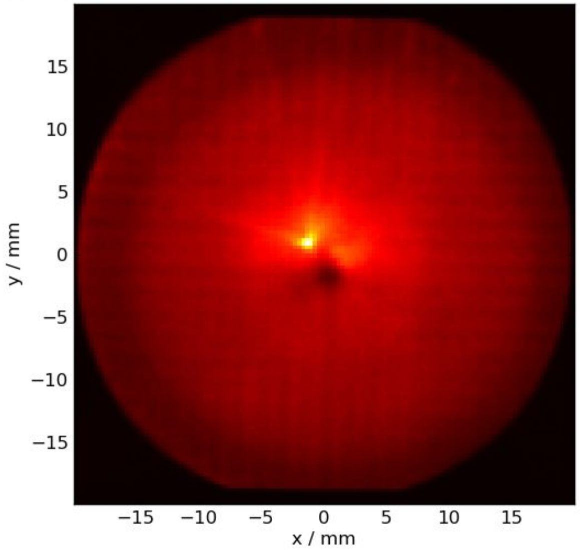
- Difficult to focus; diffraction patterns were unclear



Simulated Diffraction Pattern (CoO)



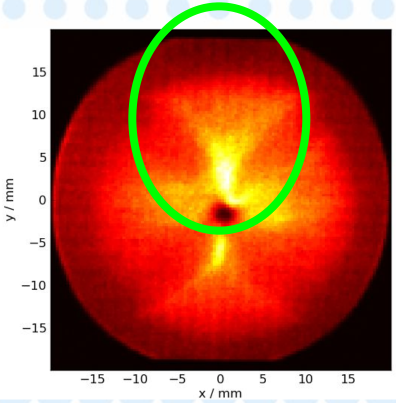
Early-stage diffraction pattern



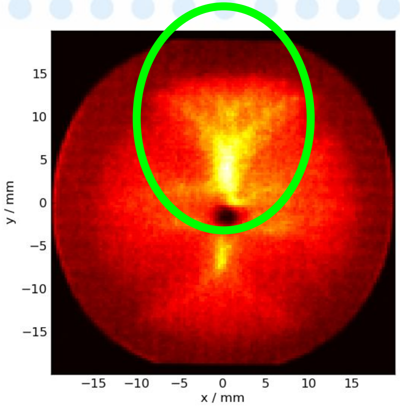
Late-stage diffraction pattern
(Instrument declared out of order)

AED Diffraction Patterns Obtained from Experiment

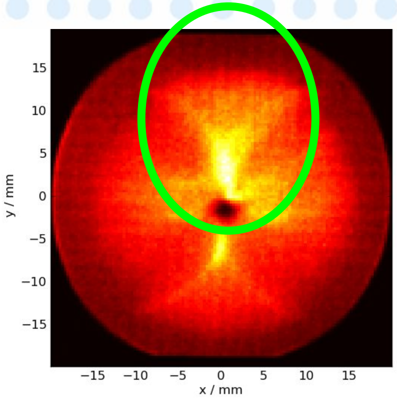
- At certain angles, differences can still be observed, indicating that the material has a specific directional arrangement.



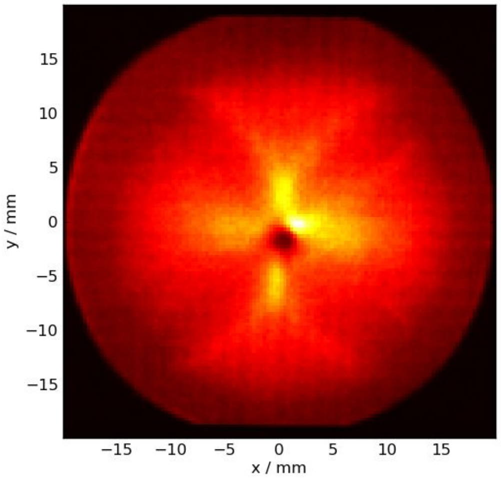
45°



225°



315°



0° (and most other angles)

Program simulation & tools

Category	Name	Purpose
Integrated development environment IDE	Spyder	Integrated development environment for codi-ng and simulation
Programming language	Python	Write code
Package	ASE	Build molecular and crystal structures
Package	MsSpec	Simulate electron or electron diffraction p-atterns
Package	Matplotlib/NumPy	Create interference figures, perform nu-merical calculations

Build atomic model and lattice structure

Simulations completed using the Atomic Simulation Environment (ASE) package

簡單氣體模型
如 H_2、O_2、CO_2

→

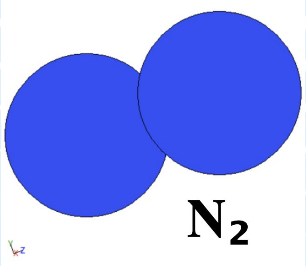
金屬固體模型
如 Cu、Al

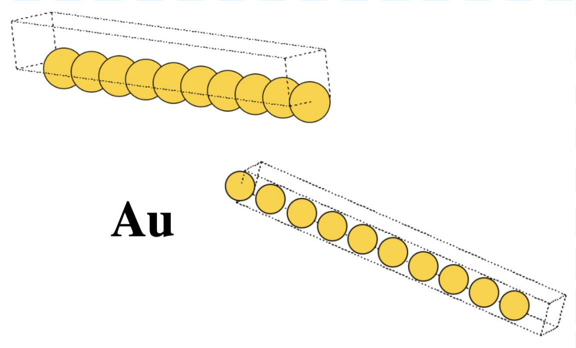
→

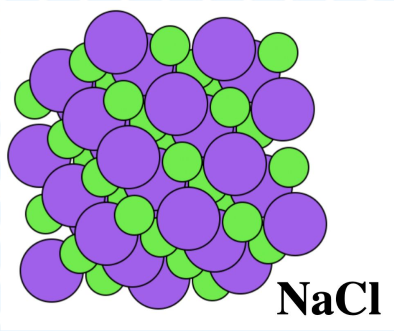
鹽類晶格模型
如 NaCl、MgO

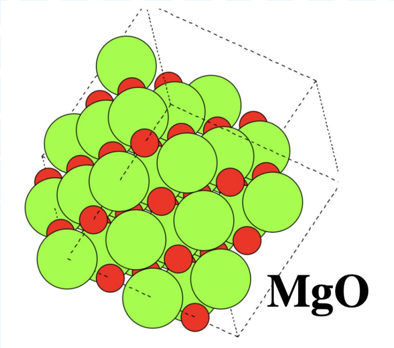
→

二硫化鉬模型
MoS_2過度金屬二硫族化合物



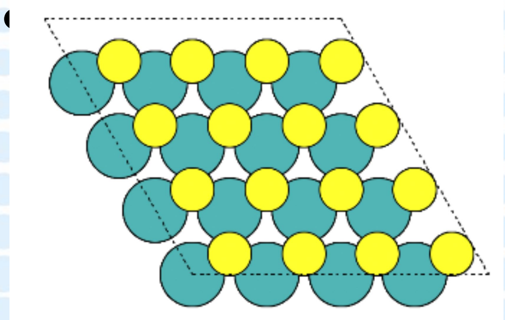


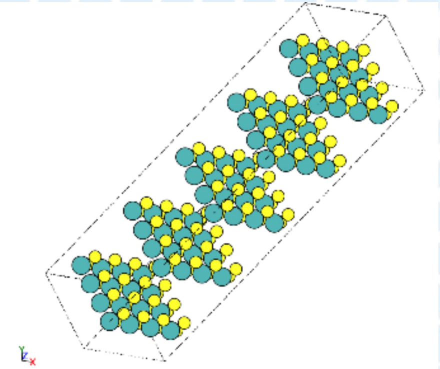




Construct the MoS_2 model and verify the bond length

- Use the Bravais lattice framework + ASE's mx2() function
- Simulate 2H-phase MoS_2 with a diameter of 25 Å



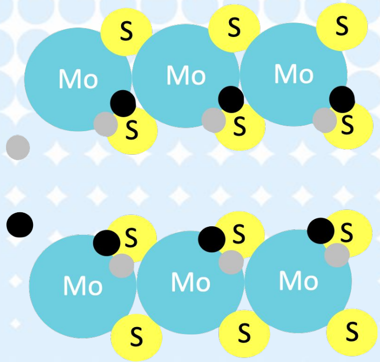


Calculate the average Mo–S bond length to validate the simulation accuracy:

Theoretical value – 2.4219 Å

Calculated result – 2.4266 Å

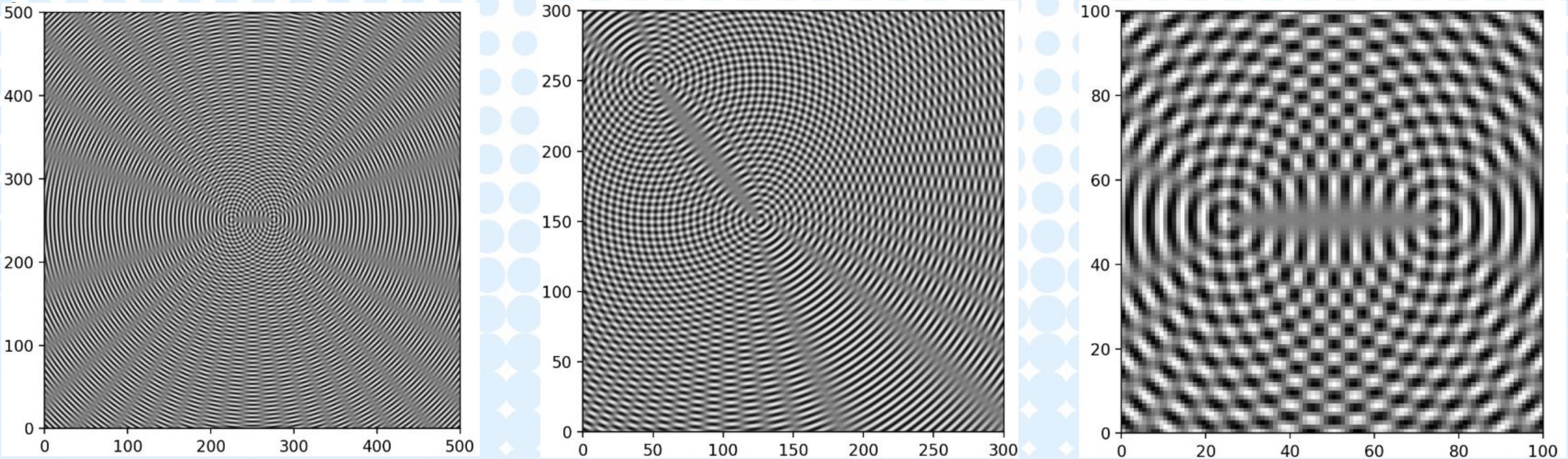
Van De Waals bonds



MoS_2 Python model

Simulating electron-wave interference and double-slit diffraction

- Simulate the superposition and cancellation of two wave sources in a 2D plane, and compute the total field value of the two sources on the plane.
- Use the imaging function imshow() with grayscale to display bright and dark fringes:



Simulated image of two-wave interference

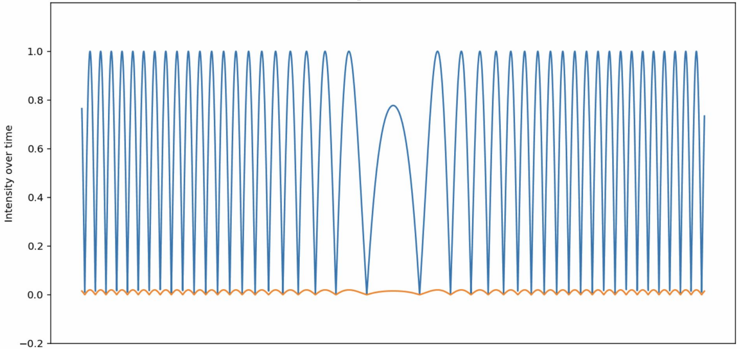
(adjusting source positions, resolution, and source spacing).

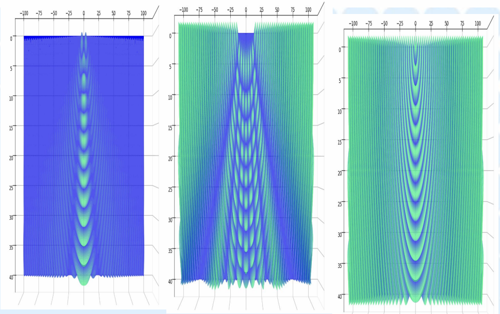
Simulating electron-wave interference and double-slit diffraction

To simulate more complex wave states and compute the total field value, the waves are divided into four types:

類別	名稱(程式函數)	說明
1	single_wave	單一波源的波動傳播
2	single_slit_diffraction	單狹縫繞射
3	double_slit_no_diffraction	雙狹縫干涉但無繞射
4	double_slit_diffraction	雙狹縫干涉 + 繞射

Simulation of multiple-wave interference.



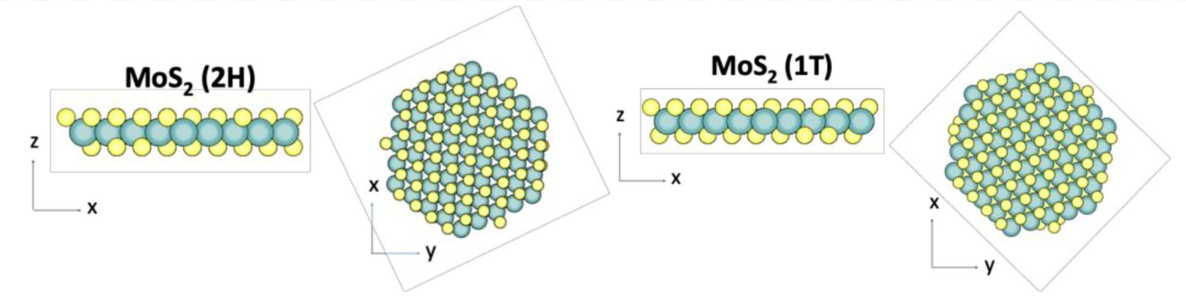


Generate GIF images via matplotlib.animation.

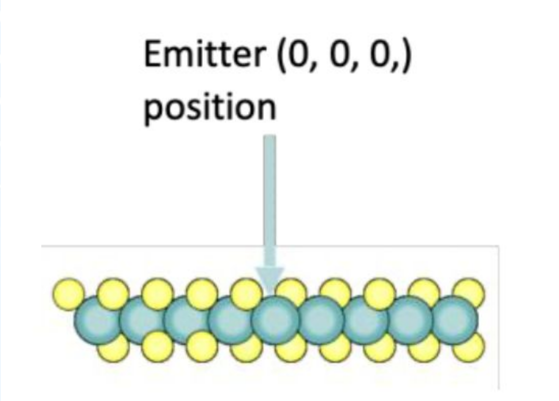
MsSpec diffraction simulation: PED instead of AED

Using the MsSpec package, the Single Scattering Cluster (SSC) model is applied to simulate the spherical diffraction pattern of monolayer MoS_2.

MsSpec1.0 Package



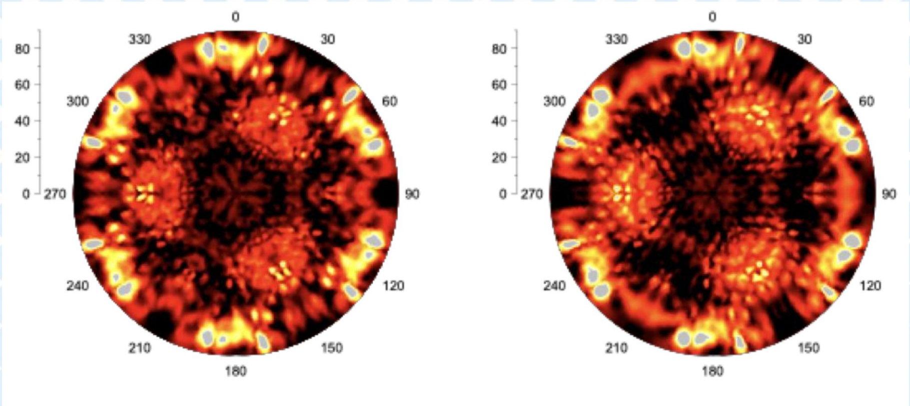
Lattice simulation of the 2H and 1T phases



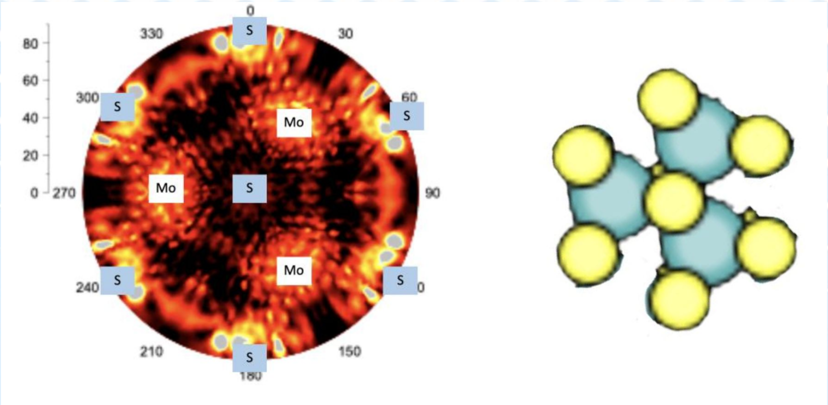
Schematic of incident electromagnetic-wave simulation (modeled with the 2H phase)

Simulation Results

Using the hemispherical_cluster() function in the MsSpec package, a hemispherical atomic arrangement model was employed to predict diffraction patterns in all directions, simulating the diffraction of high-energy electromagnetic waves on a monolayer of molybdenum disulfide (MoS_2).



The **left image** shows the simulated diffraction pattern of MoS_2 in the **2H phase**, while the **right image** corresponds to the **1T phase**.



Elemental structures corresponding to the MoS_2 diffraction patterns

Conclusion

Achieved

- Successfully simulated atomic structures and electron interference/diffraction models using Python.

To Be Completed

- Prepare material samples suitable for analysis (large-area, flat surfaces).
- Conduct a full AED material analysis using the prepared samples.
- Compare experimental data with simulated results.

Future Outlook

Improving Sample Materials

- Develop self-made UV tape and adjust its composition ratio.
- Replace the material with strontium calcium copper oxide (SrCaCuO).

Repeated Experimental Verification

- After instrument repair, repeat AES/AED experiments multiple times to collect more data.
- Verify the accuracy of experimental data through computational modeling.
- Integrate AI-assisted analysis to improve AED data recognition efficiency.
- Apply the technique to broader material analysis in the future.

Conclusion & Acknowledgments

This research combined theory, experimentation, and simulation to deeply explore the applications of quantum physics. Although we encountered many difficulties and challenges throughout the process, these experiences allowed us to truly understand the obstacles that real scientists often face in their work.

During this project, we received valuable guidance from professors at the National Synchrotron Radiation Research Center, who also provided us with opportunities to access advanced experimental instruments.

We would like to express our special thanks to Senior Student Liao Ze-Ming, who patiently assisted and instructed us in every experiment. His mentorship greatly enhanced our understanding of quantum physics and deepened our passion for the subject.

Thanks for listening!