# Preparation of an Optical Microscopy Dataset for Machine Learning–Based Detection of Two-Dimensional Material Flakes

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## Abstract

Building on recent advances in machine learning for automated two-dimensional (2D) material identification, optical microscopy was used to identify suitable fragments of transition metal dichalcogenides (TMDs) for use in training the machine learning framework developed by Uslu et al. to autonomously detect similar 2D material flakes. High-quality optical micrographs were collected and manually annotated to generate a representative training dataset spanning a range of flake sizes, shapes, and optical contrasts. These labeled data were used to adapt the pre-trained foundation model to our experimental imaging conditions, enabling reliable identification of 2D material flakes with minimal additional training data. By leveraging transfer learning from a model trained on synthetic microscopy images, this approach reduces the manual effort traditionally required for flake identification while maintaining high detection accuracy. The resulting workflow provides a scalable method for automated characterization of exfoliated 2D material samples and represents a step toward high-throughput material discovery and device fabrication.

## Introduction

Properties of 2D Materials and TMDs

Two-dimensional (2D) materials and transition metal dichalcogenides (TMDs) have recently attracted great interest due to their material properties. Taking graphene for example, it has an unparalleled tensile strength and Young's modulus, and an excellent electrical and thermal conductivity. 2D materials in general exhibit strong light–matter interactions, tunable band structures, and exceptional mechanical properties. These properties make 2D materials prime candidates for applications in optoelectronics, nanoelectronics, and even excitonic devices.

Detection of 2D Materials and TMDs

Fabrication of these devices usually involve mechanical exfoliation, producing flakes of varying sizes that must be identified and characterized before device fabrication. Optical microscopy has been the most common technique used for locating suitable flakes because it doesn't alter the fragile material.

MaskTerial

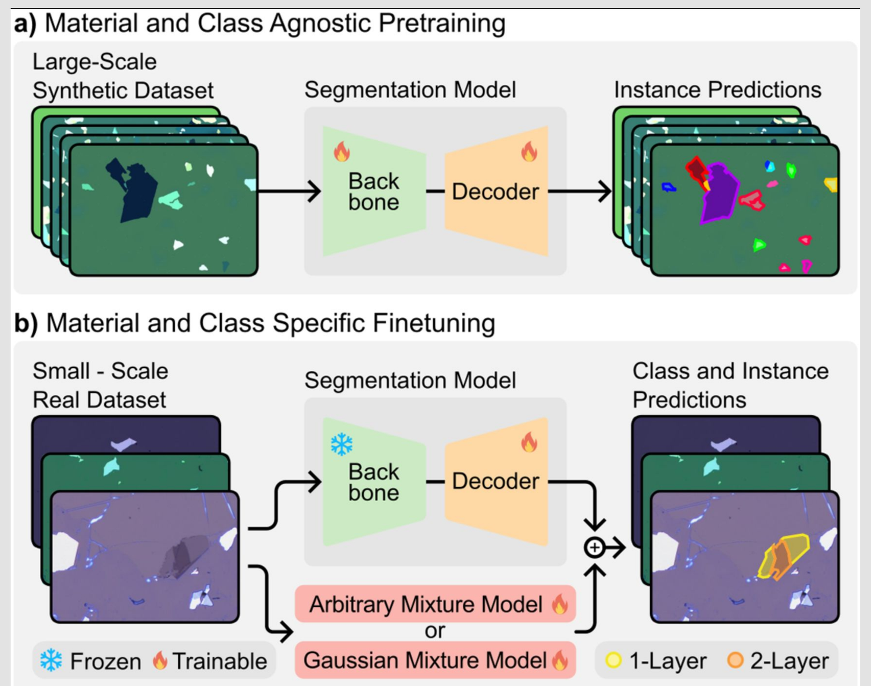
A recent framework named "MaskTerial" developed by Uslu et al.[1] combines synthetic pre-training with transfer learning to accurately detect 2D material flakes using labeled experimental images. This model helps automate and speed up the slow and monotonous process of flake detection done by humans. In this project, optical microscopy was used to identify and annotate suitable TMD flakes for training the MaskTerial model under our laboratory imaging conditions. This work contributes toward an automated workflow for quick and reliable detection of exfoliated 2D materials.

## Methodology

The inference system uses a two-stage search framework. The first stage is a segmentation model pre-trained on millions of synthetic images and fine-tuned using tens of images of specific materials. It identifies regions that may contain flakes.

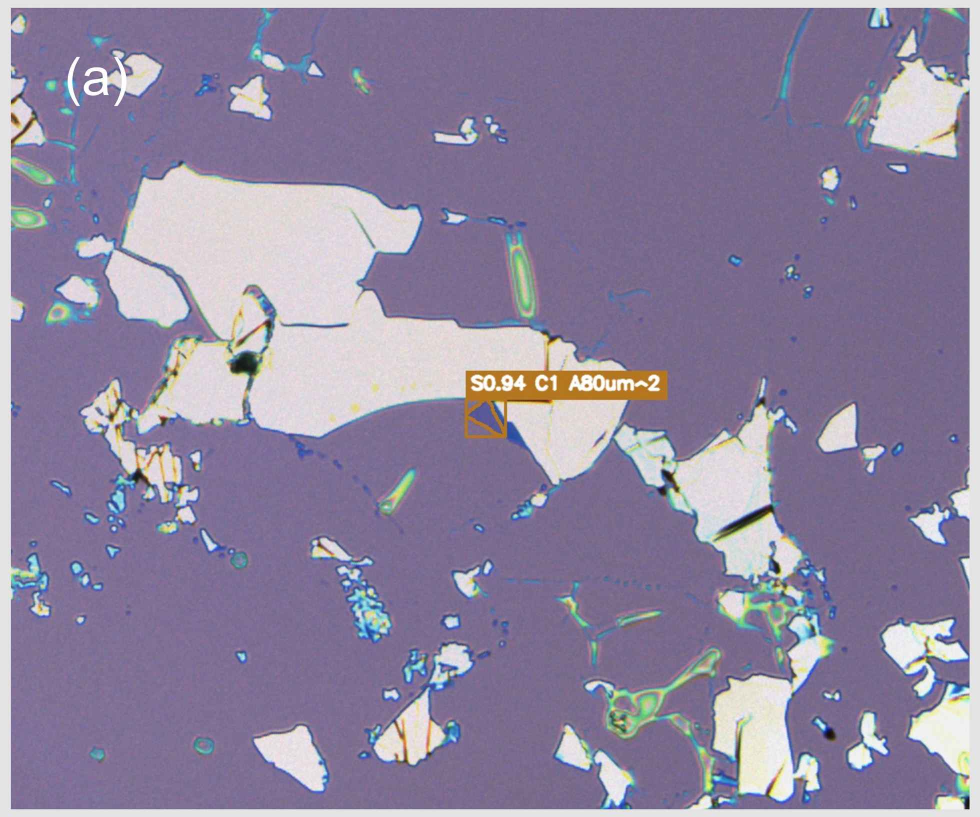
The second stage uses an arbitrary mixture model (AMM) to determine the number of layers in each detected region based on its optical contrast. Together, the two models determine whether flakes are present in an image and, when flakes are detected, report their positions, layer numbers, and areas.

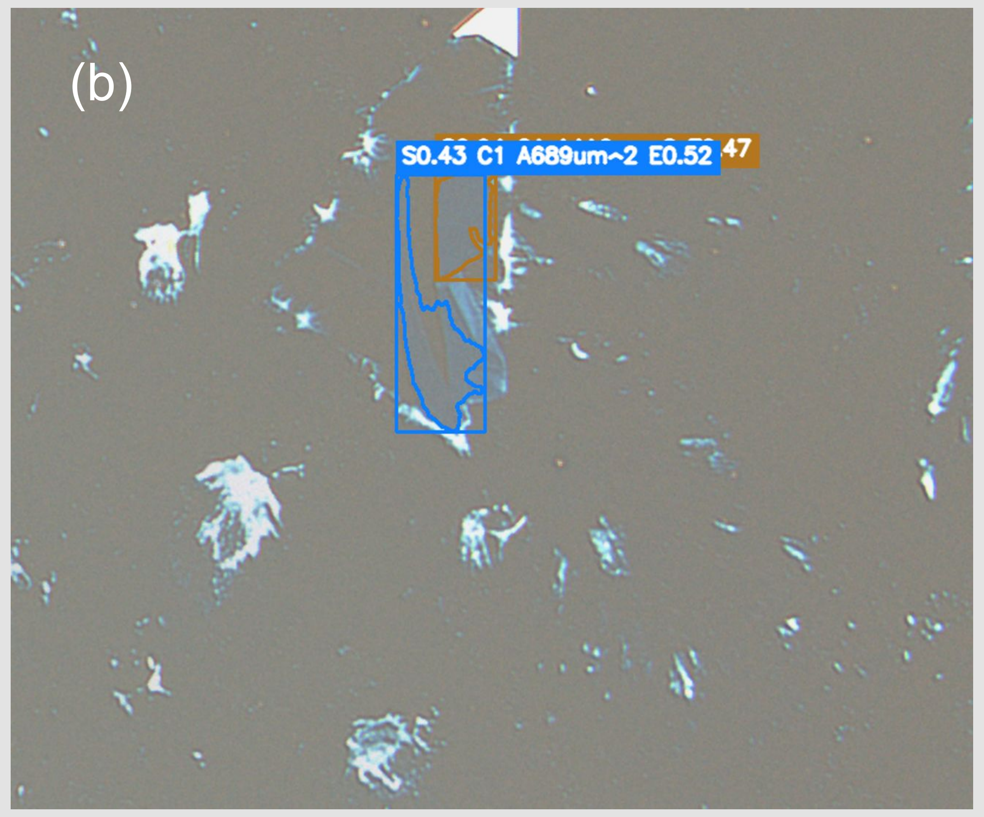
We integrated the inference system with a motorized scanning stage and an optical microscope. The complete platform can automatically scan multiple wafers, analyze the acquired image tiles, and report the locations and properties of the detected flakes.




## Results

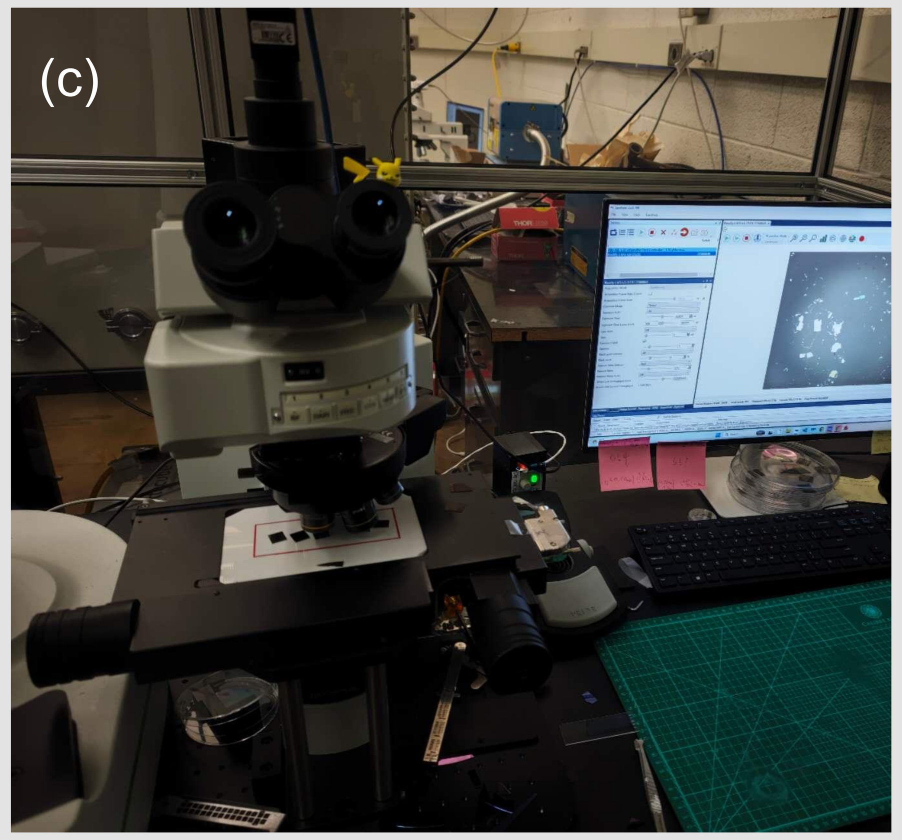
We fine-tuned the segmentation model and trained AMM model in the inference system by at least 30 images. It's now able to detect multiple kinds of materials such as tungsten diselenide ($WSe_2$), tungsten disulfide ($WS_2$) and hexagonal boron nitride (hBN).




Figures (a) and (b): Detection results from the inference system.
(a) A detected monolayer $WSe_2$ flake. (b) Two detected thin hBN flakes. The confidence score, area, and layer number are annotated in each bounding box.

Figure (c): Experimental setup of the automated scanning system.
An XY translation stage is installed beneath the microscope, while the microscope focus is controlled by a motorized Z stage. Images are captured by a camera mounted on top of the microscope. After the wafers are placed on the stage, the system automatically scans each wafer and captures an image of every tile. The acquired images are then sent to the inference system for flake detection and analysis.

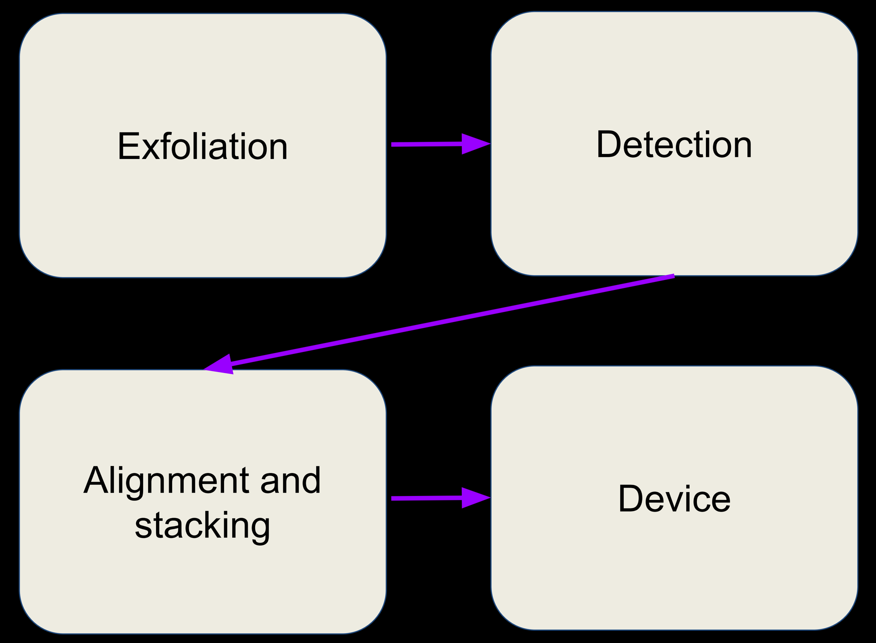



## Future Goals

Future work will focus on expanding the training database to include a wider range of materials, substrates, layer numbers, illumination conditions, and imaging systems. A larger and more diverse dataset will improve the model's accuracy, robustness, and ability to generalize to new samples.

The automated flake-detection platform developed in this work represents the first step toward a fully automated device-fabrication workflow. The next stages will involve integrating an automated exfoliation robot for sample preparation and an automated stacking system for identifying, aligning, and assembling selected flakes.

Ultimately, these components will be combined into a unified platform capable of performing material preparation, flake detection, selection, and heterostructure assembly with minimal human intervention.




## References

1. Jan-Lucas Uslu, Alexey Nekrasov, Alexander Hermans, Bernd Beschoten, Bastian Leibe, Lutz Waldecker, Christoph Stampfer; MaskTerial: a foundation model for automated 2D material flake detection. Digital Discovery 2025; 4 (12): 3744–3752. https://doi.org/10.1039/d5dd00156k

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