Automated Image Analysis of exfoliated van der Waals material

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Abstract

Van der Waals materials, like graphene or transition metal dichalcogenides, are very promising for the field of spintronics due to their unique properties. Fabricating devices from these materials requires isolating well defined flakes, a process typically done manually via scotch tape exfoliation and microscopy. This approach is labor-intensive and limited in scope. We introduce a software tool that automates flake identification from microscope images, allowing for rapid and accurate analysis of larger areas. This advancement streamlines the fabrication process and supports the development of high-performance spintronic devices.

Keywords: Software Automatization, Python, Van der Waals Materials, $TaRhTe_4$, Device Fabrication

Introduction

Van der Waals (vdW) materials, consisting of atomically thin layers held together by weak van der Waals forces, have become central to advancements in spintronics and other emerging technologies due to their exceptional electronic, optical, and mechanical properties. These materials, including graphene, transition metal dichalcogenides, or hexagonal boron nitride, are particularly promising for spintronics, which leverages electron spin in addition to charge to enable faster and more efficient information processing [1].

A key challenge in fabricating devices from these materials is the isolation of a well defined, thin flakes from bulk crystals. The widely used scotch tape exfoliation method, shown in Figure 1, involves applying adhesive tape to a bulk vdW crystal and then peeling it away to transfer thin layers onto a silicon substrate [2]. These layers are subsequently characterized and processed to create functional devices [3]. The process of making electrical contacts to these flakes is crucial, whether for measuring fundamental properties or integrating them into functional devices, such as transistors. This step is complex and requires precision identifying a suitable flake which is sufficiently isolated to provide sufficient space for the lithographic processing.

Currently, the selection of suitable flakes for device fabrication is a labor-, and time-intensive task. Researchers manually examine microscope images to determine flake size, thickness, and morphology, which limits the scope and efficiency of the process. To address this, we present a software tool that automates the identification of vdW flakes from microscope images. This tool significantly speeds up the analysis and allows for the examination of much larger substrate areas. Our software enhances the flake selection process, which is particularly beneficial for working with materials known for their unique electronic properties.

In this work, we test our approach on a vdW compound that hosts type II Weyl nodes—topological features that offer promising electronic properties [4, 5]. By improving the efficiency of flake selection, our tool supports the advancement of devices utilizing these unique materials, facilitating both fundamental characterization and the development of functional spintronic devices.

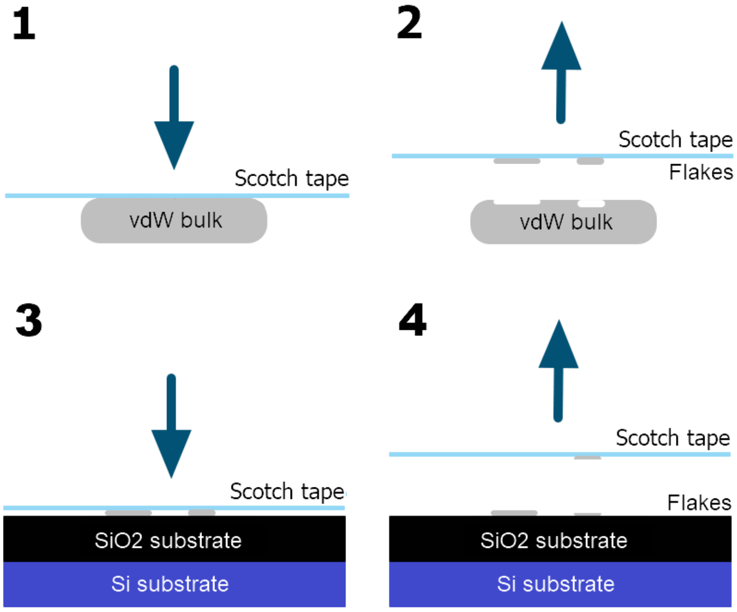


Figure 1: Scotch tape exfoliation of thin van der Waals (vdW) flakes onto a thermally oxidized silicon (Si) substrate. The process is illustrated in four steps: 1) Applying scotch tape to a bulk vdW crystal. 2) Removing the tape with attached flakes. 3) Transferring the flakes onto the substrate. 4) Carefully peeling off the tape to release the flakes.

Test Material for Flake Identification

To test our software, we use exfoliated flakes of $TaRhTe_4$, a low-energy topological material known for its four type-II Weyl nodes when in thin-layer form. Raman spectroscopy has confirmed the presence of Weyl fermions in this material, indicated by the absence of inverse symmetry. These fermions disrupt Lorentz covariance in type-II Weyl semimetals [6].

The $TaRhTe_4$ bulk is grown from tellurium (Te) flux and provided by collaborators at the Leibniz Institute for Solid State and Materials Research - IFW Dresden, Germany. The synthesis involves heating a mixture of tantalum (Ta), rhodium (Rh), and tellurium powders to 1000 °C and then cooling it to 700 °C [7]. The crystal structure, detailed in Figure 2, belongs to the orthorhombic $Pmn2_1$ space group. Rietveld analysis yields the following lattice parameters: a = 3.75670(11) Å, b = 12.5476(5) Å, and c = 13.166(3) Å. For flake separation, the (001) and (010) planes are ideal due to their cleavage properties [8].

To identify suitable flakes for further investigation, we employ the scotch tape exfoliation technique. This method involves applying adhesive tape to the bulk $TaRhTe_4$ crystal and carefully peeling it away to transfer thin layers onto a substrate. This process allows us to isolate and analyze flakes with the desired properties for subsequent experiments [2].

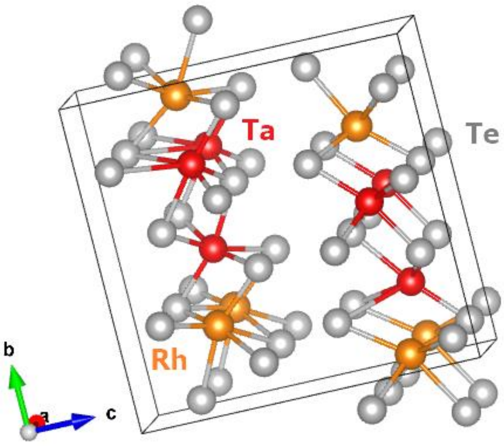


Figure 3: TaRhTe$_4$ lattice. Parameters were adopted from [8]

Criteria for Flake Detection

For effective device fabrication, the ideal van der Waals flakes should possess the following properties: good crystallinity, thin and uniform thickness, isolated position with respect to other objects.

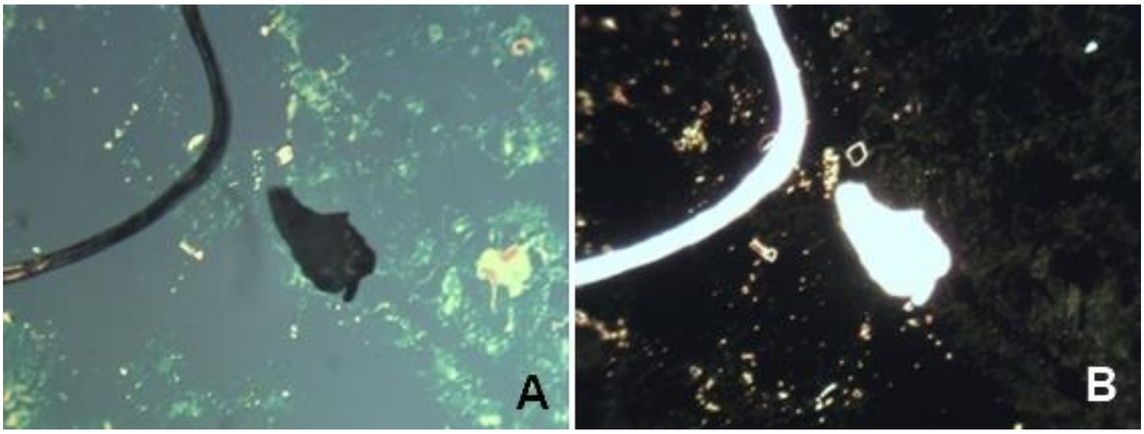


Figure 3: Example photo of substrate with flakes in bright-field (left) and dark-field mode (right) with 20× zoom taken by the microscope camera. There are flakes, adhesive, and impurities.

Figure 3A shows a microscope image of a substrate with flakes, adhesive residue, and other impurities. Similar images are commonly used to identify suitable flakes by manual inspection. In our tests, however, we identified that to improve contrast and differentiate between glue residuals, irregular objects, and the best vdW flakes dark-field microscope images are more suitable. This imaging technique enhances the visibility of flake contours, both thin and thick, while making impurities and adhesive residues more distinguishable against the background. In these dark field images (Figure 3B) the desired vdW flakes with homogeneous thickness are indicated only by their outlines. Straight outlines and 90-degrees corners (due to the orthorhombic symmetry of the material) indicate a good crystallinity of the objects.

Figure 4 presents four frames of isolated flakes. Three frames do not contain suitable flakes as they fail to meet the established criteria (Figures 4A, 4C, and 4D). Frame 4B includes one defective flake (top) and one suitable flake (bottom).

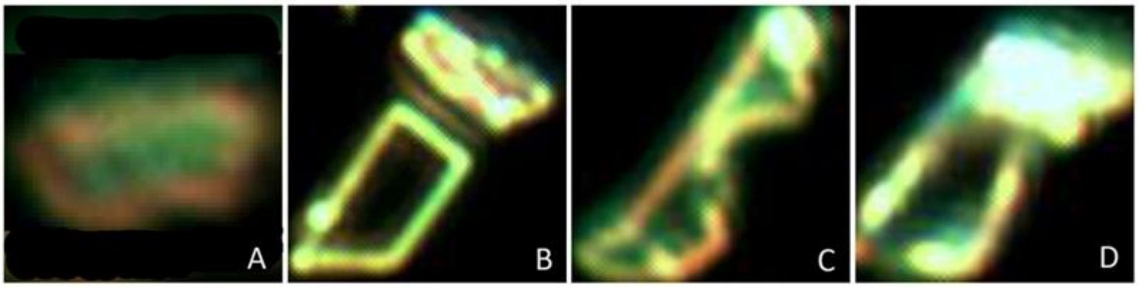
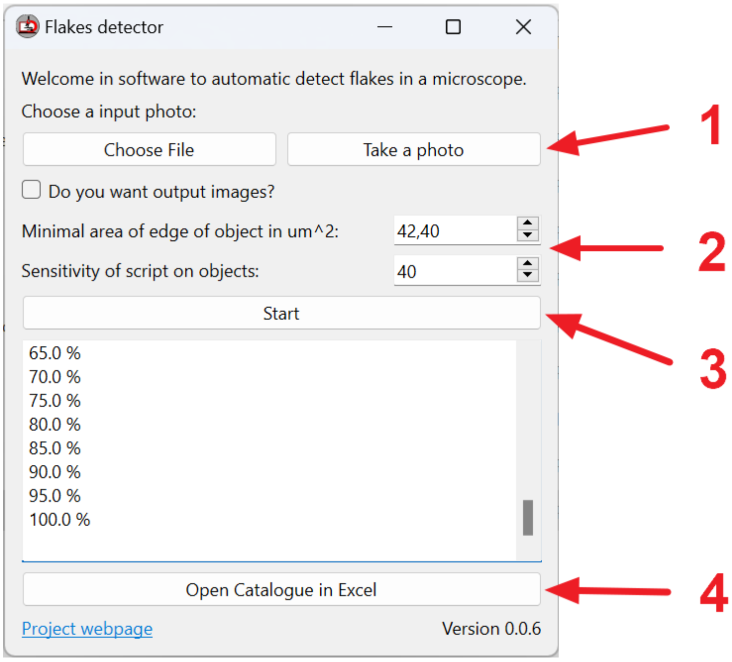


Figure 4: Illustration of a suitable flake (B) and various defects in flakes (A, C, and D). Frame A shows a flake lacking uniform thickness. Frame C depicts a flake without orthorhombic symmetry. Frame D displays two connected flakes. Images were captured using a microscope camera in dark-field mode.

Automatization of the flake detection

We developed software for detecting candidates to suitable flakes for following analysis in object-orientated Python 3. The software is available at GitHub and provides a graphical user interface (Figure 5) and terminal version (Figure 6) While both versions can be used interactively the terminal version can be also used in batch processes using various command line arguments. Installation files and a user manual are provided at https://github.com/dkriegner/micro-flakes/.


Flakes detector

Welcome in software to automatic detect flakes in a microscope.

Choose a input photo:

☐ Do you want output images?

Minimal area of edge of object in um^2: 42,40

Sensitivity of script on objects: 40

```
65.0 %
70.0 %
75.0 %
80.0 %
85.0 %
90.0 %
95.0 %
100.0 %
```

Version 0.0.6

Figure 6: Screenshots of the graphical version of the flake classification software. The process involves four steps: 1) selecting the source of the input photo, 2) setting sensitivity and minimum flake size, 3) initiating the search process, and 4) opening the output catalog in an MS Excel table.

```
Welcome in software to automatics detect object in microscope.
Project webpage: https://github.com/dkriegner/micro-flakes/tree/main/Detector
Version: 0.0.7

Working path: C:\Users\jirka\Documents\Test\input
Do you change the path? [y/N]:
You can upload existing photo or take a new photo by webcam.
Do you upload existing photo? [Y/n]:
Files in input:
['black3.jpg', 'calibration.jpg', 'input', 'output', 'Samle1.jpg', 'Test.jpg', 'Test6.jpg']
Write name of photo from microscope.
.../calibration.jpg
Do you want to get image output after 1st iteration? [y/N]:
Write minimal area of edge of object in um^2. Smaller object will be deleted [42.4]:
Write sensitivity of script on objects in dark field. Script will mark all pixels with RGB values bigger than
 the user's input. [40]: 
```

Figure 5: Screenshots of the terminal version of the flake classification software. Users must select a working directory, choose an image file or capture a new photo, and set the minimum flake size and sensitivity.

The software algorithm operates in two steps. In the first step, it colorizes light pixels (Figures 8a–8b) and divides the image into 7×7 pixels groups. If a group contains more than 70% colored pixels, the entire group is colorized; otherwise, the group is removed (Figure 8c). Small objects (10×10 µm) are deleted, and the centers of gravity are determined (Figure 8d). In the second step, the first step is repeated at a higher resolution (3×3 pixels). Finally, a catalog is created in MS Excel (Figure 9).

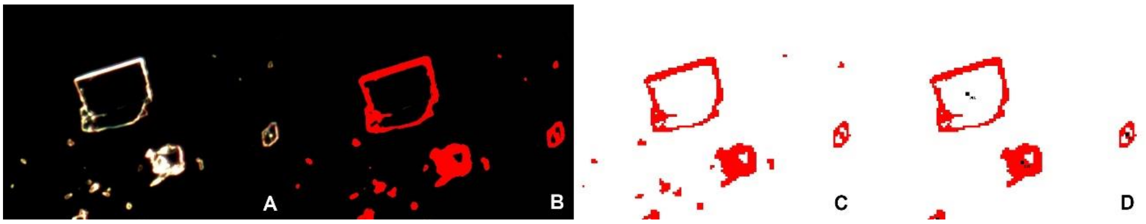
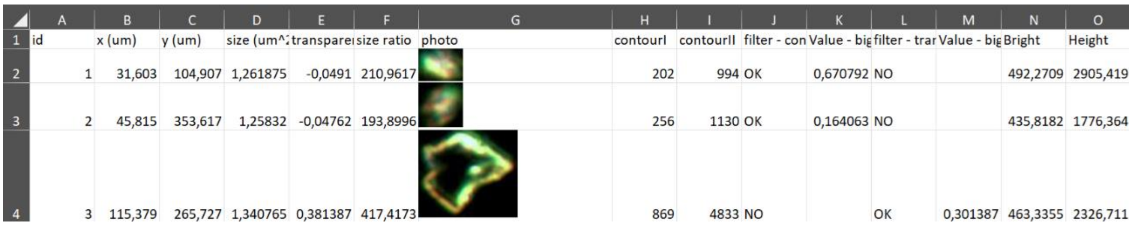


Figure 8: Algorithms in our software for selecting suitable flakes. There is the original photo on the left and the photo with a candidate selecting suitable flakes with ideal size on the right.

The output catalog includes the identification number, x and y coordinates (originating from the top left corner), area in µm², transparency (ratio of dark to total pixels in the flake), estimated size ratio (calculated by equations for rectangle from circumference and area), flake photo, brightness (mean RGB value), contour (ratio of light pixels to circumference), and estimated height (calculated from the linear relationship between brightness and measured height by Dektak Stylus Profilometer).



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	id	x (um)	y (um)	size (um^	transpare	size ratio	photo	contourI	contourII	filter - con	Value - big	filter - trar	Value - big	Bright	Height
2	1	31,603	104,907	1,261875	-0,0491	210,9617		202	994	OK	0,670792	NO		492,2709	2905,419
3	2	45,815	353,617	1,25832	-0,04762	193,8996		256	1130	OK	0,164063	NO		435,8182	1776,364
4	3	115,379	265,727	1,340765	0,381387	417,4173		869	4833	NO		OK	0,301387	463,3355	2326,711

Figure 9: Screenshot of the initial section of the flake catalog. It includes ID, x and y coordinates, size, transparency percentage, height/width ratio, contour contrast and intensity, and estimated height.

Discussion

The flake identification software proves highly effective, especially considering that many researchers typically locate flakes on the substrate manually. Using a 20× magnification, each frame covers an area of 500(10)×375(10) µm, within which approximately 400–500 flakes are visible. Our software identified 30, 19, and 20 candidate flakes in three trials, of which 5, 4, and 5 flakes (16–21% of fond flakes), respectively, were suitable for lithography. The software significantly reduces the number of flakes to be inspected manually to less than one-tenth, thus saving considerable time.

We are also working on automating the microscope stage, as it is currently moved manually by the user. Capturing the entire substrate requires approximately 100 frames. We are in the process of securing a motorized stage, which the software will control to streamline the imaging process.

In future developments, we plan to integrate a neural network to automate the final decision on flake suitability, further minimizing user involvement. And eventually automate also the design of electrical contacts to the selected flake.

Conclusions

We developed software capable of reducing the number of candidate flakes to less than one-tenth of the total. The software generates an MS Excel table cataloging the potential flakes along with their physical properties and the location on the substrate.

The selected flakes are used to fabricate electronic devices via electron-beam lithography, enabling measurements of their electrical properties. Additionally, we plan to conduct electron diffraction on the flakes using transmission electron microscopy (TEM) for structural analysis.

Acknowledge

We would like to thank Iryna Galstian and Mahdi Behnami from the Leibniz Institute for Solid State and Materials Research Dresden for their assistance in preparing thin-layer samples of $TaRhTe_4$. This research was supported by the Grant Agency of the Czech Technical University in Prague under grant No. SGS22/183/OHK4/3T/14.

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