Identifying the Crystalline Orientation of BP

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Purpose of the project

As a layered material, BP has a great anisotropic nature because of its structure (figure 1). Our final purpose is to find the electronic property of a BP device under stretching or compressing (figure 2). While the first step is to identify the crystal orientation of few layer BP.

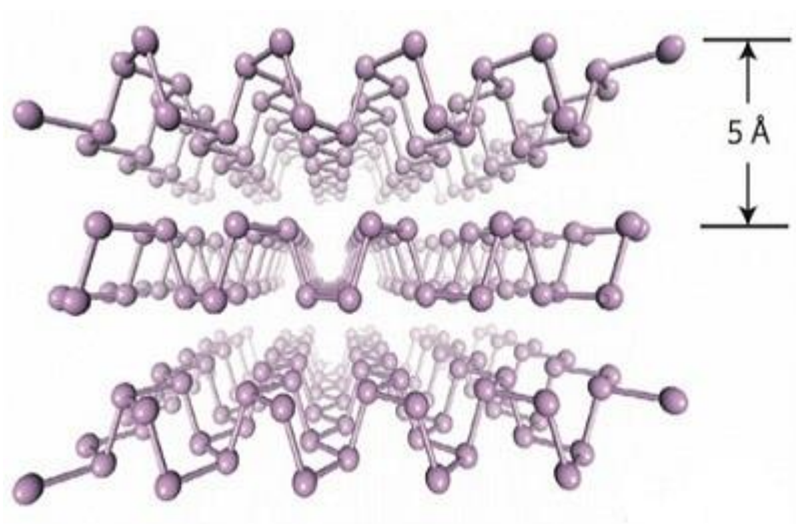


Figure1.structure of few-layer BP Li *et al*.

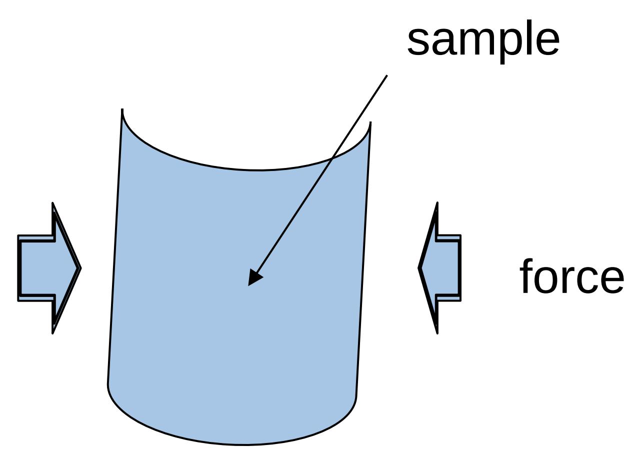


figure 2. our experiment configuration

I. Utilizing the angle resolve Raman spectrum

Raman peaks of black phosphorus

- Among the many ways to identify the crystal orientation the optical method is quick, easy and nondustuctive.
- One can observe 3 typical Raman peaks, that is, A_g^1 at 363 cm^{-1}, B_{2g} at 440 cm^{-1}, and A_g^2 at 467cm^{-1}. And the corresponding vibration modes are as follows:

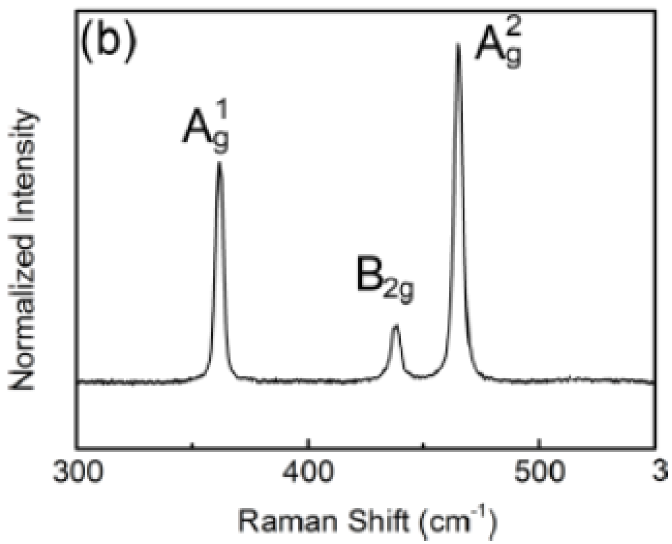


figure3.BP Raman spectrum

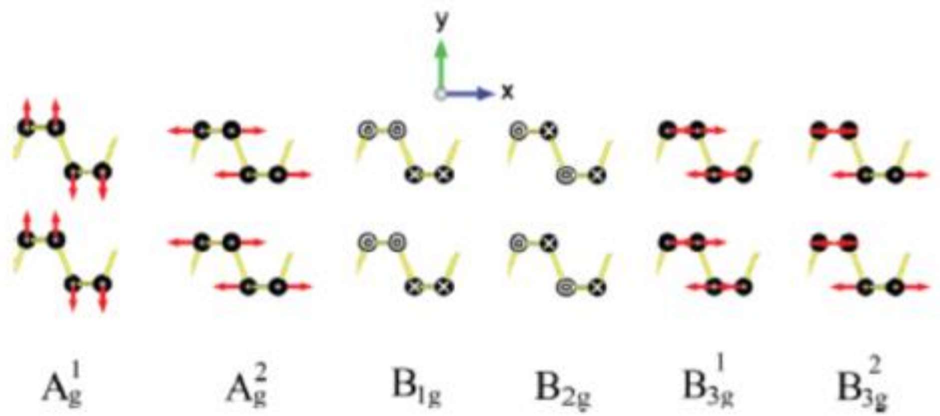


figure4. vibration modes

Device setup -- first generation

Method I : using one quarter wave plate and two polarizers to creat a polarized light with constant light intensity and changable polarization direction. (Figure 5) In this configuration we can only measure the parallel component of the scattered light.

Failed – Difficulties in producing and maintaining circular polarized light

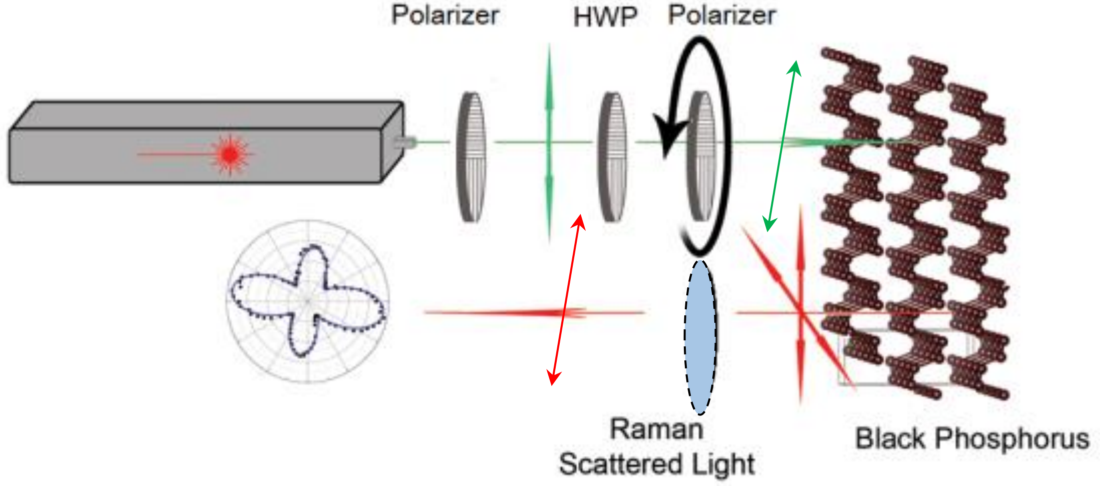


Figure 5.in this figure, polaroid2 is only the one we use to control the direction.the angle between fast axis of the QWP and the polariz-ation direction is 45° , which could create circle polarized light.

Results

We rotated the polariod2 from 0° to 180° ,and gained the data of bp raman peak intensity. (Fig 6a) To indicate the circle polarized light is accurate, we do the same operation to the Si substrate. The data was shown in figure 6b.

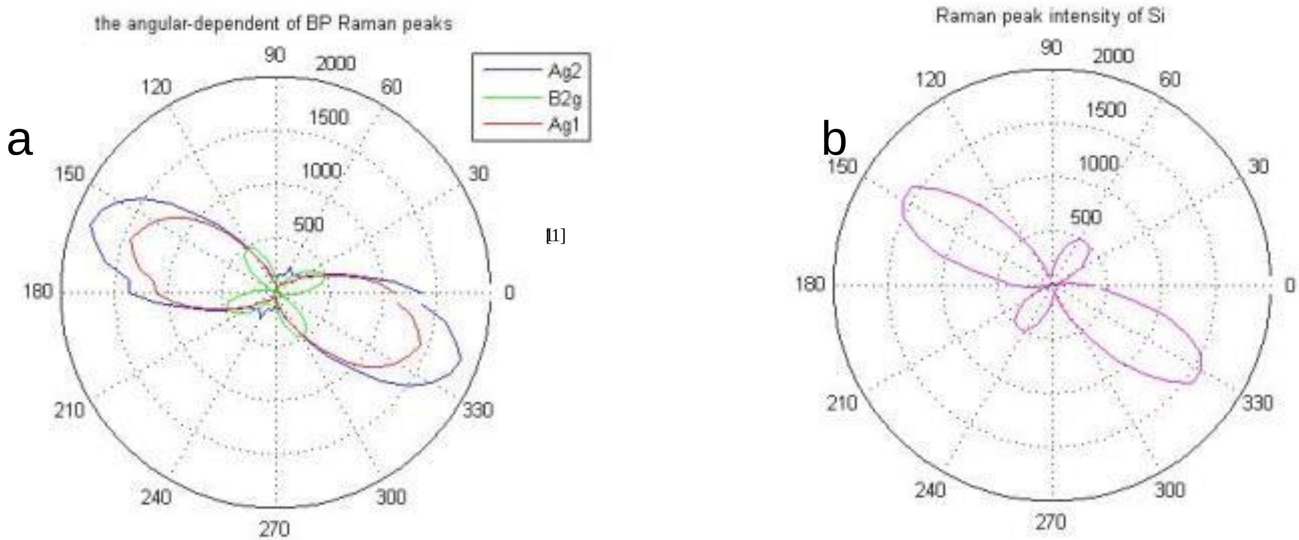


Figure 6a shows the angular-dependence of the blackphorsphorus layers. As we have mentioned,this is the parallel configuration data.As the Raman tensor theory can predict, the parallel confoguration of Ag1 and Ag2 changes following the same law.Unfortunately, we gained the data of the Si (Fig. 6b),which shows our divice did not perform well.Because the lattice plane of the Si is (1 0 0),which should result in four identical local maximun in a round. So it's too difficult to creat a ideal polarized light,this mathod should be reformed.

Device setup -- second generation

Method II: As prof. Wang suggested,we finally use a polariod and a half wave plate(HWP) to create the polarized light. HWP can change the direction of polaried light without changing the intensity. (Fig 7)

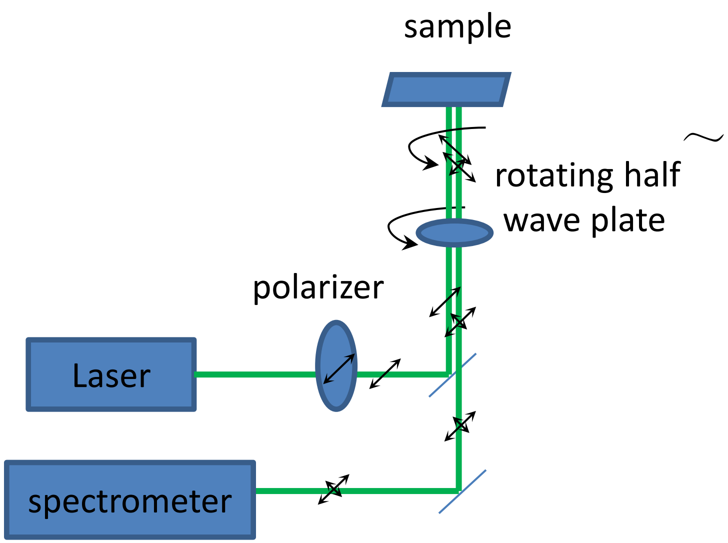


Figure 7.The divice we final used.The linely polarized light changed it's direction for 2θ as the HWP rotated θ. In case the polarization light in other direction would appear,we put the polariod along the horizontal direction. And we rotate the HWP with a rotation stage drived by a computer program.

Results

We carryed out this experiment,and get a group of data. We plot them as Fig 8

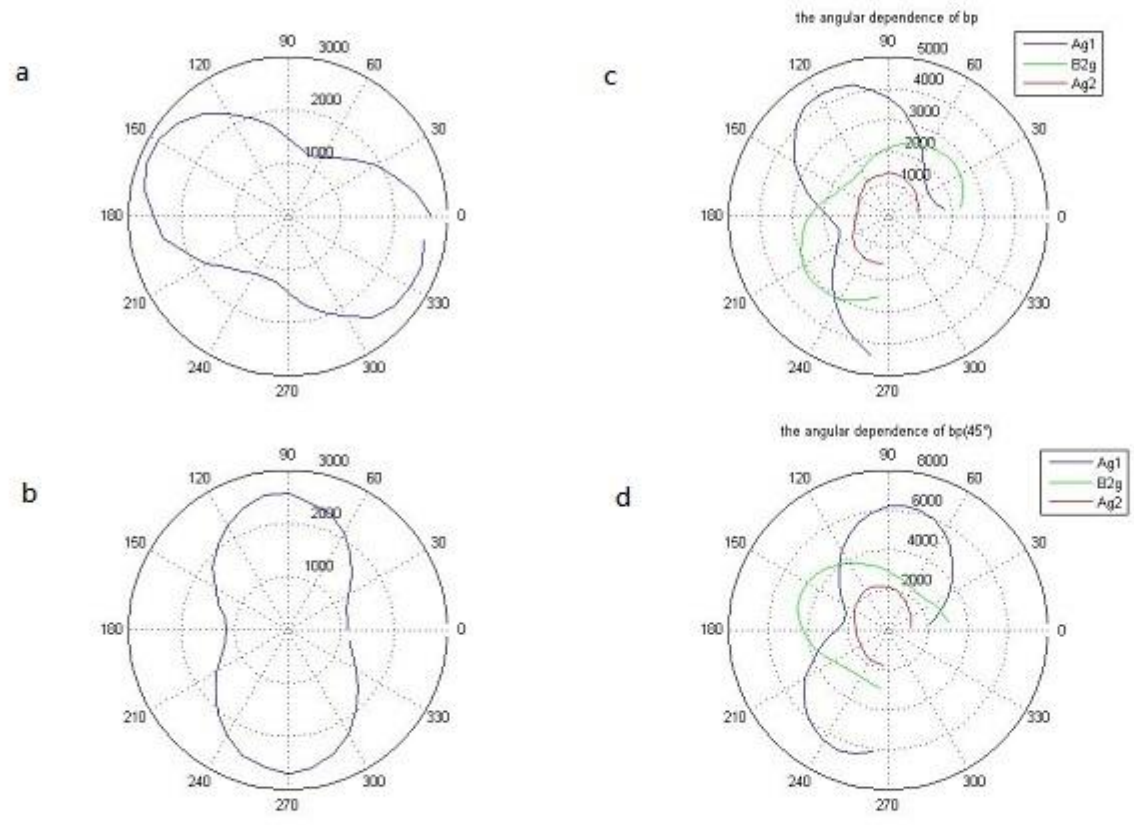
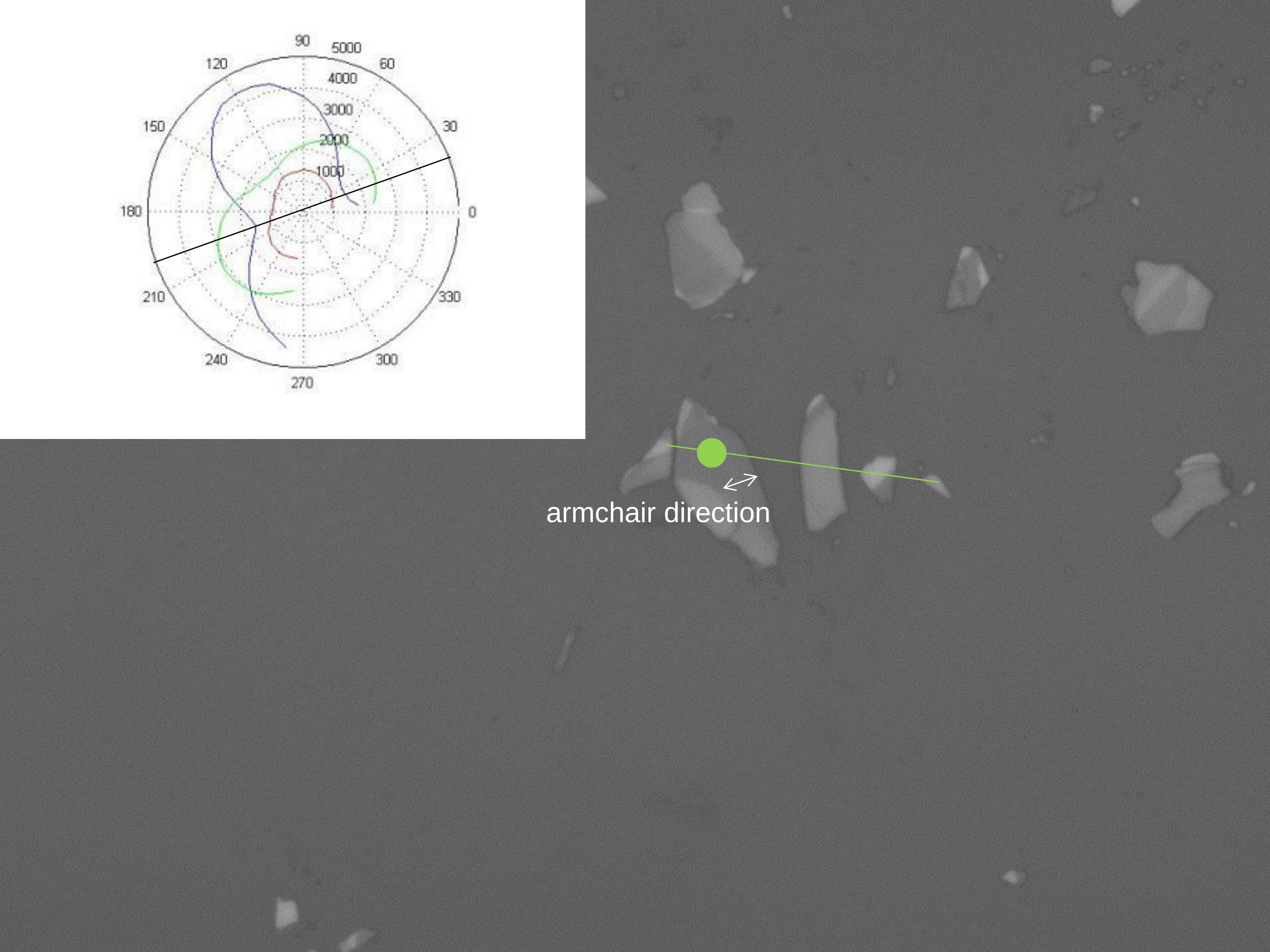


Figure 8.a&b shows the Si peak of this system,the angle this picture rotated is exactly that we rotated the sample,so the peak change has nothing to do with the light and divice. so the data of bp is reliable. c&d shows the angular dependence of the bp,that's what we want to explore. Clearly,the Ag2 peak shows the most strong anisotropy nature,we can use it to identify the crystalline orientation.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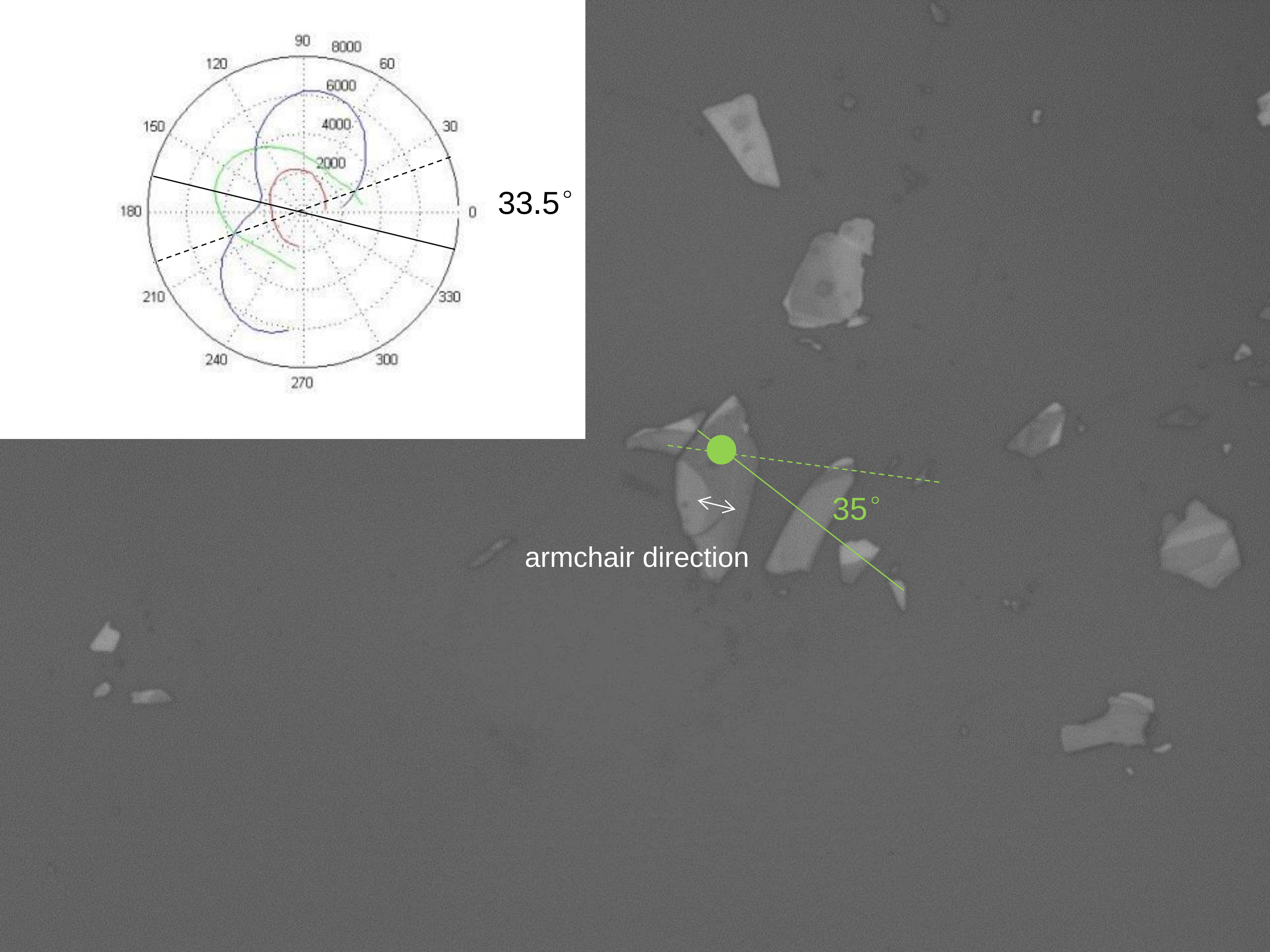
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Data fitting

- Theories of Raman scattering gives the following result about the intensity versus the direction of polarization of the incident beam

$$S_{A_g^2} = \frac{1}{2}(a^2 + c^2) + \frac{1}{2}(c^2 - a^2)\cos(2\theta)$$

$$S_{B_{2g}} = f^2$$

- where *a*, *c* and *f* are all Raman tensor elements. And *θ* is the angle between incident beam polarization direction and zigzag direction (10.1021/acsnano.5b00698)
- A_g^2 peak maximum ↔ polarization along zigzag direction
- A_g^2 peak minimum ↔ polarization along armchair direction

Data fitting

- We fitted the data of A_g^2 peak with *sum of sin* mode in matlab
  - $y = 4342 + 2075 \sin(2.17x - 1.52)$
- The parameter before *x* is supposed to be 2. The discrepancy may due to imprecise of the rotation stage

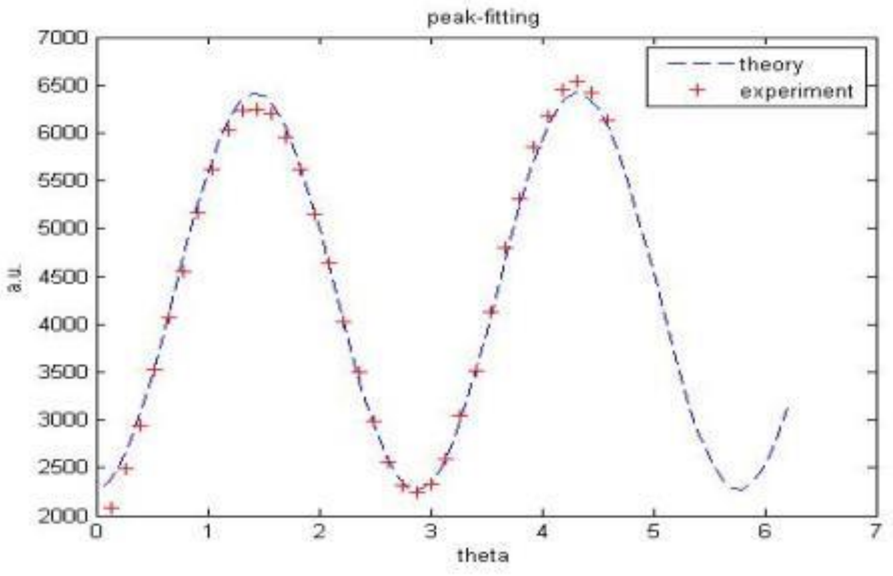


Figure 6.the red "+" is the experimential data of Ag2 peak, the dotted line is the fitted curve,Data fitting gives
$y = 4342 + 2075 \sin(2.17x - 1.52)$
the phrase difference and the angular velocity.

Conclusion and unsolved problems

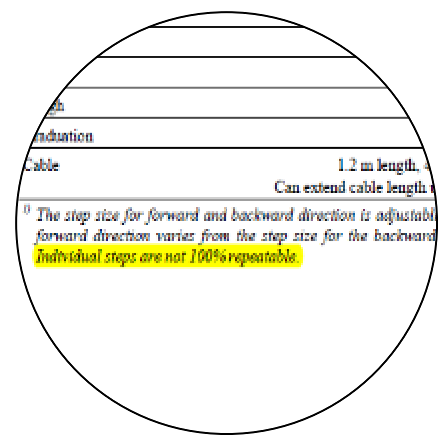
- At the very beginning the incident beam is polarized horizontally in the vision field. As the stage rotates, the polarization direction rotates anticlockwise.
- The A_g^2 peak reaches the maximum at x = 0.700 rad = 40.1 ° that is the zigzag direction.
- The precision of the system is limited by the rotation stage

3.0 AG-PR100 Rotation Stage

3.1 Specifications

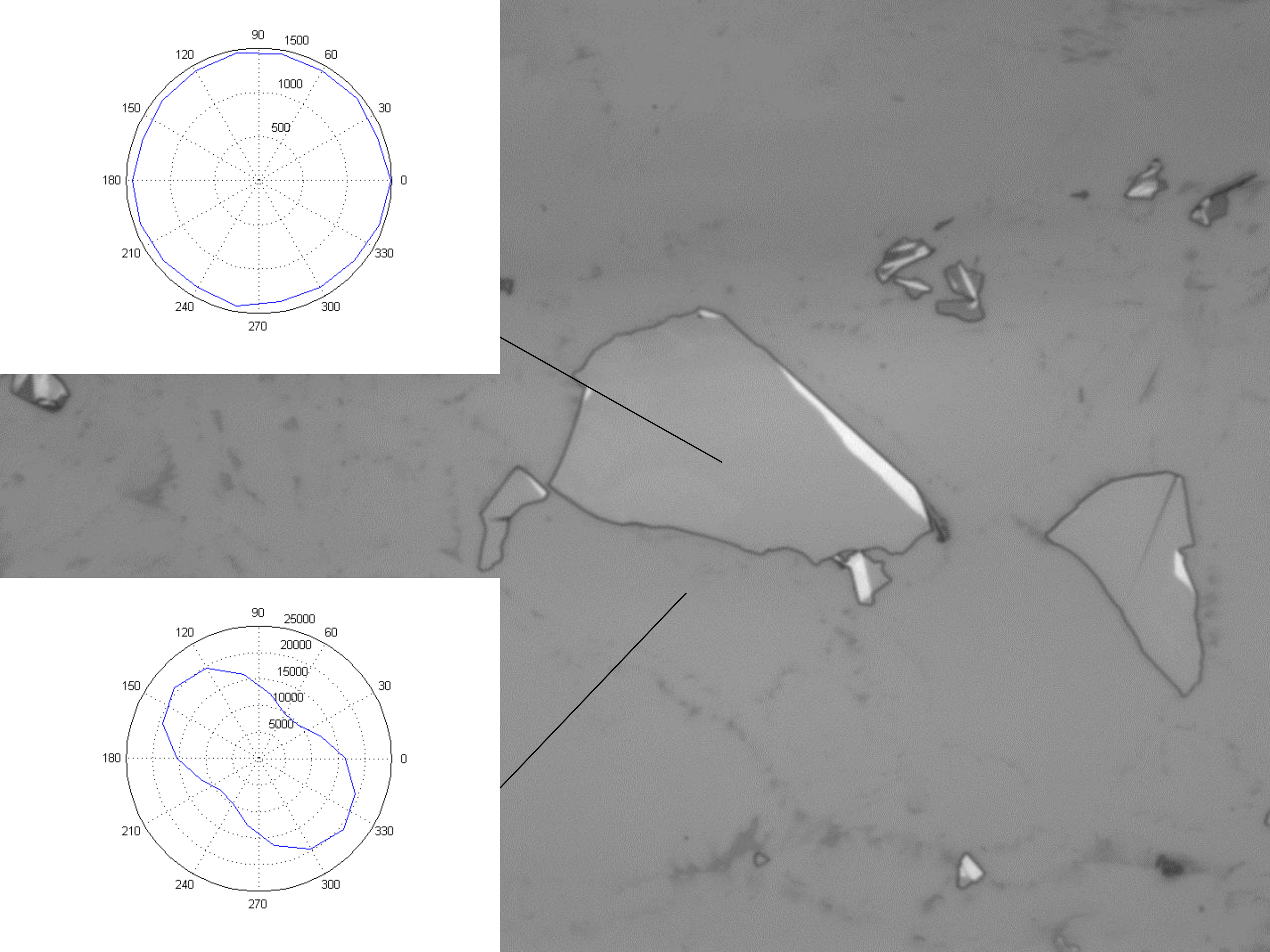
Optics diameter	1.0 in (25.4 mm)
Max. optics thickness	0.40 in. (10 mm)
Travel range	360° continuous
Minimum incremental motion [1]	5 µrad (1 arcsec)
Maximum speed	2 °/s
Wobble	100 µrad
Limits	None
Weigh	135 g
Graduation	2°
Cable	1.2 m length, 4-wire mini-Din connector. Can extend cable length using AG-MD4-1.5 extension cable.

[1] *The step size for forward and backward direction is adjustable. With default settings, the step size for the forward direction varies from the step size for the backward direction and may be larger than 5 µrad. Individual steps are not 100% repeatable.*



Supplementary Information

- To ensure that the intensity of the beam remains unchanged when the HWP is rotating, we took the angle-resolved Raman spectrum of graphene and the silicon substrate.
- The result indicated that for material with high symmetry like graphene, the Raman peaks show little anisotropic characters.
- For Silicon, when the incident beam is perpendicular to the [1,0,0] face



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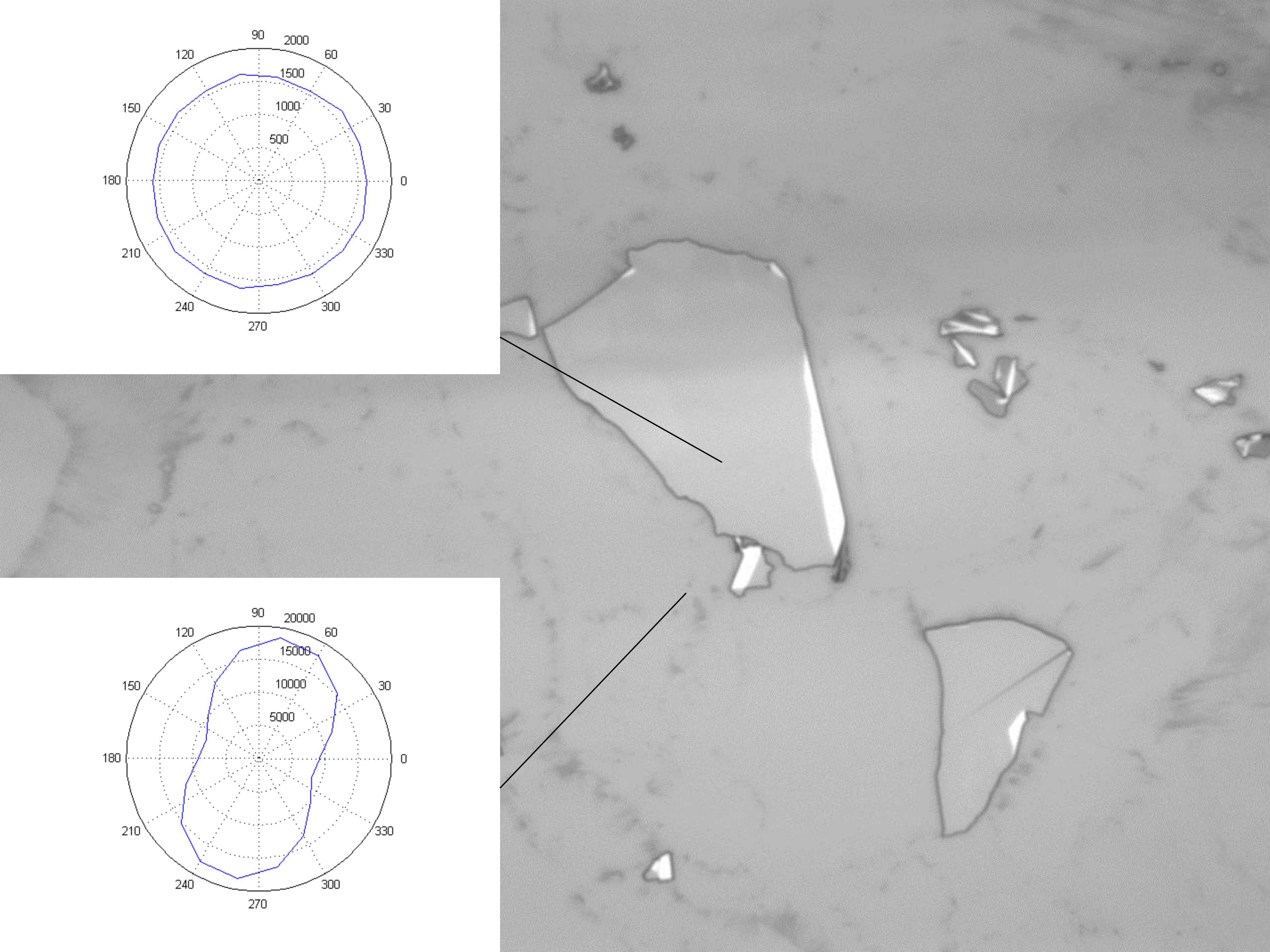

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THANK YOU