# Optical reflectance-based software for automated characterization of nanomaterials: outcomes of the NSF Nanohub's NanoMFG node

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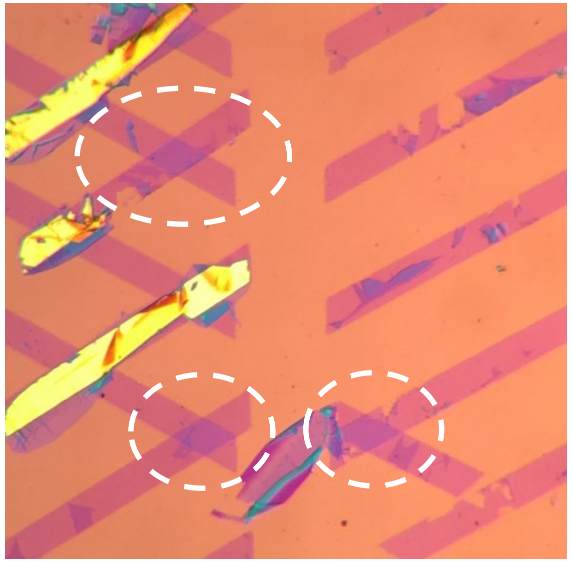
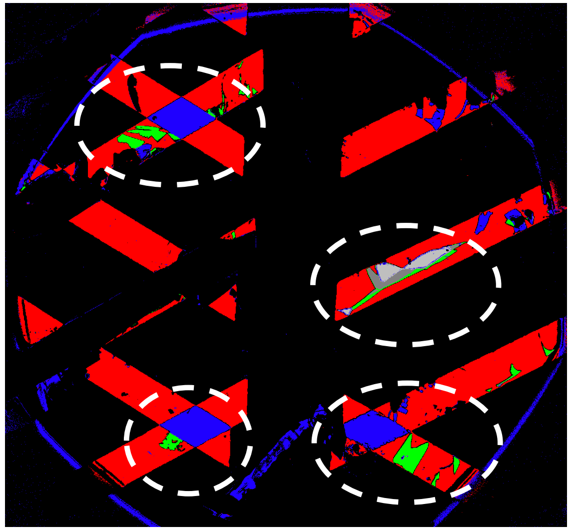
# Outline: NSF nanoMFG node outcomes

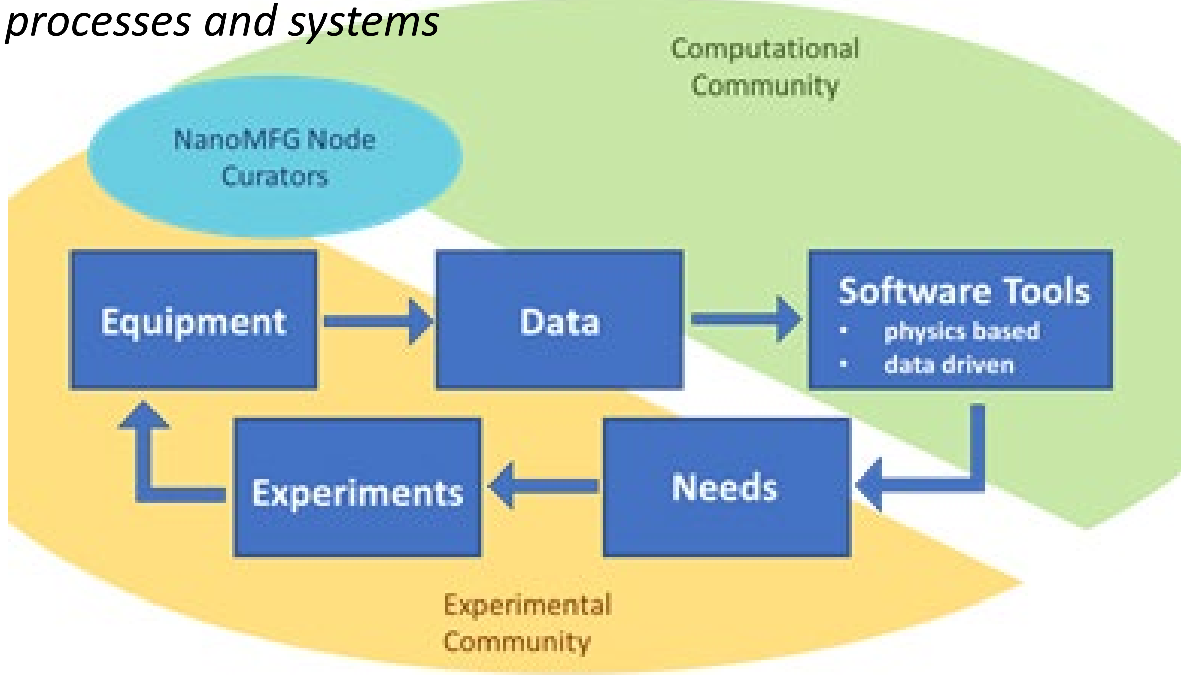
- Introduction to the NSF nanoMFG node
- Nanomanufacturing simulation needs survey
- Two recently released nanoMFG tools: applications of optical reflectance in nanoscale characterization
    - In-situ viscosity determination for nanoimprint resists: *nanovisc*
    - Determination of 2D material heterostructure composition: *2dreflect*
- Future areas of interest





# nanoMFG – the NSF nanomanufacturing node

***Vision***: *The nanoMFG node aims to assemble, develop, and implement advanced cyberinfrastructure tools for research, education, and industrial deployment of integrated, nanoscale manufacturing processes and systems*




**Goals**:

- Develop and deploy software tools and make them available through the NCN-Cyber Platform (“nanoHUB”)
- Engage with the nanomanufacturing community to address critical needs
- Address the challenges of integrating data from the computational and experimental community
- Provide a streamlined process for software development


**Adams**


**Aluru**


**Bauer**


**Ertekin**


**Ferreira**


**Katz**


**Roloff**


**Taylor**

***HIGHLIGHTED ACTIVITIES***

| Enabling Software for the Nanomanufacturing Community | Community Outreach | Data-Science Enabled Advances in Nanomanufacturing (DSEAN) Workshop |
|---|---|---|

# Getting involved with nanoMFG

## Workshop on Data-Science Enabled Advances in Nanomanufacturing

- ✓ Annual workshop held in Febr/Mar
- ✓ Bring together members of the nanoMFG community from industry, labs, and academia
- ✓ Presentations, hands-on activities, panel discussions, poster sessions, and networking

## Call For Tool Proposals

- ✓ Focuses on a targeted need for the nanomanufacturing community identified in Needs Assessment Report
- ✓ Includes full support for a graduate research assistant or partial support for a post-doc
- ✓ Includes two weeks onsite to work with our software development team on site; continued support for remote development
- ✓ Call released annually in early spring for next academic year

## Opportunities for Students

- ✓ Opportunities for graduate students
- ✓ Two-year graduate fellowship for URM students
- ✓ Summer fellowships at Illinois and Berkeley
- ✓ Research Experience for Undergraduates via NCSA FoDOMMaT, NCN SURF


The nanoMFG node is committed to promoting diversity and providing an inclusive environment for all participants. Students, post-docs, and faculty from backgrounds traditionally underrepresented in STEM are especially encouraged to apply.

Questions? contact ertekin@Illinois.edu or jayr@Illinois.edu

# Nanomanufacturing simulation needs survey

- Help us to shape the next phase of simulation tool development
- Paper survey in your conference materials; collection box at registration desk
- Also available online: https://bit.ly/2VCsWRg or use QR:
- Looking to schedule one-to-one conversations as well
- Contribute your free-to-use nanomanufaturing simulation tools to the Nanohub and get a citable DOI

nanoMFG **Nanomanufacturing simulation needs survey 2019**

Thank you in advance for taking the time to complete this survey/request for information. The NSF Nanohub's Nanomanufacturing Node (nanoMFG), https://nanohub.org/groups/nanomfg, seeks to build a sustainable infrastructure for the creation of high-quality, free-to-use nanoscale simulation software tools. We are currently surveying the NNT community to discover unmet simulation needs that will inspire the next phase of our work.

If you'd rather complete this survey online, you can do so at https://bit.ly/2VCsWRg or via the above QR code (please complete either the paper or online version, not both).

We are also keen to speak directly with anyone who has views or ideas surrounding nanoscale simulation software. Please drop Prof. Hayden Taylor a line (HKT@berkeley.edu or telephone/text 510 646-3344) and he would be grateful for an opportunity to speak with you, either in person at NNT or remotely at a later date.

1. Please check any areas below where you believe there are unmet needs for simulation software ('simulation' can be interpreted broadly):

- [ ] NIL pattern formation including residual layer uniformity
- [ ] NIL stamp/template layout and design checking
- [ ] NIL demolding process or template lifetime prediction
- [ ] NIL overlay/process-induced distortions
- [ ] Nanoscale aspects of injection molding
- [ ] Planarization
- [ ] Plasma etch processes
- [ ] Optical propagation in photonic materials/structures

diffractive optics
eposition, particularly of 2D materials
w-D materials: e.g. nanowires, graphene
ification
ıg relating to nanofabrication processes
cribe below)

a few words describing what you

ɜam used tools or materials from

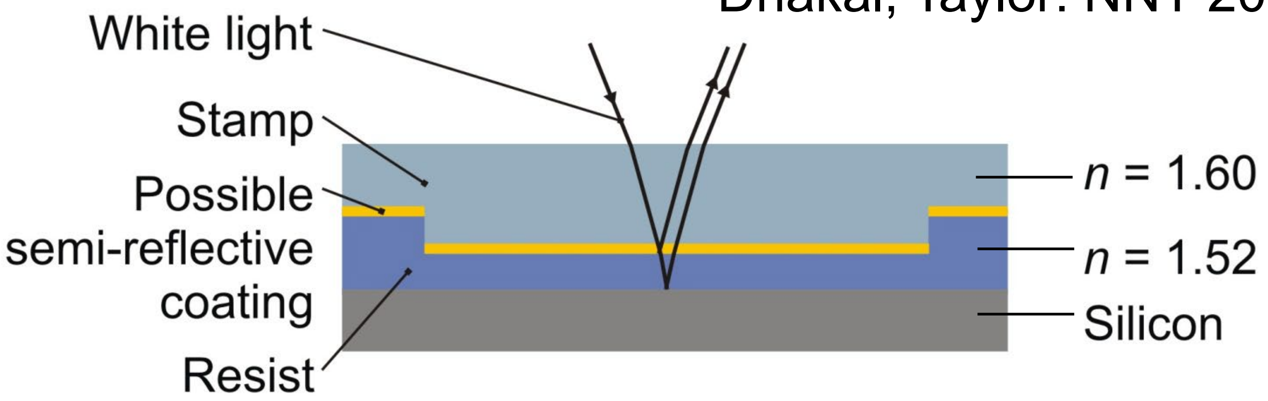
NSF Network for Computational

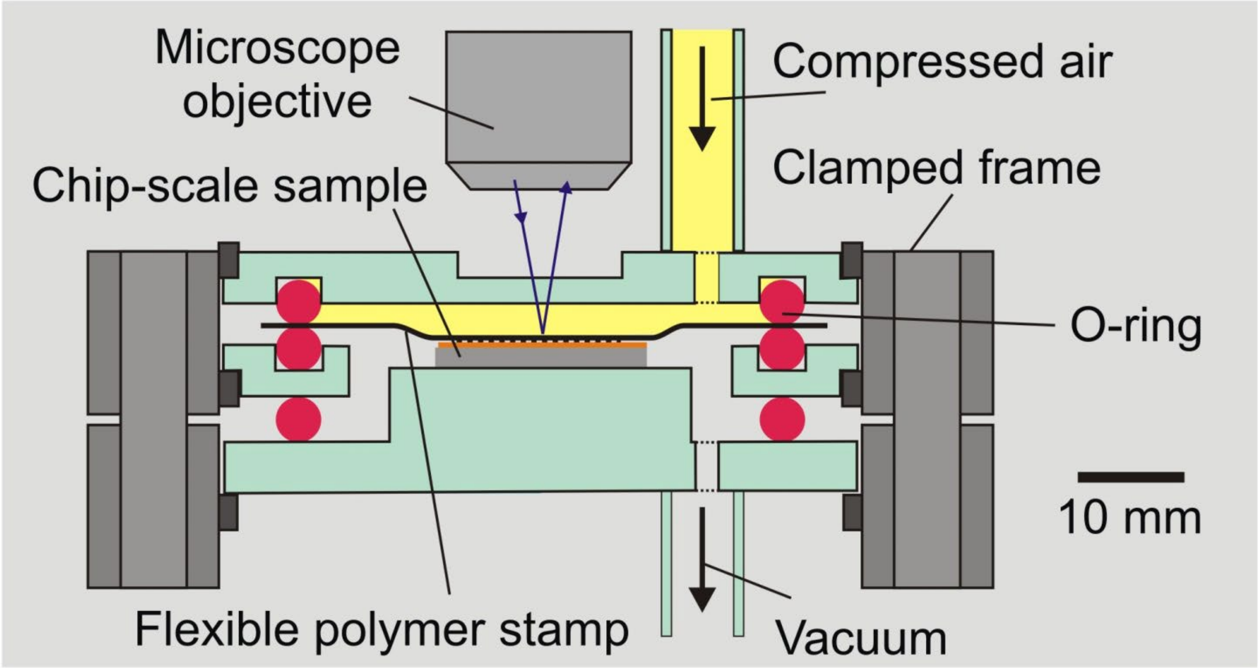
ılation in addressing a particular
tion alone and/or hand analysis)?

# Viscosity measurement of nanoscale-thickness films

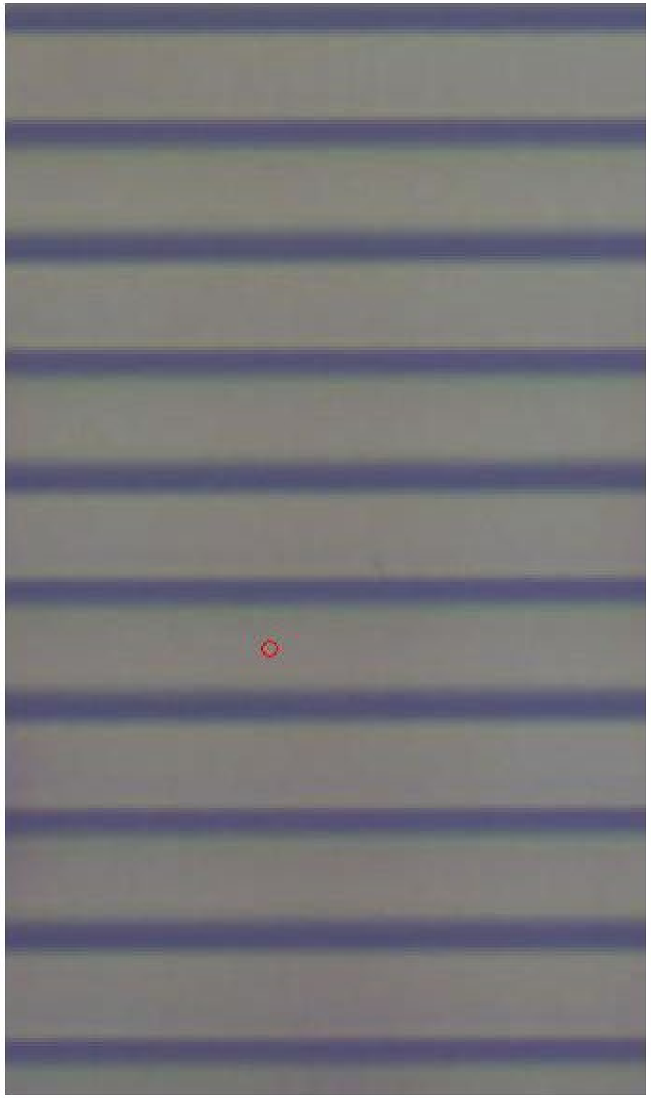
Dhakal, Taylor: NNT 2013

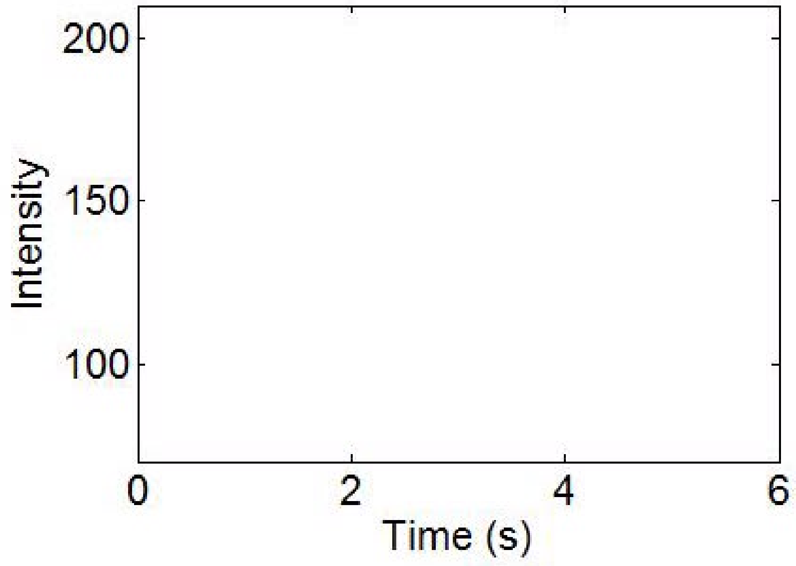
- Need to determine rheological behavior in realistic environment:
  - Molecular confinement
  - Solvent evaporation extent
  - Solid-liquid boundary conditions
- Approach: observe squeezing flow of resist via optical reflection through stamp
- Pair intensity maxima/minima with modeled RLT values
- Extract viscosity by relating temporal RLT evolution to squeeze-film model



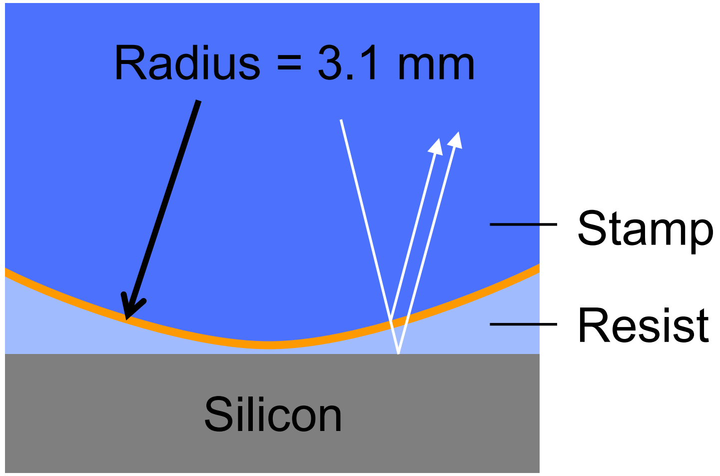
# Viscosity measurement of nanoscale-thickness films

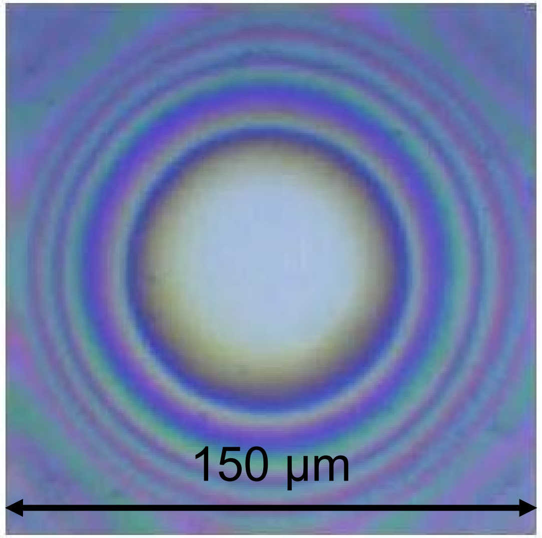





- **Material: MRT mr-UVCur-21**
- **Stamp-average pressure 20 kPa**
- **Consistent with viscosity ~ 7 Pa.s**

- ***But*: calibration with a known thickness set is needed for white light illumination**



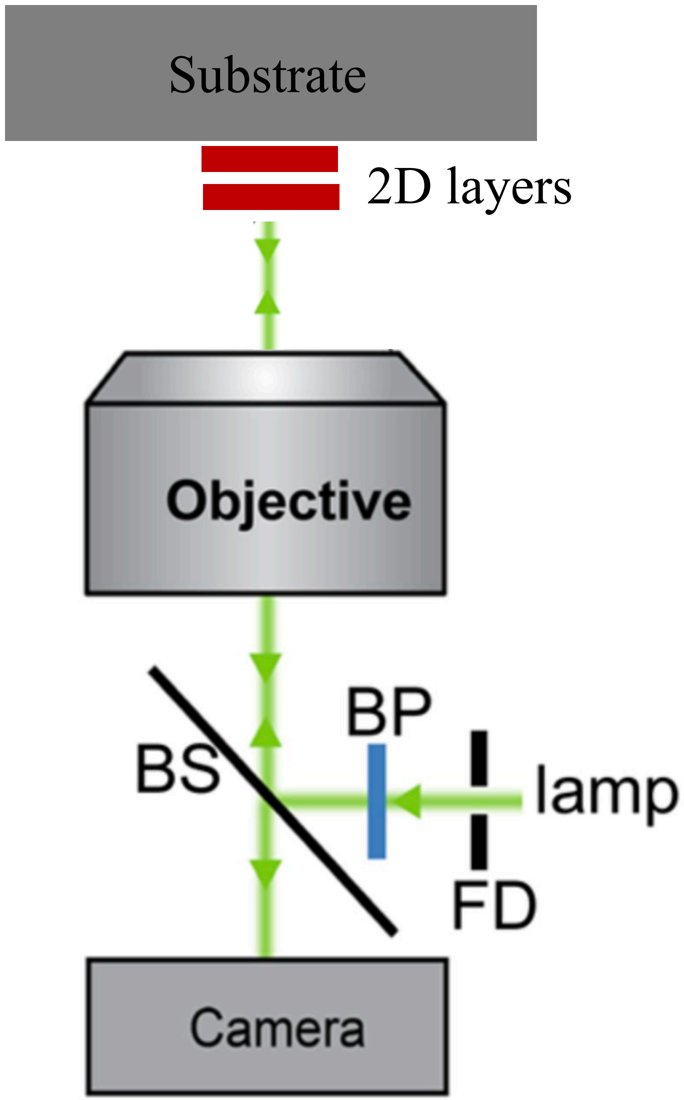




Dhakal, Taylor: NNT 2013

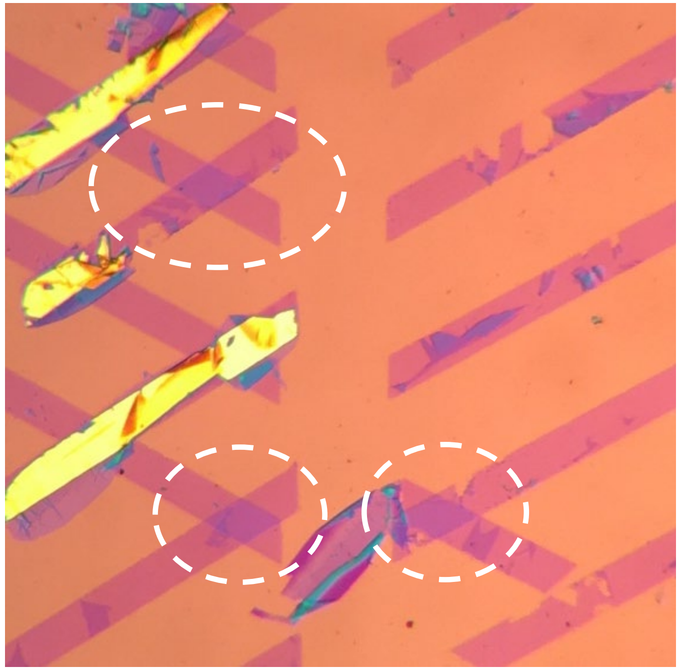
# Viscosity measurement of nanoscale-thickness films

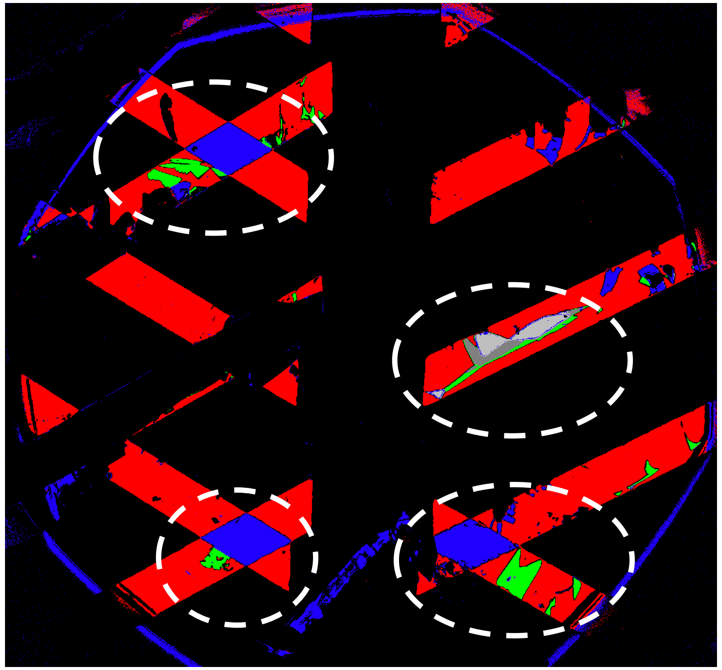
- Solution: two well spectrally separated LEDs (e.g. red, blue).
- One wavelength only → ambiguous RLT
- Two wavelengths → *sequence* of maxima and minima unambiguously determines RLT
- *Nanovisc:*
    - imports video of squeezing
    - guides max/min identification
    - extracts viscosity

# Reflectance-based characterization of 2D stacks




Two crossed arrays of $MoS_2$ by mechanical stacking



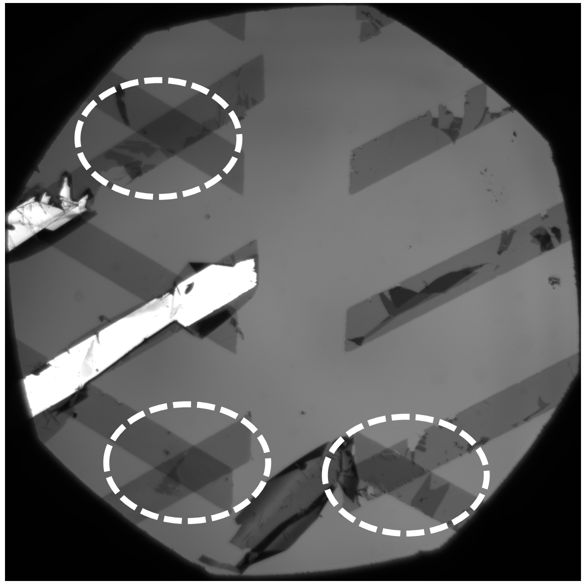


| | | |
|---|---|---|
| substrate | 2 layer-natural | 3 layer-natural |
| 1 layer | 2 layer-stacked | 4 layer-natural |

validated by AFM and photoluminescence

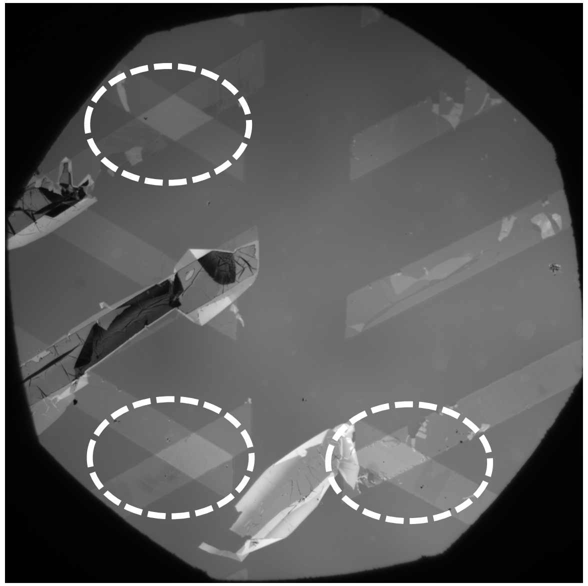
# Distinguishing *natural* from *manufactured* bilayer $MoS_2$

610 nm illumination

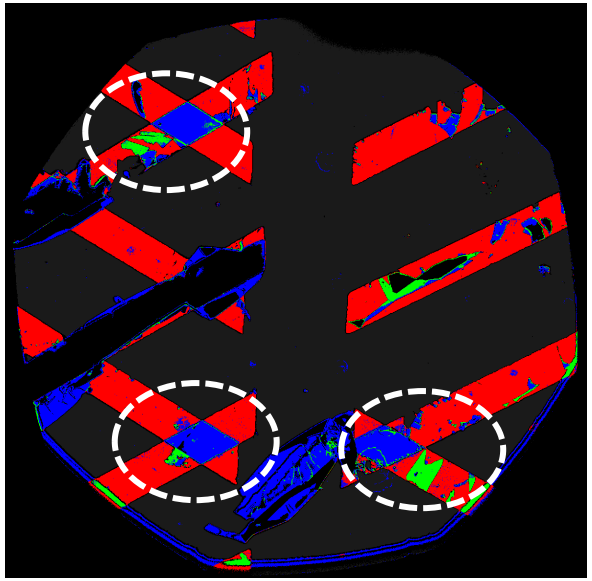


- High contrast between monolayer and bilayer
- Low contrast between closely and less closely spaced layers

450 nm illumination



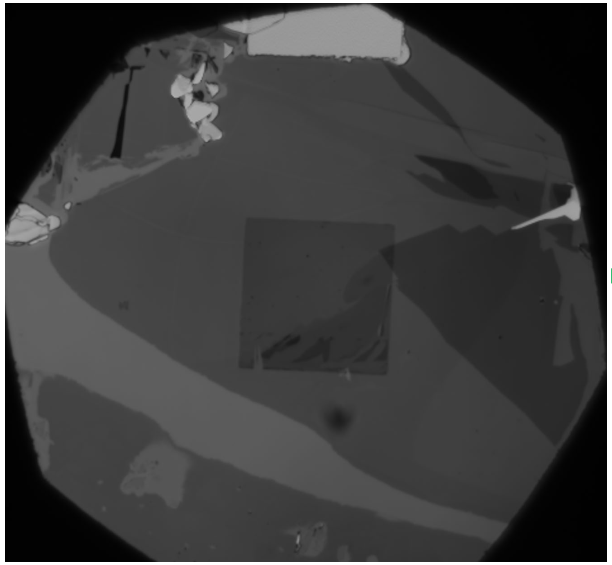
- Low contrast between monolayer and closely spaced bilayers
- High contrast between closely and less closely spaced bilayers



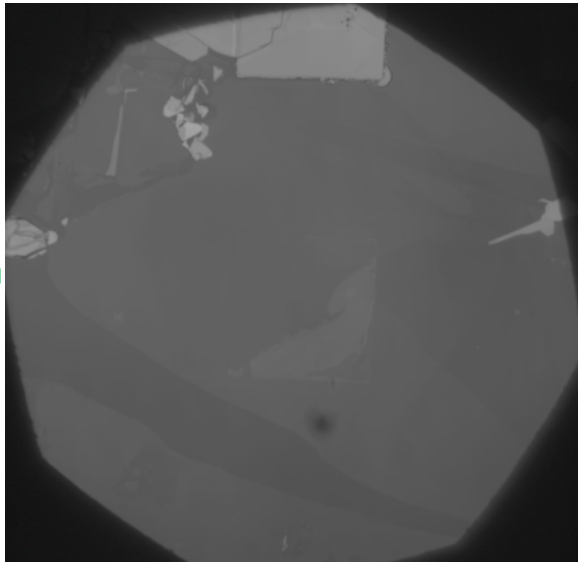
- Substrate (260nm $SiO_2$/Si)
- 1 layer $MoS_2$
- 2 layers, closely spaced
- 2 layers, less closely spaced

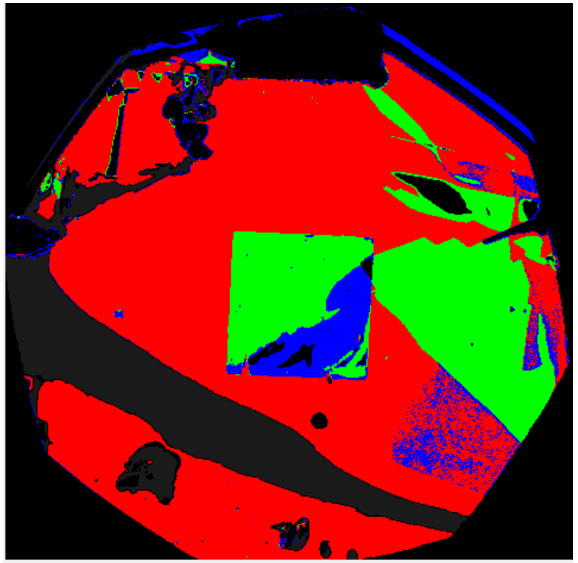
# The impact of bilayer thermal annealing can be visualized

610 nm illumination

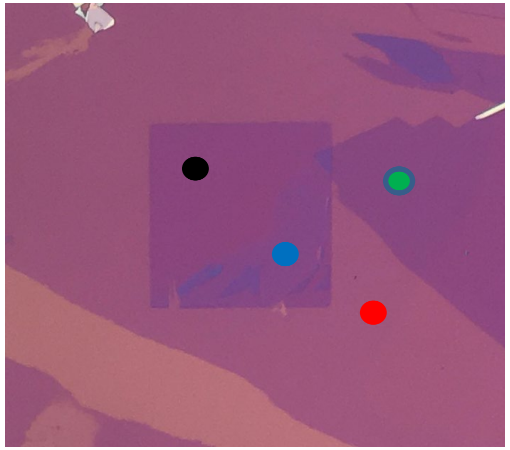


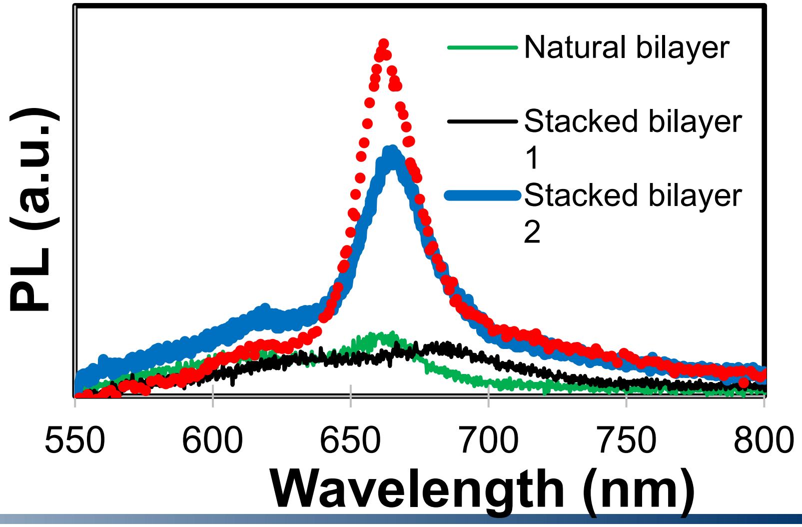
450 nm illumination






White light






Annealed stacked bilayer shows patches of optoelectronically coupled and less coupled regions – corroborated by photoluminescence (PL)

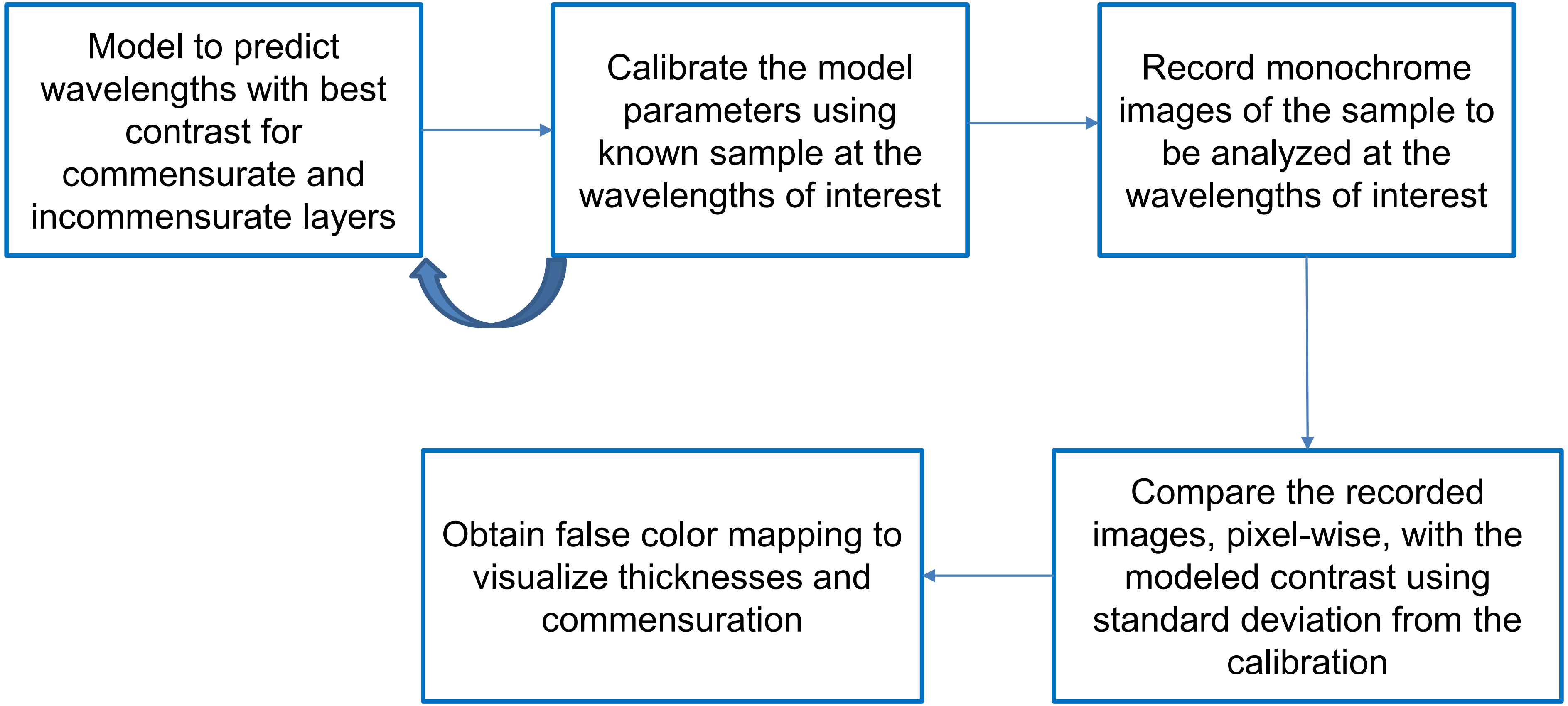
# Summary and outlook

- Nanovisc: https://nanohub.org/resources/nanovisc
  - Viscosity extraction from thin films via color video
- 2dreflect: https://nanohub.org/resources/2dreflect
  - Sub-monolayer-resolution characterization of 2D material stacks
- Possible future directions:
  - Multiplexed cell deformability characterization
  - Study curing kinetics; refractive index changes under load

- Simulation needs survey: https://bit.ly/2VCsWRg

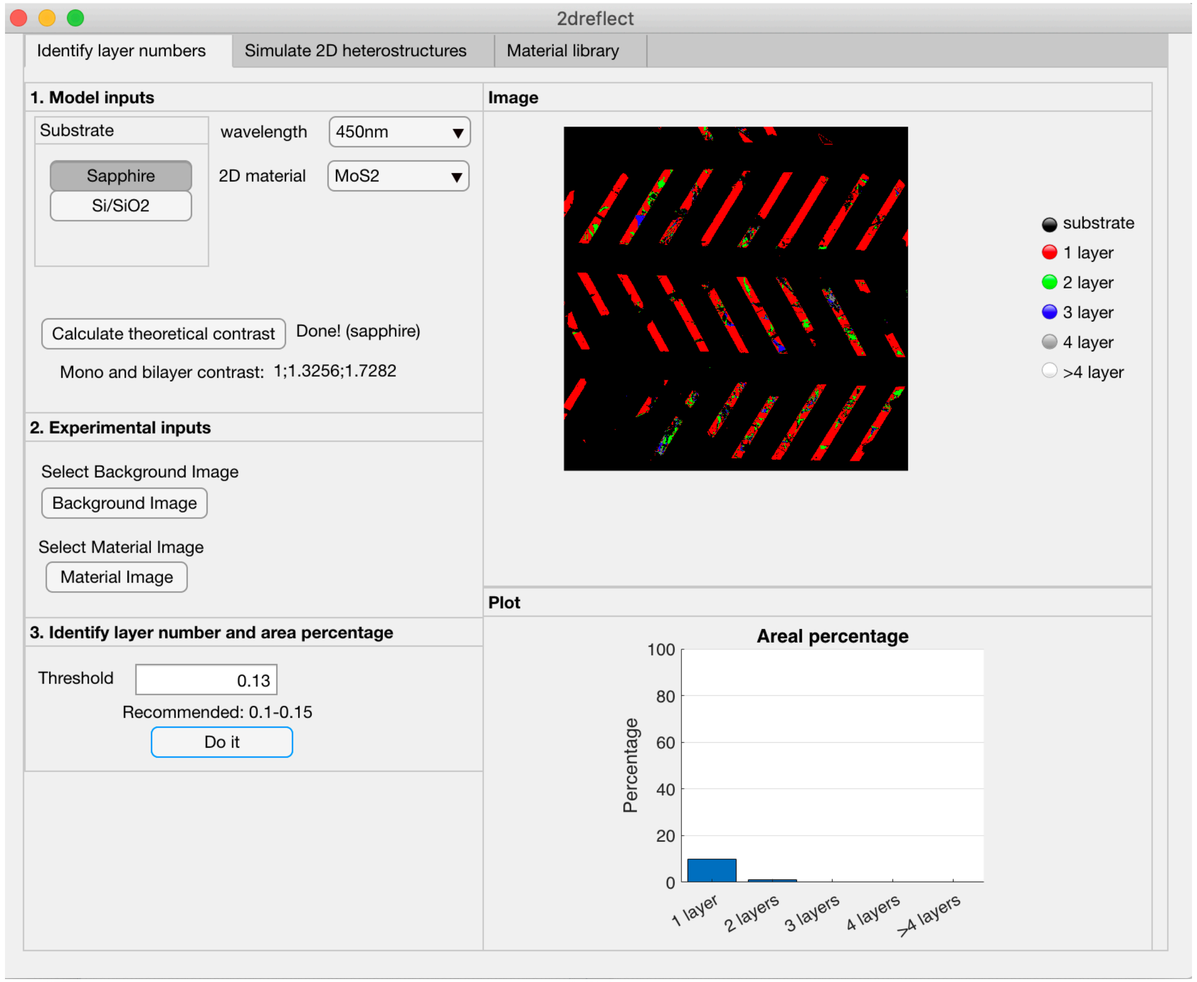
# Supporting slides

# 2dreflect: computational procedure



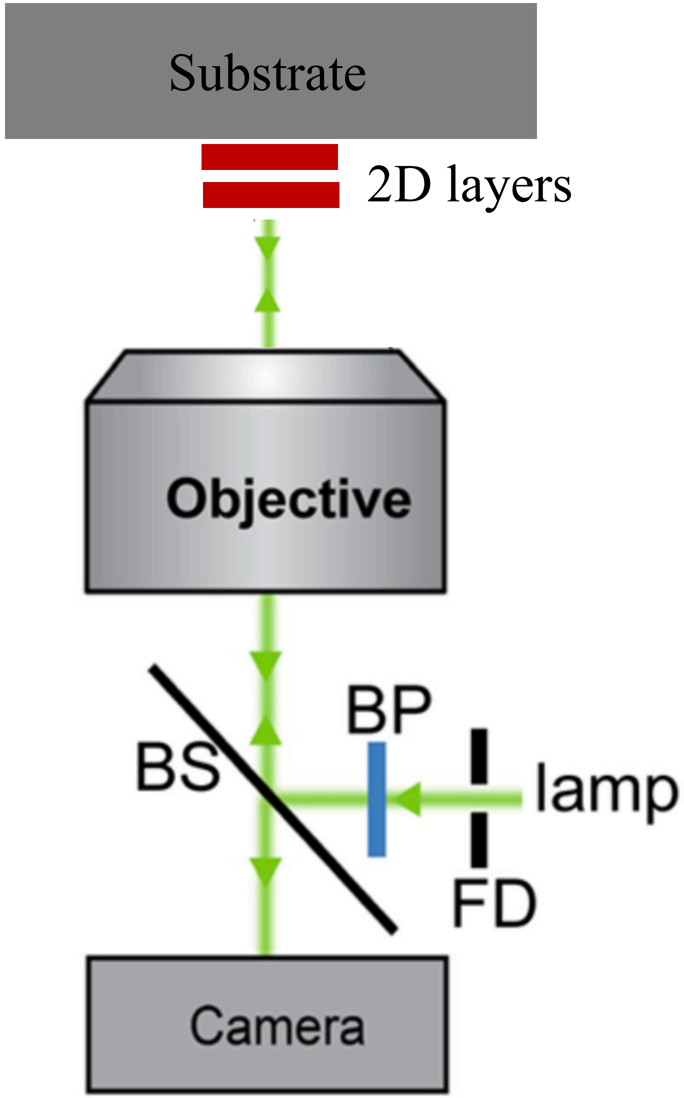
# 2dreflect: interface

User's input panels

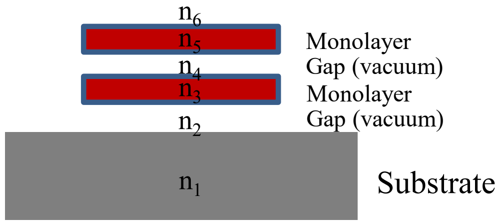



Tool's output panels

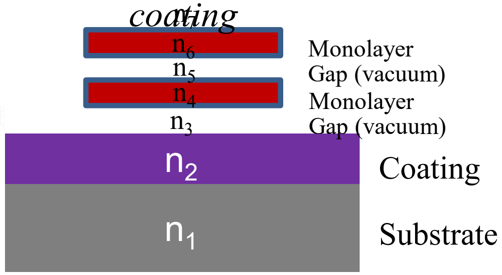
# Reflectance-based characterization of 2D stacks




*2D materials on a bare substrate*




*2D materials on a substrate with coating*




The contrast of the 2D materials is calculated using transfer matrix formulation:

Transfer matrix at interfaces

$$T^{12} = \frac{1}{t_{12}}\begin{bmatrix} 1 & r_{12} \\ r_{12} & 1 \end{bmatrix}$$

Fresnel coefficients

$$r_{12} = \frac{n_1 - n_2}{n_1 + n_2}, t_{12} = \frac{2n_1}{n_1 + n_2}$$

Transfer matrix of the layer

$$T^{2} = \begin{bmatrix} e^{i\varphi} & 0 \\ 0 & e^{-i\varphi} \end{bmatrix}$$

Phase shift

$$\varphi = \frac{2\pi}{\lambda} n_2 d_2$$

With r, t being reflection and transmission coefficients according to Fresnel's equations. The transfer matrix of the layered system is then calculated:

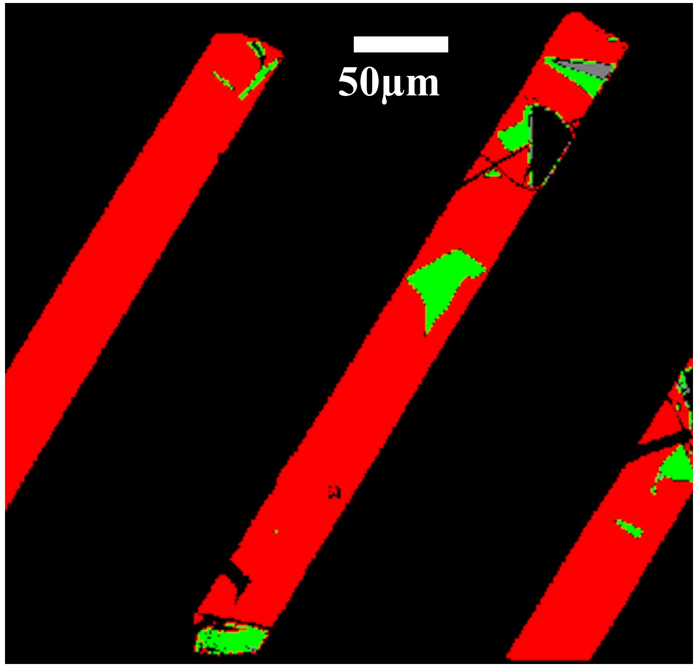
Transfer matrix of the system

$$T^{13} = T^{12} T^{2} T^{23}$$

➡ Intensities and contrasts

# 2dreflect: calibrating for the uncertainties in the substrate

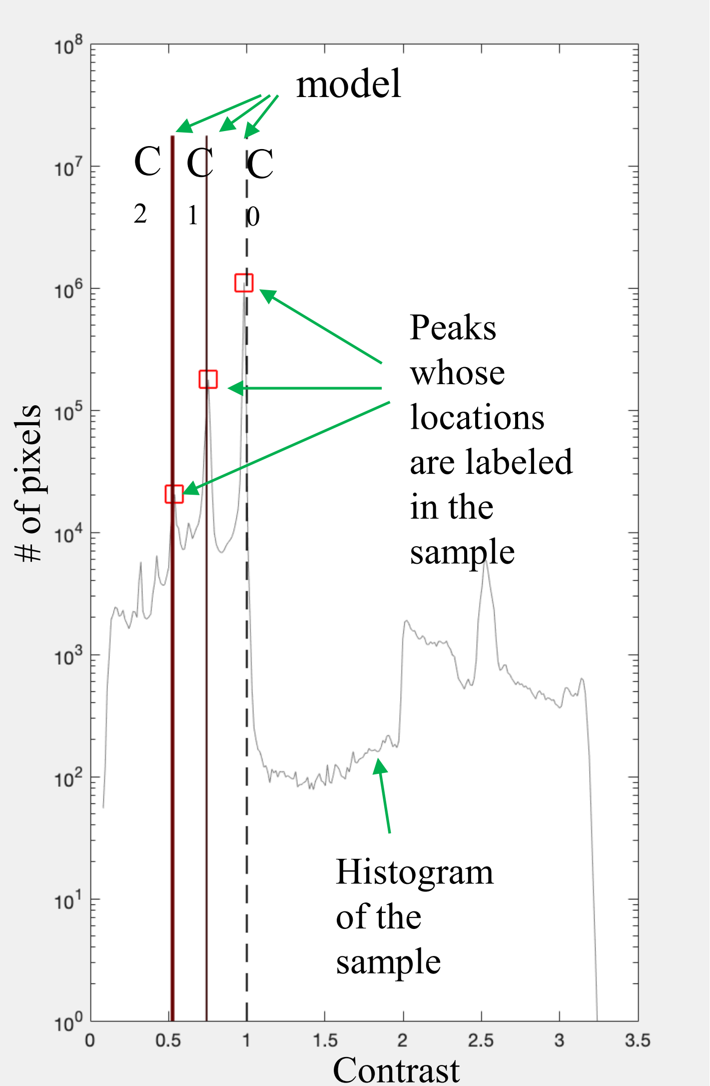
Calibration sample



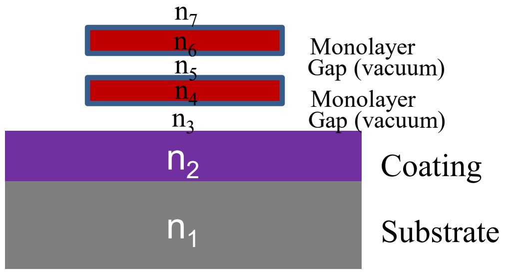

substrate — 2 layers

1 layer — >= 3 layer

Thicknesses verified by PL and AFM




*2D materials on a substrate with coating*



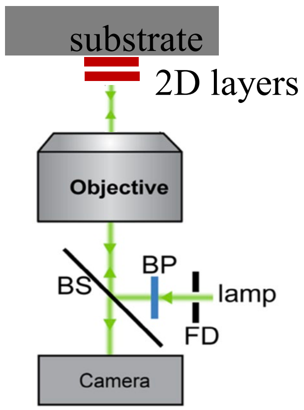

Calibrate for:

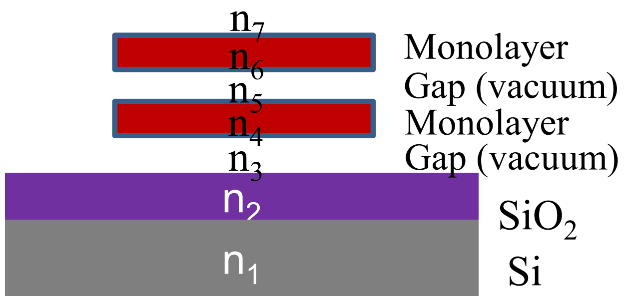
- Coating diffusive boundary with substrate
- Coating pure thickness
- Gap with the coating/substrate

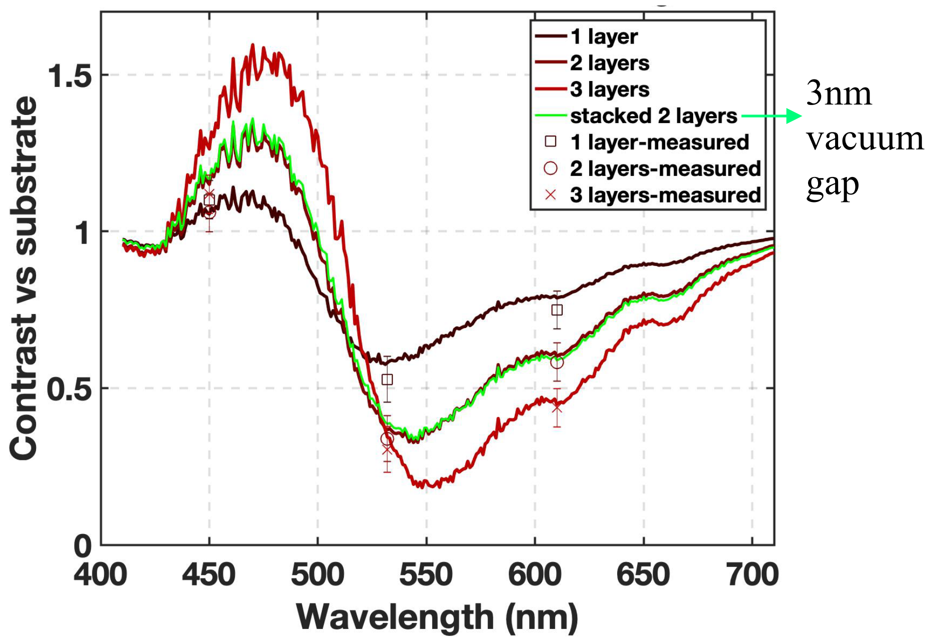
➢ Adjust until the modeled levels overlap with the peaks

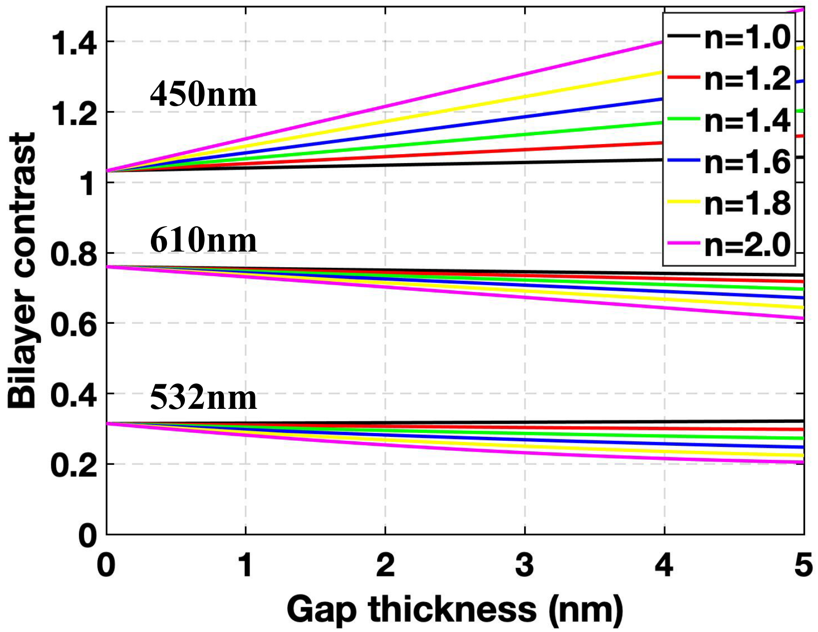
➢ Record standard deviation of the measured levels

# 2dreflect: experimental setup and modeling the effect of inter-layer gap




- 450nm illumination yields best contrast for stacked layers with inclusion
- Different SiO2 thickness will yield best contrast for stacked layers at different wavelength