

Review Report on PhD Thesis

Faculty: **Central European Institute of Technology
Brno University of Technology in Brno**

Academic year: **2024/2025**

Student: **Krishna Sampathkumar**

Doctoral study program: **Advanced Materials and Nanosciences**

Field of study: **Advanced nanotechnologies and microtechnologies**

Supervisor: **Prof. Ing. Pavel Neuzil, Dr., DSc.**

Reviewer: **Prof. Dr.-Ing. Prashanth Konda Gokuldoss**

PhD thesis title: Tailoring the physical properties of 2D materials

Topicality of doctoral thesis:

The doctoral thesis entitled: ***Tailoring the physical properties of 2D materials*** delves into one of the most dynamic and rapidly evolving areas of modern materials science, which is '***2D materials***'. Since the discovery of graphene, the exploration of atomically thin materials (2D materials) has surged, driven by their unique physical properties. This thesis is notably topical, addressing a critical need to understand and control the physical properties to harness the full potential of 2D materials in both fundamental research and technological applications.

Meeting the goals set:

The present thesis aims to exploit the strain engineering of graphene and TMDs to elucidate the hidden scientific phenomena from fundamental and application perspectives. It aims to identify the single monolayer graphene layer on opaque materials and by imposing the biaxial strain using a simple supporting polymer swelling. (1) A modified dry transfer technique is aimed at fabricating both suspended and supported heterostructures of a 2D material on any substrate. (2) Detection of graphene thickness on an optically opaque surface using the Raman peak from the silicon substrate and using the machine learning techniques. (3) Controlled formation of graphene wrinkles and imprinting nanopatterns onto the substrates. (4) Elucidate the exciton dynamics in a biaxially strained TMDs using the polymer swelling technique.

Based on the research objectives, the present thesis successfully developed methodologies to tailor the physical properties of 2D vdW materials through (a) controlled deformation, (b) strain engineering, and (c) functionalization. The dry transfer technique was revamped that has resulted in superior suspended

heterobilayers on SiN grids. The thesis has also developed a novel technique to determine graphene thickness on native oxide surfaces using the combination of Raman spectroscopy and ML model with accurate predictions. A technique was introduced for imprinting sinusoidal nano/microscale wrinkle patterns into soft polymer substrates using graphene as the imprinting agent. A methodology to exert biaxial tensile deformation on graphene by a swelling polymer (SU8) was established. The combination of mechanical strain and chemical modification effectively tailored graphene's physical properties, providing insights into reaction mechanisms and highlighting the need to account for non-graphene Raman bands when quantifying functionalization. The objectives/goals set were met (as desired).

Problem solving and dissertation results:

The objectives are well addressed using experimental and ML techniques. The results generated are reasonable and solves the problems to reach a conclusive conclusion and addresses the objectives/aim of the thesis.

Importance for practice or development of the discipline:

The importance of the lies in the demonstration that include the use of biaxial strain on atomically thin monolayers of graphene and MoS₂ by utilizing the swelling of polymer substrates in methanol. In graphene, the strain quantification was established via the Raman shift of the 2D band, while in MoS₂, photoluminescence (PL) tracked strain-induced changes. In addition, the utility of polymer swelling was effectively utilized to induce biaxial strain in 2D materials to tune their physical properties (electronic and optical properties).

Formal adjustment of the thesis and language level:

The language used in the thesis is readily readable and needs no adjustment.

Some formatting/typos:

- (1) At the first instance of using vdW, it should be abbreviated (especially in the keywords section).
- (2) The legends and text in the axes are difficult to read in Fig. 13.
- (3) The unit 0.35 m bar should be written as 0.35 mbar and 150W should be written as 150 W. All such typos need careful attention.
- (4) Some microstructures in Fig. 19/Fig. 23/Fig. 24/Fig. 25/Fig. 32 do not have scale bars.
- (5) The scalebars in Fig. 43 is hard to read.
- (6) Page – 96: Ref. 142 – Typo/formatting error.
- (7) Page – 97: Ref. 164 – Typo/formatting error.

Questions and comments:

- (1) The employed ML model needs further detailing. Any equations present behind the model should be furnished including the assumptions made.
- (2) The choice of employing graphene for biaxial strain experiments needs justification.
- (3) In addition, the choice of using TMDs (MoS₂ and WS₂) needs to be explained.
- (4) It may be good if the title can explain the type of physical properties that are considered in the thesis.
- (5) The effect after heating and UV exposure in Si substrate shown in Fig. 46 may include a brief explanation in the Fig. itself.
- (6) The influence of strain on the Raman spectra needs a detailed explanation and then it may be correlated with the present results.

(7) The influence of uniaxial and biaxial strain and their differences needs a detailed explanation.

Conclusion:

The reviewed thesis fulfills all requirements posed on theses aimed for obtaining a PhD degree. The thesis is well written and incorporates all scientific aspects for making the thesis complete. This thesis is ready to be defended orally, in front of the respective committee.

In Tallinn, Estonia, date: 05.02.2025

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Prof. Dr.Ing. Prashanth Konda Gokuldoss