Name: Animesh Sharma
Roll Number: 2201PH05
Title: Development of a Python-Based Framework for Scanning Probe Microscopy Data Processing

---

1. Introduction to Scanning Probe Microscopy

Scanning Probe Microscopy (SPM) techniques, including Atomic Force Microscopy (AFM) and Scanning Tunnelling Microscopy (STM), have become indispensable tools for nanoscale material characterisation. By measuring local surface interactions, mechanical, electrical, and chemical, SPM enables direct visualisation and quantification of nanoscale phenomena that cannot be accessed through conventional optical or electron microscopy. In particular, AFM has emerged as a versatile technique capable of operating in various modes (contact, tapping, non-contact) to probe both the topographical and mechanical properties of surfaces with nanometer or even sub-nanometer precision.

AFM operates by scanning a sharp tip attached to a cantilever over the sample surface. The tip–sample interaction causes deflection of the cantilever, which is measured by a laser beam reflected onto a photodetector. This deflection, proportional to interaction forces, can be converted into a **force–distance (F–δ)** curve. By interpreting these curves using models from contact mechanics, such as Hertz, DMT, or JKR, local mechanical parameters such as elastic modulus, adhesion energy, and hardness can be derived. Such mechanical insights are critical for understanding nanoscale systems like molecular films, biomaterials, and polymer composites.

---

2. Research Objectives

The main objective of this project is to develop a **Python-based computational framework** for the analysis of Scanning Probe Microscopy (SPM) data, with emphasis on AFM datasets used in nanoscale mechanical characterisation.

Specific objectives include:

1. **Design and implement data processing modules** capable of reading, filtering, and visualising raw AFM data such as height maps, force–distance curves, amplitude, and phase images.
2. **Compute physical quantities** such as elastic modulus, adhesion energy, and energy dissipation using established models like Hertz, DMT, and JKR.
3. **Generate automated maps** of mechanical properties (modulus, energy dissipation) for different material systems, including PyTp and PyTp–DNA complex films.
4. **Validate the framework** against published experimental data and ensure accuracy of physical parameters extracted.

5. **Create a modular, user-friendly design** to facilitate further development for other SPM modes and advanced analysis using machine learning.

These objectives ensure that the project bridges computational methods and nanoscale physics, offering a robust and reproducible tool for material characterization.

---

3. Physics of SPM Data and Its Processing

SPM datasets encapsulate several physical quantities: - **Height (topography)** maps showing surface morphology. - **Force curves** that describe tip–sample interaction forces. - **Phase shift data** indicating viscoelasticity, adhesion, and energy loss. - **Amplitude and frequency response** reflecting dynamic mechanical properties.

From a physics perspective, SPM data represent the probe's response to the surface potential energy landscape. For example, during indentation, deflection (d) relates to applied load (F) and indentation depth (δ) via Hooke's law ($F = k_c d$), while deformation depends on elastic modulus and surface adhesion. In dynamic (tapping) mode, the **phase lag (ϕ)** between the cantilever drive and its response encodes **energy dissipation**, caused by viscoelastic damping or adhesive hysteresis.

Energy dissipated per cycle (E_{dis}) is given by: $E_{dis} = \frac{\pi k_c A_0 A_{sp}}{Q} (\sin\varphi - \frac{f A_{sp}}{f_0 A_0})$

where (k_c) is the cantilever spring constant, (A_0) the free amplitude, (A_{sp}) the setpoint amplitude, (Q) the quality factor, and ϕ the phase lag. Processing such data transforms raw AFM signals into meaningful physical parameters: elastic modulus, hardness, and **energy dissipation maps**, enabling nanoscale mechanical insights.

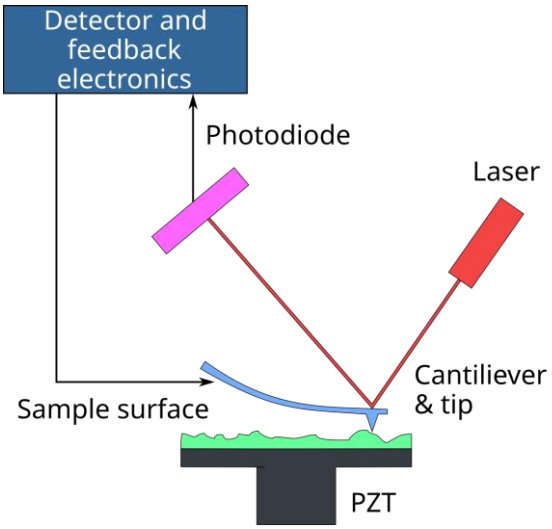

Figure 1: Schematic of AFM operation showing cantilever–tip and sample interaction.

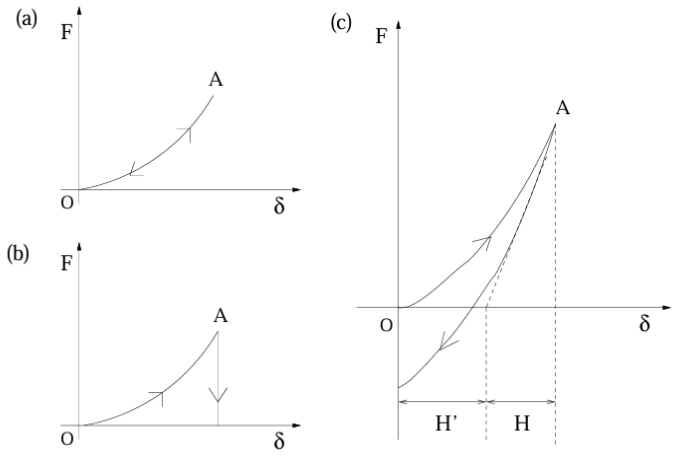

Figure 2: Typical force–distance (F–δ) curve illustrating approach, contact, and retract phases.

---

4. Need for a Python-Based Framework

Current AFM data processing relies heavily on proprietary software, limiting transparency and reproducibility. A Python-based framework will enable: - **Automated extraction** of force–distance curves and model fitting. - **Computation of mechanical property maps** using physics-based algorithms. - **Quantitative phase analysis** to derive spatial energy dissipation maps. - **Statistical correlation** between surface morphology and mechanical response.

Methodology Overview: The framework will be built in stages: (i) reading and visualising AFM datasets, (ii) implementing contact mechanics and energy dissipation models, (iii) validating parameters with literature data, and (iv) developing visualisation modules using Python libraries (NumPy, SciPy, Matplotlib, and PyQt). This will culminate in an open-source, physics-grounded tool for SPM data interpretation.

---

5. Summary

This literature review highlights the physics underpinning SPM, emphasising AFM-based mechanical and dissipative interactions. Prior research on PyTp and PyTp–DNA films demonstrates the connection between molecular interactions and nanoscale mechanics. The proposed Python framework aims to systematically process AFM data, compute physical quantities such as modulus and energy dissipation, and visualise nanoscale heterogeneity. This integration of physics and computation will enhance reproducibility and accessibility in nanomaterial characterisation.

References

[1] A. Bhaumik, M. Ramakanth, L. K. Brar, A. K. Raychaudhuri, F. Rondelez, and D. Chatterji, *Langmuir* **20**, 5891 (2004).

[2] J. O. Radler, I. Koltover, T. Salditt, and C. R. Safinya, *Science* **275**, 810 (1997).

[3] D. Putnam, *Nature Materials* **5**, 439 (2006).

[4] M. Guillot-Nieckowski, D. Joester, M. Stohr, M. Losson, M. Adrian, B. Wagner, M. Kansy, H. Heinzelmann, R. Pugin, F. Deiderich, and J. L. Gallani, *Langmuir* **23**, 737 (2007).

[5] M. P. W. Frances, L. R. Dorothy, and B. B. Marcel, *Biochemistry* **35**, 5756 (1996).

[6] M. Sastry, V. Ramakrishnan, M. Pattarkine, A. Gole, and K. N. Ganesh, *Langmuir* **16**, 9142 (2000).

[7] D. D. Lasic and N. S. Templeton, *Advanced Drug Delivery Reviews* **20**, 221 (1996).

[8] G. B. Sukhorukov, M. M. Montrel, A. I. Petrov, L. I. Shabarchina, and B. I. Sukhorukov, *Biosensors and Bioelectronics* **11**, 913 (1996).

[9] J. J. Gooding and G. C. King, *J. Mater. Chem.* **15**, 4876 (2005).

[10] L. Cui, J. Miao, and L. Zhu, *Macromolecules* **39**, 2536 (2006).

[11] D. Tranchida, S. Piccarolo, and M. Soliman, *Macromolecules* **39**, 4547 (2006).

[12] Sandeep Kumar and Santanu Kumar Pal, *Tetrahedron Letters* **46**, 4127 (2005).

[13] B. Du, O. K. C. Tsui, Q. Zhang, and T. He, *Langmuir* **17**, 3286 (2001).

[14] Alpana Nayak and K. A. Suresh, *J. Phys. Chem. B* **112**, 2930 (2008).

[15] G. Roberts, *Langmuir-Blodgett Films*, Plenum Press: New York, 1990.

[16] Alpana Nayak, K. A. Suresh, Santanu Kumar Pal, and Sandeep Kumar, *J. Phys. Chem. B* **111**, 11157 (2007).

[17] B. Bhushan, A. V. Kulkarni, V. N. Koinkar, M. Boehm, L. Odoni, C. Martelet, and M. Belin, *Langmuir* **11**, 3189 (1995).

[18] D. H. Gracias and G. A. Somorjai, *Macromolecules* **31**, 1269 (1998).

[19] V. Matti, J. Saily, S. J. Ryhanen, J. M. Holopainen, S. Borocci, G. Mancini, and P. K. J. Kinnunen, *Biophysical Journal* **81**, 2135 (2001).

[20] J. C. Wu, T. L. Lin, U. S. Jeng, H. Y. Lee, and T. Gutberlet, *Physica B* **385**, 841 (2006).

[21] K. Kago, H. Matsuoka, R. Yoshitome, H. Yamaoka, K. Ijiro, and M. Shimomura, *Langmuir* **15**, 5193 (1999).

[22] X. Chen, J. Wang, and M. Liu, *J. Colloid Interface Sci.* **287**, 185 (2005).

[23] Y. Okahata, T. Kobayashi, and K. Tanaka, *Langmuir* **12**, 1326 (1996).

[24] D. K. Schwartz, *Surface Science Reports* **27**, 241 (1997).

[25] M. Elena Diaz and R. L. Cerro, *Thin Solid Films* **460**, 274 (2004).

[26] T. Nguyen, W. E. Byrd, and D. Bentz, *J. Adhes.* **48**, 169 (1995).

[27] D. Raghavan, X. Gu, T. Nguyen, M. VanLandingham, and A. Karim, *Macromolecules* **33**, 2573 (2000).

[28] T. Akihiro, M. Sasaki, K. Hane, and S. Okuma, *Sensors and Actuators A* **40**, 71 (1994).

[29] M. Binggeli and C. M. Mate, *Appl. Phys. Lett.* **65**, 415 (1994).

[30] R. C. Thomas, J. E. Houston, T. A. Michalske, and R. M. Crooks, *Science* **259**, 1883 (1993).

[31] C. S. Braun, G. S. Jas, S. Choosakoonkriang, G. S. Koe, and J. G. Smith, *Biophysical Journal* **84**, 1114 (2003).

[32] W. Pisula *et al.*, *Adv. Mater.* **17**, 684 (2005).