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Goal of MiDA Lab research:

The research aims to establish an **intelligent**, closed-loop **nanometrology** framework that addresses the critical challenge of **measurement uncertainty** at the sub-nanometer scale. As semiconductor scaling approaches atomistic dimensions and novel advanced materials exhibit increasingly complex mechanical properties, conventional characterization paradigms face fundamental resolution and throughput bottlenecks. Tracing the evolution of metrology, this study targets the **research and development of metrology intelligence and subsequent data analysis,** especially with localized Atomic Force Microscopy (AFM) and high-throughput Optical Critical Dimension (OCD) metrology.

To overcome conventional limitations, this research presents a unified framework that combines artificial intelligence (AI), multi-physics Finite Element Method (FEM) simulations, and real-world experiments. The framework will be validated through rigorous experimentation to map physical property variations in 2D materials and optimize inline critical dimension profiling for next-generation semiconductor nodes (e.g., Gate-All-Around FETs). Ultimately, the research would deliver a traceable, high-accuracy, and uncertainty-aware intelligent metrology framework, significantly lowering measurement costs while accelerating time-to-market for advanced manufacturing and nanomaterials discovery.

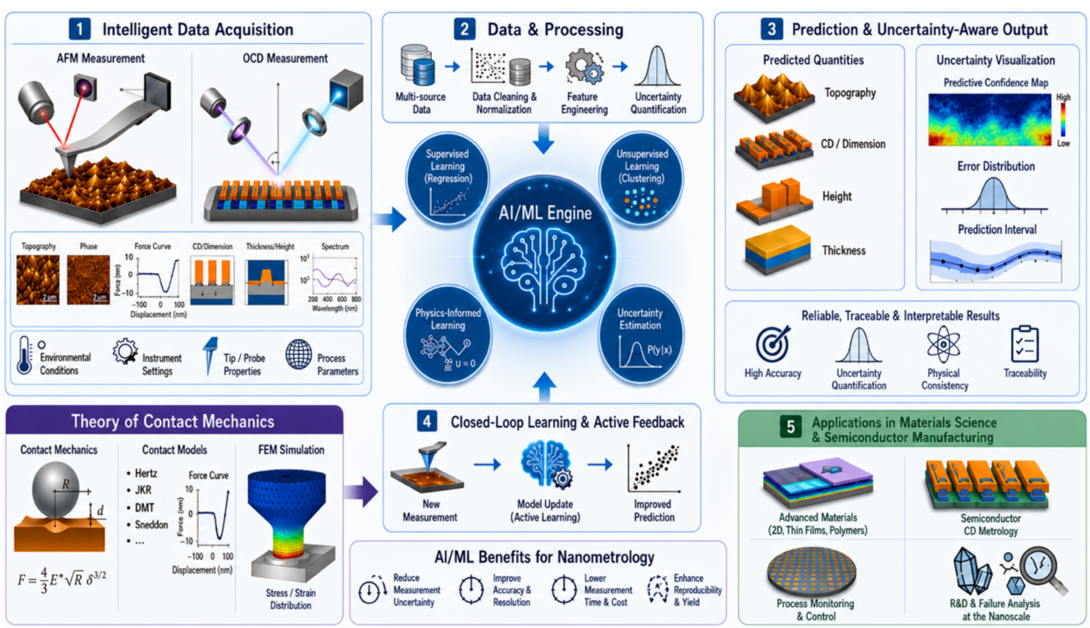

Figure 1. Representative machine learning (ML)/ AI approach benefit for Nanometrology in Materials Science and Semiconductor Manufacturing. (Not in scale)

1. Machine Learning (ML)/ AI Applications to Reduce Uncertainty in Metrology

Data-driven machine learning (ML) methods provide a promising approach for predicting the properties of both existing and emerging materials and for developing new material design strategies. Previously, ML approaches have been proposed for suggesting appropriate contact model, and forward to determine the elastic modulus of engineering materials based on the force-curve features, without the need of tip geometry needed. Therefore, in the future research, ML frameworks are continuously developed for predicting the adhesion energy of components, e.g., high entropy alloy films, based on several input variables, for example, elastic modulus, half-buckle width, Buckle height, thin-film thickness, etc. Besides, the ML framework can be used for classification purposes, such as classifying materials/components based on the elastic modulus, adhesion energy, deformation, etc.

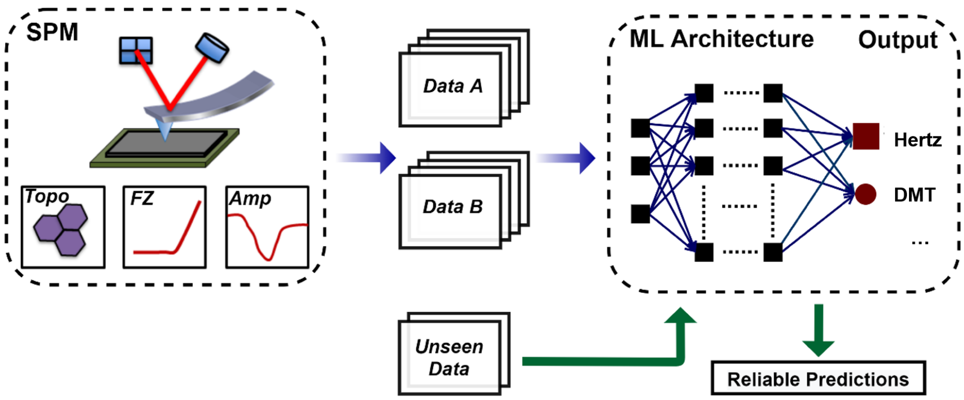

Figure 2. ML approach used in SPM-based measurements to learn data features and provide predictions of appropriate contact model. *(LTP Nguyen, BH Liu - European Journal of Mechanics-A/Solids, 2022)*

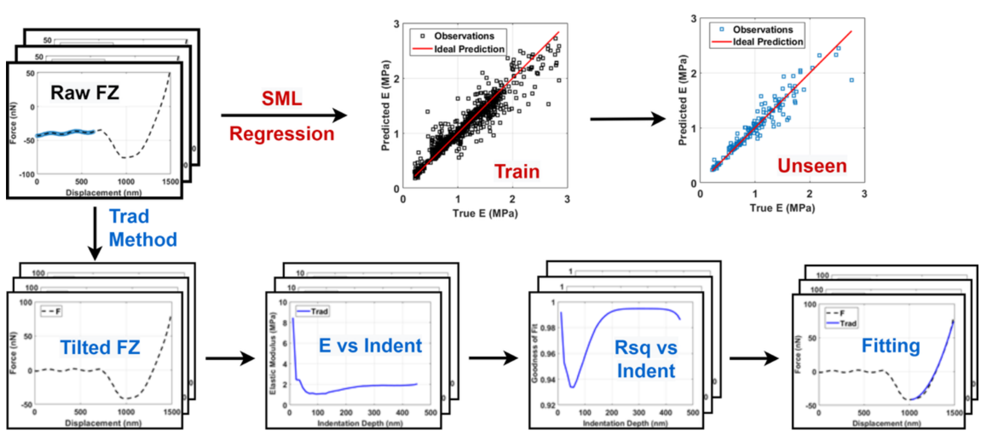

Figure 3. ML framework is capable of determining the elastic modulus of materials without contact model fitting. *(LTP Nguyen, BH Liu - International Journal of Solids and Structures, 2022)*

2. Computational and Data-Driven Methods Solving Issues in Contact Mechanics

Contact mechanics is essential for high-load mechanical components like gears and bearings, where surface curvature and microgeometry induce severe contact stresses and plastic deformation. In these systems, maintaining a precise lubricant film thickness is critical to prevent damaging metal-to-metal contact and ensure operational reliability. Furthermore, the extreme pressures generated within these tribological interfaces induce significant elastic deformation of the contacting bodies, which directly aids in building and maintaining the fluid film.

Future research aims to study consecutive impact EHL and PEHL behavior in anisotropic and inhomogeneous materials. Together with that, the research will integrate ML-based models offer the potential to predict contact stress, deformation, and lubricant film behavior. Particularly, machine learning (ML) models can be trained using simulation or experimental data, which learns the relationship between data feature and output parameters, then predicts these contact stress, deformation, and lubrication film thickness.

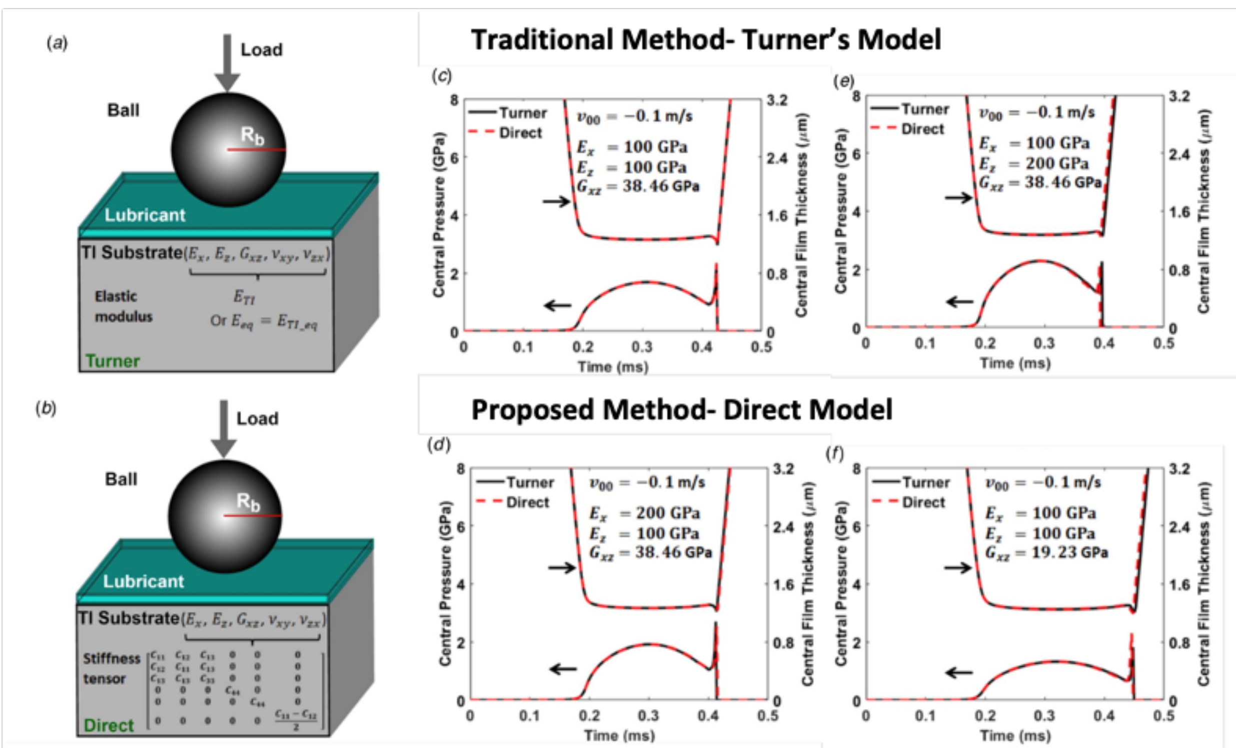

Figure 4. An EHL model based on a direct solving method for investigating the point contact between a rigid ball and a transversely isotropic substrate under impact loading. *(LTP Nguyen, WL Li - Journal of Tribology, 2024)*

3. Research and Development of AFM in Materials Science and Engineering

Many methods are applied to reduce measurement uncertainty in AFM data acquisition and subsequent data analysis, e.g., an increase of experimental replicates, development of automatic software, and improve the theoretical of calculation method. The previous proposed a self-designed 3D-printed AFM fluid cell to improve the resolution of AFM image as well the accuracy of determining quantitative values for bacterial adhesion and elastic modulus. The future research is aimed to develop theoretical model and establish autonomous package to speed up and improve the accuracy and precision of the AFM measurements.

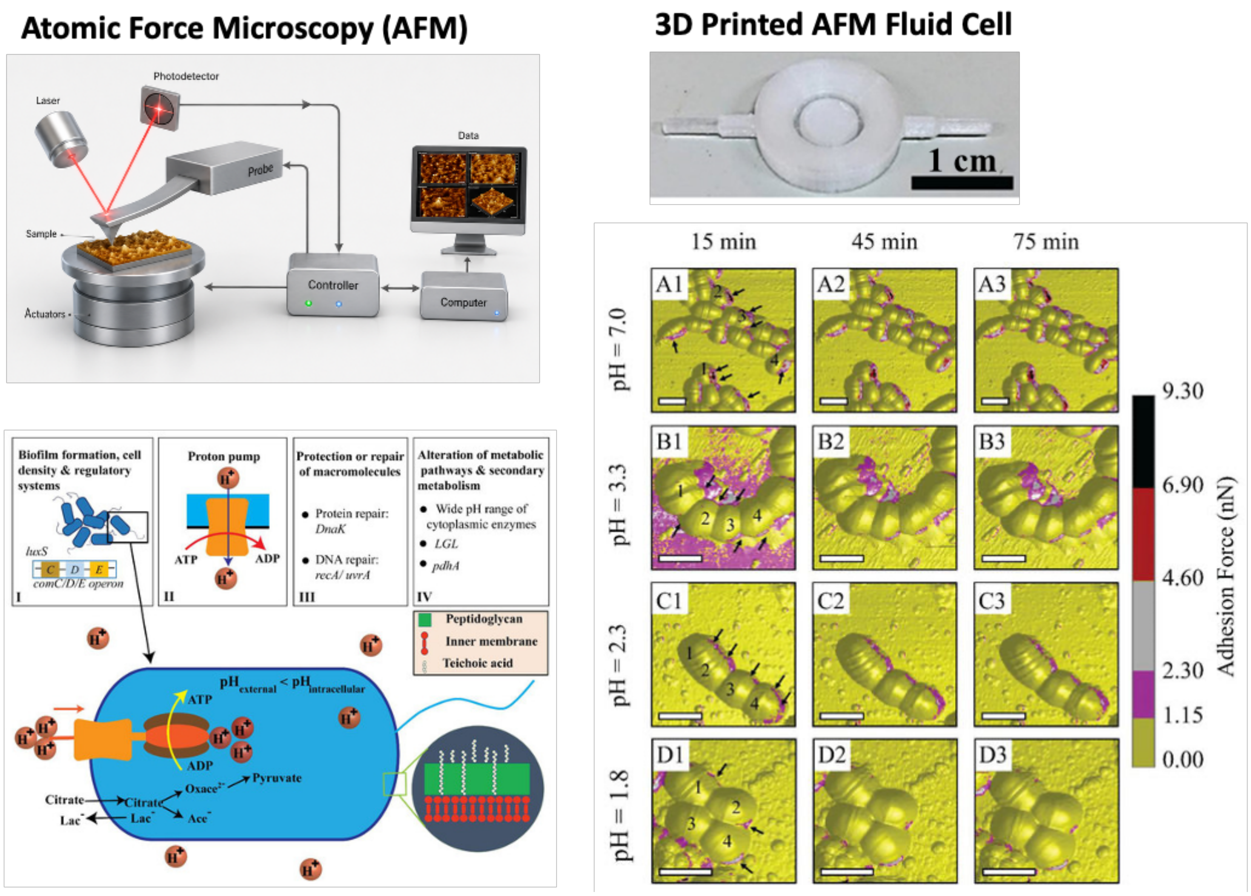

Figure 5. 3D printed AFM fluid cell proposed to investigate in-situ nanomechanical properties of Streptococcus mutans in citric acid. *(LTP Nguyen, BH Liu - International journal of molecular sciences, 2020)*

4. Research and Development of Ellipsometry in Semiconductor Manufacturing

Optical Critical Dimension (OCD) metrology is a vital technique in semiconductor manufacturing due to its non-destructive and highly efficient measurement capabilities. However, OCD metrology does not capture a direct image of a nanostructure. Instead, it shines a broadband beam of polarized light onto a specimen and records the resulting intensity and polarization changes in the reflected light, known as a spectrum. Because this inherently indirect measurement relies on a pre-built model to retrieve dimensional information from the spectrum, OCD ellipsometry requires prior knowledge of the target structure and specialized expertise to develop a regression model based on Rigorous Coupled-Wave Analysis (RCWA). With the increasing complexity of advanced semiconductor devices, OCD modeling also suffers from parameter correlation and regression instability. Future research aims to combine the complementary advantages of OCD and Atomic Force Microscopy (AFM) to improve the robustness of advanced metrology design.

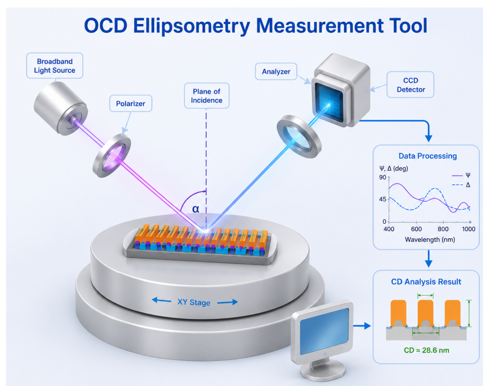

Figure 6. Reprentative working principle of ellipsometry measurement tool in semiconductor manufacturing.

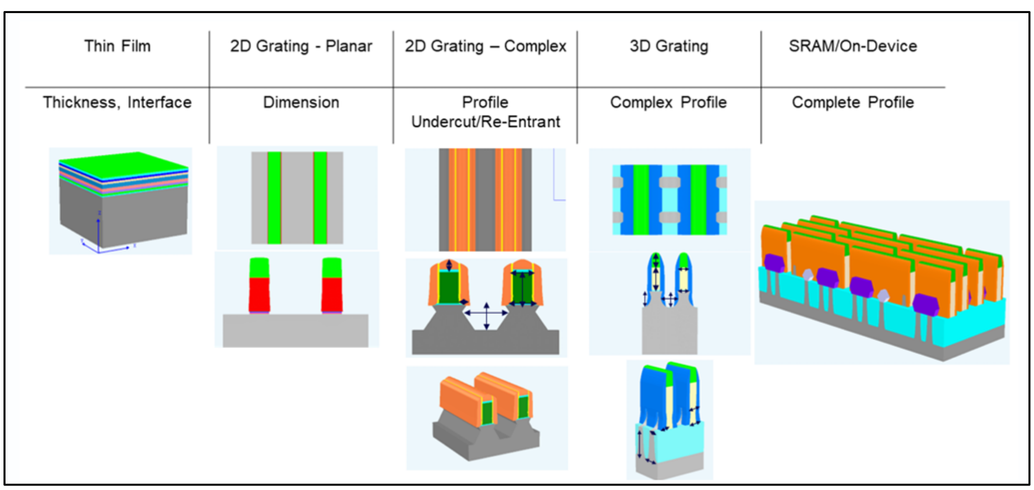

Figure 7. Summary of semiconductor structures measured using OCD. (Optical critical dimension Metrology with Spectroscopic Ellipsometry, Nick Keller)