SHORT ABSTRACT

This dissertation, entitled Predicting and Analyzing the Thermal and Electrical Properties of Materials Using Advanced Machine Learning Models, develops correction and prediction frameworks for thermal conductivity (TC) and electrical conductivity (EC) characterization in thin films by combining experimental methodology, physics-based modeling, and advanced machine learning (ML). The work is structured into two main parts. The first focuses on TC determination using Scanning Thermal Microscopy (SThM), addressing roughness-induced artifacts through simultaneous thermal–topographical mapping, quartz-referenced normalization, and ML regression. The second focuses on EC determination using Four-Point Probe (4PP) measurements and mitigates geometry-induced distortions through both Finite Element Method (FEM) simulations and a fully experimental ML-based correction framework.

The thesis is guided by two hypotheses. The first proposes that integrating SThM thermal mapping with detailed surface topography analysis and ML models trained on physically meaningful descriptors can overcome the limitations of conventional SThM analysis and enable accurate and reproducible thin-film TC estimation. The second proposes that both FEM and ML can generate effective correction factors for 4PP conductivity measurements by compensating geometric distortions such as edge effects and probe placement sensitivity, where FEM provides physics-based corrections and ML offers a scalable simulation-free alternative with comparable accuracy.

For the TC component, the thesis highlights the limitations of optical pump–probe methods such as TDTR/FDTR, which are accurate but spatially limited by optical diffraction and cannot resolve submicron TC variations. In contrast, SThM provides submicron resolution but suffers from strong dependence on probe–sample interaction, surface roughness, and contact variability. The measured thermal signal is shown to be a convolution of intrinsic TC, topography-dependent contact effects, thermal contact resistance (TCR), and substrate contributions, particularly for films below ~100 nm. To address this, the thesis develops an integrated TC methodology combining normalization and topography-based ML descriptors.

A core contribution is a quartz-referenced normalization procedure, defining a dimensionless thermal ratio Γ_i based on static and dynamic probe resistances measured on the sample and quartz reference. This reduces probe-dependent variability and improves cross-sample comparability. The experimental framework uses a multi-scale mapping strategy: each sample is mapped over a 2×2 μm^2 region divided into a 16×16 grid, and each region includes localized 375×375 nm^2 subwindows divided into 3×3 grids, enabling spatially correlated datasets linking thermal response to topography. Micro-scale descriptors include RMS roughness and surface skewness, while submicron descriptors include surface inclination, peak-to-valley variation, and local height distribution variability. A substrate–thickness factor C is introduced as a key ML input to distinguish bulk-like transport from substrate-dominated thin-film behavior.

Instead of directly predicting TC, the thesis defines a continuous target variable $\chi = \kappa^{s}/\sigma^{s_i}$, where σ^{s_i} represents localized height variation, improving regression stability and generalization. Feature relevance analysis using Spearman correlation identifies Γ_i as the dominant predictor, with strong contributions from submicron topography descriptors and C, while phase difference contributes negligibly. The TC dataset includes 3,332 measurements, with 2,352 for development and 980 for independent validation, spanning thin-film systems (annealed ITO on glass, ZnO on Si) and bulk references from 0.17 to 450 W m^{-1} K^{-1}. ML model development compares Random Forest and Gradient Boosting regressions, with extensive hyperparameter tuning across 279 models. Random Forest consistently performs best, achieving strong agreement with reference TC values across multiple orders of magnitude, particularly for low and moderate TC materials, with acceptable deviations at extreme TC ranges.

For the EC component, the thesis addresses limitations of vdP and 4PP methods. While vdP provides reliable sheet resistance under strict conditions, it is time-consuming and requires contact fabrication. The 4PP method is more practical but highly sensitive to geometry, probe spacing, and measurement position, requiring correction for edge-induced current distortions. The electrical dataset includes 553 measurements obtained using a custom-built 4PP system with Keithley instrumentation. Measurements cover irregular ITO films and metallic samples, using multiple probe positions and systematic sample rotations to capture diverse edge-effect regimes. Inputs include sample dimensions, diagonals, probe coordinates, and applied current.

A 3D FEM model in COMSOL validates geometric distortions and generates correction factors based on simulated vs intrinsic conductivity, producing FEM-corrected EC. In parallel, the thesis introduces an ML correction framework based purely on experiments by defining a continuous regression target Θ derived from the analytical 4PP relationship. The ML model predicts Θ from geometry and current, enabling calculation of corrected conductivity without simulations. Spearman correlation confirms current as the most dominant contributor to Θ, and Random Forest regression is optimized over 170 hyperparameter combinations. Performance comparisons using Relative Difference (RD%) show that both FEM and ML effectively correct EC under strong edge distortion conditions. For metals, FEM yields a mean RD% of +5.66% and ML -3.15%, while for ITO films FEM yields -4.30% and ML -2.93%, with ML showing tighter residual distributions. Final results demonstrate ML predictions typically within ±15% of reference values and strong consistency across ITO samples.