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**Review**

**of the doctoral dissertation of Mr. Mohsena Dehbashi, MSc. „Predicting and Analyzing the Thermal and Electrical Properties of Materials Using Advanced Machine Learning Models" was made at the Institute of Physics - C.N.D. of the Silesian University of Technology in Gliwice.**

The 104-page doctoral thesis submitted for evaluation, Mohsen Dehbashi MSc, analyzes the thermal and electrical properties of materials using advanced machine learning models. The PhD student addressed a crucial issue in the contemporary design, production, and use of optoelectronic devices – the study of the thermal and electrical properties of materials used in their production. These properties are thermal conductivity (TC) and electrical conductivity (EC). As the size of active devices in optoelectronic devices decreases, especially in electronics, efficient heat dissipation is one of the most important factors determining their performance. Importantly, in thin films and submicron structures, heat transfer mechanisms differ from those observed in their bulk counterparts. Accurately determining the electrical conductivity of thin films also poses a challenge in materials characterization.

The idea behind the work is excellent and aligns with contemporary trends in using machine learning methods to improve measurement processes, experimental interpretation methods, and their quality.

**Aim of the work**

The main aims of the work are presented in several places, only after an introductory discussion of the literature on the subject, which makes it somewhat difficult to organize them systematically:

• On page 6, the PhD student writes that the work aims to improve the accuracy of thermal conductivity measurements in thin films performed using Scanning Thermal Microscopy (SThM) by taking into account the influence of the surface roughness of the materials being tested. In this work, the author analyzes the advantages and limitations of existing methods and proposes improvements to data interpretation methods to characterize heat transport at the submicron scale more accurately.

• The problem description and research objective are also presented in Chapter 4 (on page 24), where it is explained that the research is divided into two main components: the determination of thermal conductivity (TC) and electrical conductivity (EC) in thin films.

• It was emphasized that the goal for TC research is to develop an integrated methodology that combines high-resolution spatial mapping, simultaneous thermal-topographic data acquisition, normalization procedures, and machine learning (ML) models. This aims to increase the reliability and repeatability of thin-film TC measurements, creating a scalable platform (by converting physical topography into numerical datasets) using topography-based descriptors (e.g., slope, peak-to-valley height) and combining experimental SThM data with computational predictive modeling.

• The goal of the EC component is to create a standardized and adaptable correction system that operates on experimental data. The author proposes a data-driven approach in which ML models learn and correct geometric distortions directly from measured data using the Four-Point Probe (4PP) method, eliminating the need for rigid geometries or destructive procedures while enabling more practical and scalable EC characterization. A correction system based on the finite element method (FEM) was also developed in parallel, enabling comparison of the obtained results.

**Research Objects and Methods**

Commercial 170 nm-thick indium tin oxide layers deposited on glass substrates and annealed in six different atmospheres were used in the research. Annealing processes were previously performed at 400°C in vacuum, air, oxygen ($O_2$), nitrogen ($N_2$), carbon dioxide ($CO_2$), and a mixture of nitrogen and hydrogen ($N_2$–$H_2$). Similarly, thin zinc oxide films were obtained as prefabricated samples. These were previously fabricated by atomic layer deposition (ALD), a technique that enables precise control over thickness and composition. Available ZnO films were deposited at 100°C and 200°C with varying numbers of ALD cycles, thereby varying film thickness and structural properties. Bulk materials with isotropic thermal characteristics were also considered in the study. These materials were chosen for their well-defined thermal properties and structural homogeneity, which are essential for accurate model calibration. The bulk materials studied included glass, glassy carbon, a single crystal of SiC, a single crystal of yttrium aluminum garnet (YAG), bulk ZnO, and polymethyl methacrylate (PMMA). The bulk materials served as reference standards to improve model calibration by providing well-characterized thermal properties. Information on sample sizes appears on page 58 of Chapter 7. The thermal conductivity (TC) measurements of the thin-film samples listed in Table 5.1 were previously performed using an atomic force microscope (AFM) (Park Systems XE-70) and two different thermal probes to ensure repeatability and minimize experimental error. A SThM probe (KNT-SThM-3an, Kelvin NanoTechnology) was used for TC measurements in this work. The 4 Point Probe Technique (4PP) with machine learning-based interpretation methods was used for electrical conductivity measurements. By systematically varying the probe position and sample orientation, a dataset was generated to train a model that can compensate for the inherent experimental complexity. Electrical measurements were performed using a Keithley Model 6221 current source for ITO samples, a Keithley Model 2231A-30-3 current source for metallic samples, and a Keithley Model 2182A nanovoltmeter to measure the net voltage for both sample types. Measurements were obtained using a 4-probe device with a 4-pin, 2-row, straight male connector (RS PRO) with a standard 2.54 mm pitch. To account for geometric effects and verify the experimental 4PP measurements, a 3D FEM model was developed in COMSOL Multiphysics.

This work is divided into two parts: one covering thermal measurements and the other covering electrical measurements, each divided into sections on the experiment and the interpretation of results. It would be easier to read if all the experimental information were presented in a single section, but the decision was left to the author.

A significant part of the work involves Machine Learning (ML). Its methods, Random Forest Regression and Gradient Boosting, demonstrate remarkable accuracy in capturing complex, nonlinear relationships in material datasets. The author demonstrates that integrating high-resolution thermal mapping with detailed surface topographic analysis, combined with advanced machine learning algorithms, can overcome the limitations of conventional SThM techniques. For EC measurements, the author demonstrates that both the Finite Element Method (FEM) and ML can generate effective correction factors that mitigate geometric distortions in 4PP measurements. Distortions (such as edge effects and probe position deviations) significantly affect the current distribution and voltage measurement, leading to inaccuracies in electrical conductivity determination. The author posits that machine learning -based frameworks offer an alternative to FEM, providing comparable accuracy with significantly shorter computational time. This demonstrates that machine learning is particularly suitable for scalable, high-throughput electrical conductivity characterization, where efficiency and adaptability are key.

**The organization of the paper and the characterization and evaluation of the content of individual chapters**

The paper consists of 13 chapters, the first of which provides an introduction to the literature on thermal issues, and the last contains a reference list of 74 references. All entries in the list have a DOI, allowing easy access to the articles. The chapters are divided into short subsections, making it easier to follow the author's argument and providing a better understanding of each section. This is a good solution. The author begins unusually, not with the aim of the work, but with a chapter that serves as an introduction and simultaneously presents the literature on the subject of measuring thermal properties (of materials). The chapter itself is interesting and comprehensively describes the topic, demonstrating the importance of studying these properties and presenting methods for doing so. It is noted that for small sizes, theoretical models based on classical laws often do not accurately describe thermal behavior, and heat transport becomes strongly dependent on surface and dimensional effects. The PhD student then describes methods for studying thermal properties: Time-Domain Thermoreflectance (TDTR), Frequency-Domain Thermoreflectance (FDTR), and Scanning Thermal Microscopy (SThM). The author discusses the limitations of TDTR and FDTR, noting that the accuracy of the extracted parameters depends largely on prior knowledge of the experimental input data, such as layer thickness, beam spot sizes, and heat capacities. The limitations of the methods motivate the PhD student to explore innovative techniques enabling higher-resolution TC measurements. The PhD student presents the basics of his SThM method, which uses a thermal probe that systematically scans the sample surface while simultaneously detecting temperature-dependent changes in the probe material's resistance. A schematic of the AFM-SThM system, combining atomic force microscopy (AFM) with a thermal probe, is presented. SThM enables ultrahigh-resolution thermal mapping along with topographic imaging.

The author points out that inconsistencies in SThM measurements (especially those related to surface roughness) are particularly problematic at the submicron-scale tip-sample interface. He

emphasizes the need for next-generation techniques that will more faithfully capture the complex interplay of forces, heat transfer mechanisms, and material reactions at the submicron scale. Advanced computational algorithms separate material properties from measurement artifacts, and machine learning (ML) techniques identify patterns in complex, multidimensional datasets.

Chapter two is another introduction, but also a literature review on electrical conductivity measurements. The PhD student emphasizes that reliable EC measurements in thin films are hampered primarily by edge effects, in which proximity to sample boundaries disrupts the current distribution, leading to uneven current paths and complicating overall measurements. The two most commonly used methods for measuring TC in thin films are described: the four-point probe (4PP) technique and the van der Pauw (vdP) method, which was previously used to measure reference materials. The 4PP method is widely used to determine material resistance because it effectively eliminates errors caused by contact resistance. Factors such as sample geometry and probe position influence measurement accuracy. Sample geometry plays a significant role in determining accurate conductivity values. The size, shape, and thickness of the material affect the current distribution, necessitating the use of correction factors to ensure reliable results. The PhD student emphasizes that to increase the accuracy of 4PP techniques, numerical simulations and computational methods were incorporated into the experimental work, allowing for refinement of the measurement techniques.

Chapter three presents the research background for the work, continuing the ideas from the previous chapters, in which the PhD student demonstrated knowledge of the literature. In electrical conductivity studies, the main challenge in EC measurements is the influence of sample geometry. This complexity increases significantly as the device characteristics decrease, causing the assumptions underlying theoretical formulas to break down. This requires adopting methodologies such as FEM modeling, which accounts for complex geometries and boundary conditions, as well as developing data-driven approaches, such as ML, to automate correction processes and handle multiparameter nonidealities. The research motivations and hypotheses are presented in Chapter 4, which was already described at the beginning of this review in the section on the work's objective. Chapter 5 presents the methodology and experimental (thermal) procedures, and the first subsection describes the materials tested and the measurement methods used, which were also summarized at the beginning of the review. A note comes to mind: in the case of indium tin oxide (ITO), samples were used after six different annealing processes. Information is lacking on why these thermal treatments were chosen and on their impact on surface properties (e.g., roughness). The author previously wrote that surface properties influence the measurement and accuracy of the chosen method, and even small topographic features on a submicron scale can disrupt the interaction between the measuring probe and the sample surface. To investigate this effect, it would be useful to select several material samples that undergo the same surface treatment (e.g., annealing) but with different surface parameters, and test how the author's model performs.

The title of subsection 5.3. "A Factor as ML Input for Substrate and Thickness Consideration" likely lacks the letter C, referring to the substrate thickness factor introduced as an additional ML input parameter to quantitatively account for the influence of thin film dimensions and substrate properties.

In the next section, the author describes the influence of surface topography on the study of thermal parameters. The thermal characterization methodology used a framework in which the effective thermal resistance of each discrete grid cell in the sample matrix (initially set to 5.2) was evaluated relative to the corresponding thermal resistance of the reference material. This differential approach was used to normalize measurement deviations and isolate the intrinsic thermal properties of the tested samples. The definition of this cell and the structure (framework) are omitted here, but this will be discussed later in the chapter. The author notes that surface roughness increases thermal resistance by reducing the actual contact area between the probe and the sample. The tip contacts only high-roughness points (irregularities), while air-filled cavities act as insulating gaps. In contrast, a surface with an atomic structure is smooth, ensuring near-perfect contact, maximizing contact area, and minimizing resistance by creating efficient thermal-conduction paths. For the author, it is crucial to develop analytical data to train the ML model to distinguish between bulk and thin-film samples, as thin films exhibit fundamentally different heat transfer properties that, if not accounted for, would introduce significant inaccuracies in the measured TC. The study uses thin films on silicon substrates and bulk silicon; the thermal conductivity results (Table 5.1) show a significant difference (an order of magnitude) between the two. To illustrate the capabilities of the methods used by the author, it would also be useful to compare materials where the ZnO layer is deposited on a different substrate. This would better demonstrate how, and whether, the substrate affects the ability to determine the properties of the layer above. Comparison is not possible for ITO, as the properties of the bulk material were not measured. This chapter introduces the substrate thickness factor (C factor) as an additional ML input parameter to quantitatively account for the influence of thin-film dimensions and substrate properties on TC measurements during ML model development. At the beginning of the next section, the author describes the framework (platform) described earlier. This study utilized a microstructural analysis framework, focusing on a precisely defined $2 \times 2$ μm² region, divided into a high-resolution $16 \times 16$ measurement grid. The designed microgrid architecture enables comprehensive characterization of surface morphology and its influence on thermal transport phenomena at the submicron scale. This grid-based analytical framework enables several improvements in thermal metrology. The PhD student then introduces Microscale Topographical Parameters and Submicron-scale Topographical Parameters. The analytical protocol incorporates standard statistical surface metrology, with particular emphasis on two topographic parameters: root-mean-square roughness and surface skewness. This approach enables the study of local thermophysical phenomena by capturing submicron-scale parameters that govern interfacial heat transfer mechanisms. Table 5.2 provides an overview of the data collected and documented during the laboratory experiments. It's unclear whether the data refers to all samples or just a selection. What's the significance of this table? Besides showing the range of variables used for ML training, what conclusions can be drawn from it? The PhD student uses a machine learning (ML) framework specifically designed to mitigate the experimental errors inherent in submicron-scale thermal characterization, arising from the complex interactions among multiple variables. The ML model is trained on a multidimensional dataset encompassing the full range of experimentally measured thermal and topographic parameters. Before training the model, the methodology employs a rigorous feature selection protocol based on Spearman's rank correlation.

This statistical preprocessing step serves several key purposes: it quantitatively assesses the predictive importance of each measured parameter relative to the target TC values. It

systematically identifies and eliminates variables with statistically insignificant correlations, retaining only those parameters that demonstrate strong physical relationships with the thermal transport phenomena under study. The PhD student develops a machine learning model using a regression framework to provide accurate and generalizable TC predictions. By integrating thermal, topographic, and material properties while preserving TC's continuous nature, his model aims to overcome the limitations of categorical classification methods. The model architecture is specifically designed to predict a continuous multiplicative variable, $\chi = \kappa_s/\sigma_{si}$, where $\kappa_s$ represents the TC of the sample and $\sigma_{si}$ denotes the standard deviation of the surface height obtained from topographic measurements. In Chapter 5.7, the PhD student introduces new concepts in machine learning, stating that he strives to explain them as clearly as possible and provides references to the primary literature. Model performance is quantified using statistical metrics such as $R^2$, RMSE, MAE, and AARD%, which collectively indicate how well the predictions match experimental values. For these typical statistical analysis variables, it would be helpful to recall their names in the text (although they are provided at the beginning of the paper), briefly explaining their possible values and their meaning in the fitted data. This would facilitate analysis and understanding of the results. The author describes two ML models, Random Forest Regression and Gradient Boosting Regression, which have proven effective, demonstrating remarkable accuracy in capturing complex, nonlinear relationships within material datasets. Random Forest Regression and Gradient Boosting Regression are two advanced machine learning methods based on ensembles of decision trees. They are used to predict continuous values but differ in their model-building and optimization approaches. A key advantage of Random Forest Regression is its ability to model nonlinear relationships between input variables and material properties without relying on predefined mathematical formulas. The Gradient Boosting method uses a sequential ensemble approach, in which each new decision tree is trained to correct the residual errors of previous trees.

Chapter 6 presents measurement results and a discussion that evaluates ML models for predicting thermal conductivity, with a focus on hyperparameter optimization, model selection, and performance validation. The author presents an evaluation of the Gradient Boosting and Random Forest models using an extensive grid search approach combined with cross-validation to identify optimal hyperparameter configurations that maximize prediction accuracy. The experimental design relies on training and evaluating 279 separate models (each with a different set of hyperparameters). Unfortunately, the author does not provide information on how these models were selected or why this number was selected. The hyperparameters of the ML models that were tested and analyzed in this study are presented in Table 6.1. It is valuable to provide definitions and explanations of these quantities below the table, though this is not convenient for the reader. The hyperparameter tuning for the Gradient Boosting and Random Forest Regression methods, model selection, and validation are presented next (6.1). Comparative evaluation showed that the Random Forest model consistently outperformed the Gradient Boosting method in terms of predictive accuracy, as confirmed by numerous statistical performance metrics. Table 6.4 presents a comparison of the actual and predicted thermal conductivities ($\kappa$) for the samples. For some samples, very good agreement with the reference data was achieved. It would have been beneficial if the table also included basic information on the surface properties of these samples.
Chapter 6 concludes the section on thermal measurements, and the next chapter is devoted to electrical conductivity measurements and refinements using ML.

I'm not sure whether this arrangement is convenient for the reader, i.e., separating the experimental section for thermal properties in Chapter 5 and Chapter 7 for electrical properties, or whether it wouldn't be better to split it into the experimental section and present both

experiments (thermal and electrical in one) at the beginning of the thesis, but this was the PhD student's decision.

The electrical measurements are presented in Chapter 7; the apparatus used by the PhD student is described in the introductory part of the review. The study uses a precise 4PP system integrated with machine-learning-based interpretation methods. By systematically varying the probe position and sample orientation, a dataset was generated that allowed for training a model capable of compensating for the real-world experimental complexities. Table 7-2 presents summary information on sample dimensions and probe position, as well as a statistical summary of the experimental measurements. The data represent 553 observations per parameter. I'm not convinced this data was worth tabulating. The following short sections present the mathematical foundations and the machine learning model.

Results and discussion of the electrical measurements are presented in Chapter 8, which begins with FEM simulations. The goal of this simulation was to replicate the experimental setup under controlled numerical conditions and develop a physics-based correction that would improve the accuracy of the conductivity measurements. The effectiveness of the FEM correction is quantitatively presented in Table 8-1, which compares the measured, numerical, simulated, actual ($\sigma_a$), and FEM-corrected ($\sigma_{FEM}$) conductivity values for the iron (Fe) sample for different probe configurations. Model performance was evaluated for various Random Forest Regression hyperparameter settings. A total of 170 distinct hyperparameter combinations were evaluated to fine-tune the model for improved generalization. The question was, what was the key to selecting these parameters? Table 8-4 shows the best-identified hyperparameters for each ML model and their corresponding prediction accuracy. Radar plots are presented next to aid in selecting the best hyperparameters. I don't fully understand how these plots were constructed – they show parameters with significantly different values across three axes. The plots depict triangles that are close to isosceles, while, for example, model a has RMSE = 16.208, AARD% = 3.328, and MAE = 5.088. However, considering the values in the table alone allows for a correct interpretation of the results. The evaluation shows that of the four Random Forest models (a–d), model "a" is the optimal choice due to its superior performance across all measured metrics. In the training set, model "a" achieved the lowest RMSE (16.208), AARD% (3.328%), and MAE (5.088), significantly outperforming the others. This advantage is visually illustrated in Figure 8-4, where the polygon for model "a" is the smallest, confirming its best fit to the training data. The performance of ML- and FEM-based approaches for estimating EC is presented in turn. Predicted EC values ($\sigma_{ML}$) are derived from Equation 7.4 using the ML-predicted $\Theta$ values, while simulated EC values ($\sigma_{FEM}$) are calculated using Equation 7.2. Figure 8-7 illustrates the relative percentage difference (RD%) between predicted and simulated EC values for metal samples. Information is missing regarding the specific samples for which this is shown, or the meaning of the circles and segments in Figures 8-7 and 8-9. However, as the PhD student writes, these results illustrate that both techniques—one based on physical laws and the other on data patterns—yield solutions that are similarly accurate yet characteristically different to the ITO characterization problem.

The results confirm that FEM and ML can serve as complementary approaches: FEM provides fundamental physical information, ML offers an effective empirical approximation, and both methods maintain good agreement with experimental reality for ITO materials. The final section and Table 8-6 present a comparison of theoretical, predicted, and actual EC values for nine different samples, including four ITO samples and five metal samples (Cu, W, Ni, Fe, Sn).

The predicted EC values ($\sigma_{ML}$, derived from Eq. 7.4) were obtained by averaging the EC values predicted by the ML model using a new set of unseen data for each sample. Similarly, the simulated EC values ($\sigma_{FEM}$) were calculated by averaging the results across different experimental conditions for each sample using Eq. 7.2. As the PhD student writes, the results highlight the complementary strengths of both approaches: Random Forest Regression and Gradient Boosting. FEM utilizes detailed physics-based simulations and offers high performance when comprehensive material modeling is available, particularly for ITO systems. In contrast, the ML approach demonstrates promising generalization capabilities across both oxide and metallic samples, with clear potential for further improvement with expanded, more diverse training datasets. These results suggest that combining the precision of physics-based FEM with the adaptability of data-driven ML could lead to a more robust and reliable framework for electrical conductivity characterization in future research. Conclusions and plans for method development are presented in Chapter 9. This coherent, well-structured chapter clearly summarizes the PhD student's achievement. The final sections of the thesis include appendices presenting topographic and thermal maps of the samples for thermal property analysis, a plot of paired data for thermal property studies, supplementary data on electrical conductivity, and a comparison of experimental, numerical, intrinsic, and FEM-corrected EC. Unfortunately, there are no comments, conclusions, or summaries.

**The most important achievements of this work include:**

- For thermal measurements:
  - o Development, validation, and demonstration of a methodology for determining thermal conductivity in thin films that addresses the main limitations of the SThM method, in particular surface topographic effects.
  - o Use of thermal-topographic mapping, normalization and correction strategies, and machine learning.
  - o Confirmation of the effectiveness of combining physics-based strategies with machine learning for measuring thermal conductivity.

- For electrical measurements:
  - o Development of a method for accurately determining electrical conductivity in thin films using the four-point probe technique.
  - o Use of machine learning and comparison with FEM results to correct geometric artifacts and ensure the consistency of conductivity estimates using experimental measurements.
  - o Combining FEM and ML enables accurate and repeatable characterization of the electrical conductivity of thin films with non-ideal geometries.

The methods used in this work and the results obtained are of great practical importance, enabling the new method to be applied to the study of industrial structures.

**Editorial evaluation of the work:**

The work is well written and well organized, and the argument is clear and systematic. Beginning with a literature review and placing the research motivations and hypotheses in chapter four does not make the content easier to understand. Two issues concerning thermal and electrical measurements are discussed efficiently. Experimental methods are logically combined with interpellations using machine learning. A good solution was to divide the work

into many short subchapters, which facilitated the author's thoughts and systematized the information. The results, presented graphically, are generally clear and readable.

**Conclusion:**

Mohsen Dehbashi, M.A., obtained several interesting and valuable results in his work, which significantly expand current knowledge of thermal scanning microscopy and the Four-Point Probe. The proposed measurement methods and the interpretation of results using machine learning were thoroughly analyzed and experimentally verified. The author is familiar with the field in which he works, and his work aligns well with research conducted using thermal and electrical methods at other research centers. His research also aligns with the growing use of machine learning methods to interpret experimental results. Analysis of the presented results allows us to conclude that the initial goals of the work have been achieved. The work submitted for review meets all the requirements for doctoral dissertations specified in the Act on Academic Degrees and Titles. Therefore, I request that Master Mohsen Dehbashi be admitted to the next stages of his doctoral studies.

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