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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.

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

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 2×2 μm² region, divided into a high-resolution 16×16 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

The predicted EC values (σ_{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 (σ_{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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