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Review of the doctoral dissertation by

Mr. Mohsen Dehbashi

entitled ***'Predicting and Analyzing the Thermal and Electrical Properties of Materials Using Advanced Machine Learning Models'***

carried out under the guidance of the supervisor Prof. Jerzy Bodzenta and the auxiliary supervisor Dr. Justyna Juszczyk-Synowiec at the Division of Applied Physics, Institute of Physics, Silesian University of Technology

Modern technologies pose challenges for the miniaturization and integration of devices and for the use of the thin layers with desired thermal, electric or optical properties in their construction. Well-defined parameters of the layers determine the efficiency and stable performance of various systems, including those used for energy storage and the opto- or micro-electronic ones. The research described in the doctoral dissertation focuses on developing a methodology allowing for more precise ascertaining of the thermal or electric conductivity parameters of materials, especially thin layers, based on experimental results supported by advanced machine learning models. The subject matter dealt with in the dissertation is relevant not only in the scope of conducting interdisciplinary research (including materials engineering and physical sciences), but also due to the demand and need for characterization of systems in nano- and submicronic scales, allowing for the optimal use of their potential.

The doctoral dissertation submitted for review has been put together in the form of a scientific monography and comprises 104 pages. The format of the doctoral dissertation is not of a standard type; traditionally, it should begin with a title page instead of a list of chapters referring to its contents. On pages 6-21, Mr. Mohsen Dehbashi presents an introduction and literature review, divided into two parts, in which the methods used for ascertaining the thermal or electric conductivity parameters of materials are described. In further chapters, we can find the description of the challenges related to precise determining of properties of low-dimensional and thin layer functional systems. In the chapter 'Motivation and hypothesis', Mr. Mohsen Dehbasi presented the problem statement and arguments

supporting the necessity for conducting research in the scope of the chosen subject matter as well as the research aims and hypotheses. In chapters 5 and 7, the applied methodology and procedures used for ascertaining thermal and electrical properties of the studied systems are discussed at length. The obtained results and discussion are presented by Mr. Mohsen Dehbashi in a concise form in chapter 6 (9 pages (pp 45-53)) and chapter 8 (15 pages (pp 61-75)), and in chapter 9 – he presents the conclusions related to potential predicting and analyzing thermal or electrical conductivity of thin layers, based on the approaches he puts forward and the prospect of further study developments in this area. In the later part of the dissertation, annexes A-C are included, which contain supporting information related, among other things, to various activities and achievements of Mr. Mohsen Dehbashi. The volume is completed with a bibliography containing 74 items.

In the doctoral dissertation, Mr. Mohsen Dehbashi presented an interesting and original approach to ascertaining thermal conductivity of materials by means of the scanning thermal microscopy (SThM) method combined with machine learning models and normalization techniques.

In contact mode, the SThM method allows for simultaneous measurements of the thermal-topographical signal under identical conditions. A comprehensive analysis of the data enables determining a correlation between the morphology of the surface and thermal reaction of the studied material, which allows for an insight into the mechanisms governing heat transfer at small scales. Due to the impact of thin layer surface topography and the contact between a tip and a sample on the measurements of thermal properties, correct interpretation of the data acquired by means of this method may be stymied. That is why the Author proposed using a machine learning method (Random Forest regression) to enable more precise prediction of thermal properties of studied materials. He also applied a normalization procedure (referenced to quartz) and a substrate-thickness factor. This allowed for eliminating the limitations of SThM results analysis (the micro- and nano-structural (topographic) surface variability and the impact of the substrate), resulting in getting thermal conductivity results of a better quality (precise and reliable).

The models used by the Author were tested on proper sets of data and quantitative validated encompassing thermal properties of reference materials and literature-reported values. The predictive accuracy which was achieved proves that the approach proposed by Mr. Mohsen Dehbashi to a large extent reduces device-related limitations and indicates the benefits of integrating experimental technology with computational modelling.

The combination of an experiment, offering high spatial resolution (locally determined surface topography) and the ability of studying local thermal properties (analysis of heat dissipation) at the nanoscale as well as techniques of machine learning allows for limiting artefacts (variability of

contact and morphology-induced) having impact on the actual values of the parameters determining heat transport in thin layers (of thickness less than 100 nm). It would seem that, despite the complexity of thin layer characterization, the proposed approach might be applied to predict and analyze thermal conductivity for a wide range of materials. At the same time, the Author indicates potential possibilities for further developing and improving the methodology, which may allow for a standardized and scalable thermal characterization of functional thin layers.

In the doctoral dissertation, Mr. Mohsen Dehbashi also attempted to apply numerical simulations to determine the impact of various parameters on the accuracy of measuring electrical conductivity. The van der Pauw method (four-point probe) is used to measure the electrical conductivity of thin layers with arbitrary shape and thickness (including irregular thin layers). However, this particular method is sensitive to sample geometry and edge effects, which can influence the results for electrical conductivity; that is why they need to be adjusted. The Author proposed a solution in which the finite element method (FEM) and machine learning were used independently to adjust the geometrical sample distortion and the probe placement. He had assumed that taking into account the finite sample dimensions, variable placement of the probe and edge effects should allow for obtaining credible values of electrical conductivity, a parameter characteristic for the studied material.

The conducted study included a comparison of the results of numeric and experimental simulations of electrical conductivity obtained for 4 different thin layers of indium tin oxide (ITO) as well as 5 metallic samples (Cu, W, Ni, Fe, Sn) using a probe in a square arrangement (for four probes placed at the vertices of a square, on the arbitrary sample surface). Additionally, Mr. Mohsen Dehbashi built a 3-dimensional model using FEM to validate the experimental results and compared the obtained values with the actual value of the electrical conductivity used as the model parameter.

On the basis of the conducted study, Mr. Mohsen Dehbashi concluded that the proposed approach, using the FEM based model, allows for introducing the geometric constraints (eliminating the effects originating from non-ideal measuring conditions while using a four-point probe method and the sample) and obtaining corrected results for electrical conductivity much more closely consistent with the actual values. He also demonstrated machine learning algorithms being able to, when provided with empirical data, directly predict correct values of electrical conductivity across diverse experimental conditions.

It would appear that proposed by the Author the way of predicting, verifying, and validating results shows benefits resulting from applying numeric simulations and artificial intelligence methods in the analysis of experimental results, in this particular case ascertaining electrical conductivity. The presented approach has potential, which might be used not only in the field of engineering and

technology, including the study of materials but also in other fields of science or in the realm of industry and applied science.

The issues discussed in the doctoral dissertation related to the research subject matter, which he took on, were well developed, including appropriately selected literature references, which indicates that Mr. Mohsen Dehbasi has general theoretical knowledge in the discipline of materials engineering, especially in the area of methods used for ascertaining thermal and electrical properties of thin layers. The proposed research concept, the methodology used, the appropriate selection of computational methods and models and the interpretation of the results demonstrated the benefits resulting from the application of machine learning methods in analyzing experimental results, especially for measurements of the thermal properties of the sample. The chapter of the doctoral dissertation, related to describing and discussing the results, is not quite extensive, but the final conclusions have been properly expressed.

It would appear that all of the assumed research aims of the doctoral dissertation have been met. Some of the results included in the dissertation or related with its subject have been published in journals from the JCR database (*International Journal of Heat and Mass Transfer* and *Materials*), as well as included in the monography chapter, and presented at an international conference. Moreover, Mr. Mohsen Dehbashi is also a co-author of 3 publications listed in the Scopus database, which are not related to the subject of his doctoral dissertation.

During the public defence, I would like the Author to address a few questions/remarks that appeared while reading the dissertation:

1) apart from introducing additional reference data, what other way would you suggest may be used to further develop the method of determining thermal conductivity that you propose?
2) there is still a discrepancy between the corrected and actual values of thermal conductivity; would you be able to estimate to what extent they could be further corrected once the methodology has been improved?
3) can you specify what the limitations of using machine learning methods in materials science, including the characterization of thin films, are?
4) how would you explain (p. 89), the electrical conductivity values of the 'ITO (a) at Rotation 1' sample being 100-times higher than those of the other ITO samples?
5) p. 65; unfortunately, Table 8-3 has not been quoted in the text of the dissertation.

In compliance with Art. 187 sec. 4 of the Act of 20 July 2018 – The Law on Higher Education and Science (Journal of Laws of 2024, item 1571, as amended) 'The doctoral dissertation shall include an abstract in English, whereas a doctoral dissertation prepared in a foreign language – an abstract in

Polish'. With reference to the above, the doctoral dissertation of Mr. Mohsen Dehbashi,, which has already been disseminated and handed over to the library, should be annexed with the abstracts required by the law.

In summary, the doctoral dissertation demonstrates the theoretical knowledge of Mr. Mohsen Dehbashi in the area of materials engineering and informatics, in particular, improving methods for characterizing thin layers. The carried out analysis of the results and the conclusions drawn on their basis indicate that Mr. Mohsen Dehbashi presented the original solution of the scientific problem and showed his ability to independently conduct research. This doctoral dissertation contributes new information to science related to the use of advanced machine learning models to predict and analyze the thermal and electrical properties of materials.

Taking into consideration the above opinion, I conclude that the doctoral dissertation submitted for review complies with the requirements described in Art. 187 sec. 1-3 of the above mentioned Act of Law, that is why I am asking you to accept my recommendation and to allow Mr. Mohsen Dehbashi to pursue the next stages of the procedure for awarding a PhD degree in the discipline of materials engineering.

Prof. Alina Dudkowiak

/podpis odręczny/