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Review of the doctoral dissertation

by Mr. Upadesh SUBEDI, M.Sc., Eng.

entitled:

Towards Digital Twins for Quantifying Laser-Microstructure Interface in Multicomponent Alloys Using Thermodynamic Tensor Model

prepared under the supervision of:

Tomasz TAŃSKI, Ph.D., D.Sc., Eng., Professor of the Silesian University of Technology

Assistant Supervisor: Anil Kunwar, Ph.D., Eng.

1. Basis for the review

The review was prepared at the request of the Materials Engineering Discipline Council of the Silesian University of Technology.

The legal basis is Article 187 of the Act of 20 July 2018, Law on Higher Education and Science (as amended).

The opinion concerning the doctoral dissertation in question contains three elements:

1) An assessment, together with justification, of whether the doctoral dissertation demonstrates the Doctoral Candidate's general theoretical knowledge in the discipline of Materials Engineering;

2) An assessment, together with justification, of whether the doctoral dissertation demonstrates the ability of the Doctoral Candidate applying for the degree of doctor to conduct scientific work independently;

3) An assessment, together with justification, of whether the doctoral dissertation constitutes an original solution to a scientific problem.

2. Characteristics and description of the dissertation

General remarks

The doctoral dissertation submitted for review by Mr. Upadesh Subedi, M.Sc., Eng., entitled "Towards Digital Twins for Quantifying Laser-Microstructure Interface in Multicomponent Alloys Using Thermodynamic Tensor Model", was prepared at the Silesian University of Technology under the supervision of Tomasz Tański, Ph.D., D.Sc., Eng., Professor of SUT, and Assistant Supervisor Anil Kunwar, Ph.D., Eng.

The dissertation is devoted to an extremely topical and important scientific problem concerning the quantitative description, modeling, and prediction of microstructural evolution during laser processing of multicomponent alloys. The author of the dissertation indicated that the processes occurring during the interaction of a laser beam with a material include mutually coupled phenomena of heat transfer, diffusion of alloying elements, phase transformations, interfacial reactions, and meltpool dynamics. Understanding these phenomena and developing methods for their quantitative description constitute one of the most important challenges of contemporary materials engineering and are crucial for the development of modern additive manufacturing technologies and the design of new-generation materials.

The Doctoral Candidate undertook a very ambitious research task consisting in the development of a unified, thermodynamically consistent computational environment enabling the representation, quantitative description, compression, reconstruction, and prediction of the evolution of the laser–microstructure interface in multicomponent alloys. This task required the combination of advanced phase-field modeling, tensor representation of microstructural data, and machine-learning methods. A particularly important aspect of the research was the establishment of foundations for the construction of Digital Twins, enabling the prediction of microstructural changes under conditions close to real time.

It should be noted that the reviewed dissertation has an original form. It is a description of research presented in a cycle of five thematically coherent scientific publications published in renowned journals. The individual publications form a logical whole, leading the reader from issues related to the presentation of microstructural data, through the modeling of laser processes and the evolution of intermetallic phases, to the use of artificial-intelligence methods in predicting the behavior of materials.

The most important scientific achievement of the Doctoral Candidate should be considered the development of the author's Thermodynamic Tensor Model, which enables the efficient mapping, storage, and reconstruction of information on microstructural evolution. The author demonstrated the possibility of representing the results of phase-field simulations in the form of multidimensional tensor structures subjected to reduction, decomposition, and reconstruction processes without losing key information on microstructural morphology and interphase boundaries.

The use of artificial-intelligence methods to predict microstructural evolution should also be regarded as highly original. The research results demonstrated the possibility of effectively integrating multiphysics models, thermodynamic calculations, and machine learning within a unified computational environment forming the basis for the construction of Digital Twins of laser-processing operations for multicomponent alloys.

The author of the dissertation addressed a difficult and interdisciplinary research problem located at the interface of materials engineering, numerical modeling, materials informatics, and artificial intelligence. I believe that the results obtained make a significant contribution to the development of methods for modeling materials processes and provide a basis for the future development of Digital Twins of materials and their manufacturing technologies.

Editorial remarks

The doctoral dissertation was prepared very carefully, both in substantive and editorial terms. It is written in correct and precise scientific language, appropriate for doctoral dissertations in the field of materials engineering. The author uses specialist terminology consistently and correctly, and the manner of presenting the research demonstrates a very good command of both materials-science issues and the computational methods and artificial-intelligence tools used in the work.

The structure of the dissertation is logical, clear, and coherent. The individual chapters have been arranged in a way that allows the reader to become gradually acquainted with the research problem and to understand the successive stages of its solution. Particular emphasis should be placed on the fact that, despite preparing the dissertation in the form of a collection of publications, the author managed to preserve the uniform character of the study and to create a coherent scientific narrative leading from the identification of the research problem to the formulation of the final conclusions.

The first chapter presents a broad introduction to the issues of laser–microstructure interaction in multicomponent alloys, indicating the current state of knowledge, the most important research challenges, and the existing scientific gap. The second chapter contains clearly formulated objectives of the work and specific objectives, which are consistently pursued in the subsequent parts of the dissertation. In the third chapter, the Author precisely defines the scientific problem and formulates research hypotheses constituting the basis for the analyses carried out. The most extensive fourth chapter is devoted to presenting the main research results and integrating the results obtained within the individual publications. This chapter constitutes a valuable synthesis of the results contained in the publications and emphasizes their mutual relationships. The final chapter contains well-formulated final conclusions and interesting directions for further research, indicating possibilities for developing the proposed methodology in the context of Digital Twins of materials and technological processes.

The high quality of the illustrative material also deserves attention. The figures, diagrams, and tabular summaries are clear, well described, and properly linked to the content of the dissertation. The bibliography has been carefully selected and includes current publications concerning phase-field modeling, additive technologies, machine learning, and Digital Twins.

Thesis, objective, and scope of the work

The subject matter undertaken by the Doctoral Candidate fits into one of the most dynamically developing areas of contemporary materials engineering, related to the digitalization of materials-design processes and the use of artificial-intelligence methods for modeling and predicting microstructural phenomena. The Doctoral Candidate's motivation for undertaking the research was the gap observed in the scientific literature between very accurate but computationally expensive multiphysics models describing microstructural evolution and fast predictive models based on data analysis, which often lose the physical and thermodynamic interpretability of the results. This problem is of particular importance in the case of multicomponent alloys subjected to laser processing, where the course of microstructural processes depends on mutually coupled thermal, chemical, and kinetic interactions.

The analysis of the state of the art carried out by the Doctoral Candidate showed that, despite the intensive development of phase-field modeling methods, representations of microstructural data, and machine-learning tools, there is still a lack of a universal approach enabling the simultaneous preservation of thermodynamic information, efficient processing of high-dimensional data, and rapid prediction of microstructural evolution.

On this basis, the Author of the dissertation formulated the main research hypothesis, assuming that thermodynamic tensor representation is capable of preserving spatial, interfacial, and thermodynamic information to a degree that enables the effective use of machine-learning methods for predicting microstructural evolution induced by laser-beam interaction. Consequently, it becomes possible to establish the foundations for constructing Digital Twins of laser-processing operations for multicomponent alloys.

The main objective of the dissertation was to develop a unified, thermodynamically consistent computational environment intended for the quantitative description and prediction of the evolution of the laser–microstructure interface through the integration of multiphysics phase-field modeling, tensor representation of microstructural data, and machine-learning methods. This objective was developed through a number of specific objectives, including the development of a Thermodynamic Tensor Model, the construction of non-isothermal phase-field models for laser-processing operations, the development of methods for the quantitative characterization of microstructural interfaces, the creation of predictive models based on Conv-LSTM and U-Net architectures, and the integration of all these elements toward the construction of a Digital Twin of the process.

The scope of the work is very broad and distinctly interdisciplinary. The research was carried out for several representative material systems, including Ti–Cr, $Cu_x(Ti\text{-}6Al\text{-}4V)_Y$, Ti–Au, and Au, analyzing both the growth processes of intermetallic phases and the evolution of the meltpool during laser-beam interaction. An important part of the work also consisted of studies on the compression, reconstruction, and analysis of high-dimensional microstructural data and their use in predictive models.

It should be emphasized that the research methodology applied is modern, original, and consistent with current global trends in the development of materials engineering. The integration of multiphysics modeling, tensor representation, and machine-learning methods is undoubtedly one of the most valuable aspects of the dissertation and demonstrates the Doctoral Candidate's very good scientific preparation and his ability to conduct research at the interface of several advanced research disciplines.

3. Assessment of the doctoral dissertation

The doctoral dissertation submitted for review constitutes an original and valuable scientific achievement in the field of contemporary materials engineering, situated at the interface of materials-process modeling, computational thermodynamics, materials informatics, and artificial intelligence. The author addressed a research problem belonging to very topical issues currently developed in world science, related to the construction of Digital Twins of materials processes and the use of machine-learning methods to support the design of materials and their manufacturing processes.

Particular emphasis should be placed on the fact that the doctoral dissertation was prepared in the form of a cycle of five thematically related scientific publications published in renowned international journals, such as Scripta Materialia, Materials & Design, Engineering with Computers, and Computational Materials Science. Such a form of dissertation requires not only the achievement of results of high scientific value, but also their positive verification by reviewers of international scientific journals. All the publications form a substantively coherent cycle devoted to the development of methods for the quantitative description, representation, modeling, and prediction of microstructural evolution in materials subjected to laser-beam interaction.

On the basis of the presented co-author declarations, it should be stated that the Doctoral Candidate's contribution to the preparation of the publications constituting the basis of the dissertation was significant and, in most cases, dominant. In four of the five publications, the Doctoral Candidate is the first and corresponding author, and his contribution ranges from 60% to 72%. It primarily included the development of the research concept, preparation of computational models, execution of numerical simulations, analysis and interpretation of the results, development of the research methodology, and preparation of the original versions of the manuscripts. This testifies to the high degree of the Doctoral Candidate's scientific independence and his leading role in the implementation of the research presented in the publications.

Against the background of the current state of knowledge, a particularly important achievement of the dissertation is the development of a unified concept for describing the laser–microstructure interface, treated not as a classical phase boundary but as a complex, dynamic region of mutual interaction between thermal energy, chemical composition, and the changing morphology of the microstructure. Such an approach constitutes a significant extension of classical methods for modeling laser-processing operations, which most often analyze individual phenomena separately, without their full integration within a single computational model.

I consider the development of the author's concept of Thermodynamic Tensor Representation to be the most important scientific achievement of the dissertation. This solution enables the representation of high-dimensional microstructural data generated by phase-field models in a compact, mathematically ordered form that at the same time preserves the physical interpretability of the data structure. Many methods of data dimensionality reduction are available in the literature; however, they most often lead to the loss of part of the physical information. The Doctoral Candidate demonstrated the possibility of performing data compression, decomposition, and reconstruction while preserving key information on microstructural morphology, the position of interphase boundaries, and their evolution. This achievement should be regarded as an important contribution to the developing area of the application of informatics in materials engineering.

I also highly value the development of advanced multiphysics phase-field models intended to describe the processes occurring during laser processing of multicomponent alloys. Particularly valuable are the studies concerning the growth of Ti_2Cu intermetallic phases in the $Cu_x(Ti\text{-}6Al\text{-}4V)_Y$ system and the creation of a non-isothermal multiphase model for the Ti–Au system. These models take into account the coupled interaction of heat transfer, diffusion of components, material flow in the liquid meltpool, and phase transformations, thereby allowing a much more complete description of the processes occurring during laser-beam interaction than the solutions encountered in most previous publications.

Among the most valuable elements of the dissertation, I also include the use of artificial-intelligence methods for predicting microstructural evolution. The Conv-LSTM models developed by the Doctoral Candidate enable the prediction of microstructural changes in successive stages of system development, whereas the MicroTwin and FlowTwin models based on the U-Net architecture make it possible to predict phase distributions and velocity fields on the basis of temperature data. Particular emphasis should be placed on the fact that these models are not purely statistical in nature, but use data derived from thermodynamically consistent multiphysics simulations. Such an approach corresponds to current global trends in the development of Physics-Informed Machine Learning methods and constitutes an important step toward the construction of reliable Digital Twins of materials processes.

The interdisciplinary character of the dissertation also deserves attention. The author demonstrated very good knowledge of issues in the fields of materials engineering, thermodynamics, numerical methods, data analysis, and machine learning. The skillful combination of these areas of knowledge made it possible to develop a new research methodology whose significance goes beyond the material systems analyzed in the work and may also find application in other technological processes using local energy sources.

In summary, I consider the doctoral dissertation to be a mature, original, and valuable scientific achievement. The author not only solved the research problem posed, but also proposed a new methodology integrating multiphysics modeling, tensor representation of data, and artificial-intelligence methods. The solutions developed make a significant contribution to the development of modern materials engineering and create solid foundations for the further development of the concept of Digital Twins of laser-processing operations for materials.

4. Remarks

- To what extent is the developed tensor model universal? Is it possible to apply it to ceramic or composite materials, where the character of microstructural evolution is different from that in metallic alloys?

- The developed methodology was verified for selected alloy systems. Which groups of materials does the Author consider the most promising for further research using the proposed approach?

- The dissertation used data generated by phase-field models. How does the Author envisage the possibility of integrating the developed computational environment with real process data originating from monitoring of LPBF, DED, or other additive-manufacturing technologies?

- Can the developed methodology be extended to predicting the functional properties of materials (e.g. hardness, strength) on the basis of the predicted microstructure? What would be the main challenges of such an approach?

• Which elements of the developed methodology still require further development in order to make it possible to create a Digital Twin operating in real time and supporting the control of the technological process under industrial conditions?

5. Final opinion

The doctoral dissertation submitted for review by Mr. Upadesh Subedi, M.Sc., Eng., entitled "Towards Digital Twins for Quantifying Laser-Microstructure Interface in Multicomponent Alloys Using Thermodynamic Tensor Model", concerns a topical and important scientific issue related to the modeling of materials processes, the digitalization of materials research, and the use of artificial-intelligence methods for the description and prediction of the microstructural evolution of materials subjected to laser-beam interaction.

On the basis of the analysis of the dissertation, I state that the Doctoral Candidate demonstrated very broad and well-established theoretical knowledge in the discipline of materials engineering. He carried out an in-depth analysis of the current state of knowledge, correctly identifying the existing limitations of methods for modeling microstructure and indicating directions for their further development. The manner of formulating the scientific problem, research hypotheses, and interpretation of the obtained results unequivocally confirms the very good theoretical preparation of the Author of the dissertation and his scientific maturity.

The Doctoral Candidate independently carried out numerical analyses, developed computational models, critically interpreted the results, and formulated conclusions of a scientific and application-oriented nature. The author's leading contribution to the publications constituting the basis of the dissertation additionally confirms his significant contribution and research independence. The results obtained constitute an important contribution to the development of contemporary materials engineering and open new possibilities for research on the digital design of materials and technological processes.

In summary, I state that the doctoral dissertation of Mr. Upadesh Subedi, M.Sc., Eng., presents a high scientific level, confirms the Doctoral Candidate's possession of well-established theoretical knowledge in the discipline of materials engineering, demonstrates his ability to conduct scientific work independently, and constitutes an original solution to a scientific problem.

In view of the above, I state that the reviewed dissertation meets the requirements specified in Article 187 of the Act of 20 July 2018, Law on Higher Education and Science, and I request that the Materials Engineering Discipline Council of the Silesian University of Technology admit Mr. Upadesh Subedi, M.Sc., Eng., to the further stages of the proceedings for the award of the degree of doctor in the field of engineering and technical sciences in the discipline of materials engineering.

At the same time, taking into account the very high scientific level of the dissertation, the high originality of the results obtained and published in renowned international journals, and the significant contribution to the development of modern methods for modeling materials processes and the concept of Digital Twins in materials engineering, I request that the doctoral dissertation of Mr. Upadesh Subedi, M.Sc., Eng., be awarded distinction.

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