RDYMa. 512.5.2026

REVIEW OF THE DOCTORAL DISSERTATION

Candidate: Upadesh Subedi, M.Sc., Eng.

Title of Dissertation: "Towards Digital Twins for Laser Processed Multi-Component Alloys through Laser-Microstructure Interface Quantification"

Discipline: Materials Engineering

Reviewer: Dr. Hab. Francisco Javier Dominguez Gutierrez

1. Formal Assessment

The doctoral dissertation entitled "Towards Digital Twins for Laser Processed Multi-Component Alloys through Laser-Microstructure Interface Quantification" has been submitted as a dissertation based on a coherent collection of scientific publications accompanied by a comprehensive summary integrating the scientific achievements of the candidate. The dissertation addresses a highly relevant and contemporary research topic situated at the intersection of materials engineering, computational materials science, phase-field modeling, thermodynamics, machine learning, and digital manufacturing. The work focuses on the development of computational methodologies aimed at accelerating the prediction of microstructural evolution during laser processing and contributing toward future Digital Twin frameworks for advanced manufacturing. The dissertation consists of five peer-reviewed publications addressing different aspects of laser-material interactions, thermodynamic modeling, tensor representation of microstructures, machine learning-assisted prediction of microstructural evolution, and phase-field simulation of laser-induced transformations.

2. Scientific Merit and Originality

The scientific topic addressed in the dissertation is timely and important. The development of predictive frameworks capable of connecting processing parameters with microstructural evolution remains one of the major challenges in Integrated Computational Materials Engineering (ICME) and Digital Twin development.

The principal scientific achievements of the dissertation may be summarized as follows:

- Development of a thermodynamic tensor representation framework for the description and compression of multidimensional microstructural datasets.

- Application of advanced phase-field methods for simulation of laser-induced microstructural evolution in several alloy systems.

- Integration of machine learning techniques, including Conv-LSTM and U-Net architectures, for accelerated prediction of microstructure evolution and melt pool characteristics.

- Formulation of a Laser-Microstructure (L-M) interface concept as an intermediate representation between process parameters and resulting material states.

- Demonstration of a computational framework that may serve as a future component of Digital Twin architectures for additive manufacturing and laser processing applications.

The candidate demonstrates a broad knowledge of thermodynamics, phase transformations, numerical modeling, and data-driven materials science. The interdisciplinary character of the work represents one of its major strengths.

3. Evaluation of Methodology

The methodological framework combines phase-field modeling, thermodynamic calculations, tensor decomposition methods, and machine learning algorithms. The phase-field formulations are generally presented correctly and are based on accepted thermodynamic principles. The numerical implementation appears technically sound and is supported by examples involving Ti-Au, Ti-Cu, Au, Ti-Cr, and CoCrFeNi systems. The machine learning component is well integrated with the physics-based simulations and demonstrates a modern approach toward surrogate modeling of computationally intensive processes. Particularly valuable is the effort devoted to reducing computational complexity through tensor representations and data compression techniques. The candidate demonstrates the ability to combine advanced computational techniques into a coherent research framework.

4. Scientific Contributions

The dissertation contributes to several research directions simultaneously:

- Computational materials engineering.
- Phase-field modeling of laser processing.
- Materials informatics.
- Physics-informed machine learning.
- Digital Twin methodologies.

The strongest contribution is the integration of these approaches into a unified workflow rather than the development of a single isolated method. The publications included in the dissertation have appeared in recognized international journals, demonstrating the scientific quality and visibility of the work.

5. Critical Remarks

Despite the high scientific quality of the dissertation, several aspects deserve critical discussion.

5.1 Thermodynamic Tensor Model

The dissertation identifies the Thermodynamic Tensor Model as a central novelty. However, the distinction between the proposed framework and existing tensor decomposition methodologies such as Tucker decomposition, HOSVD, and other reduced-order modeling approaches could be articulated more clearly. The reviewer would appreciate a more rigorous discussion of what constitutes the fundamentally new scientific element beyond the application of established tensor methodologies to thermodynamic datasets.

5.2 Digital Twin Concept

The title and overall narrative strongly emphasize Digital Twins. While the presented framework undoubtedly represents an important step toward Digital Twin development, a complete Digital Twin generally requires continuous data acquisition, bidirectional communication, uncertainty management, and real-time updating mechanisms. In its current form, the framework should perhaps be viewed as a Digital Twin enabling technology rather than a fully realized Digital Twin implementation.

5.3 Experimental Validation

The dissertation relies predominantly on computational modeling. Although comparisons with experimental observations are provided, the validation remains largely qualitative in several cases. Additional quantitative validation against independent experimental measurements would strengthen confidence in the predictive capability of the proposed framework.

5.4 Generalization of Machine Learning Models

The machine learning models are trained primarily using simulation-generated data. The dissertation would benefit from a more extensive discussion of extrapolation capability, uncertainty quantification, and transferability to systems outside the training domain.

5.5 Transferability

The applicability of the framework to broader classes of multicomponent alloys is suggested but not yet fully demonstrated. Future work should address the limits of transferability with respect to composition, processing conditions, and microstructural complexity.

6. Questions for the Candidate:

1. What fundamentally differentiates the proposed Thermodynamic Tensor Model from existing tensor decomposition and reduced-order modeling techniques?
2. How would real-time experimental feedback be incorporated into the proposed Digital Twin architecture?
3. How would the proposed methodology perform when applied to irradiation-induced microstructural evolution rather than thermally driven laser processing?
4. What strategy would be used to quantify uncertainty in the machine learning predictions?

7. Final Assessment

The doctoral dissertation addresses an important scientific problem in contemporary materials engineering and presents original scientific achievements. The candidate demonstrates the ability to independently formulate research objectives, apply advanced computational methods, critically analyze results, and publish research in recognized international journals. In my opinion, the dissertation fulfills the requirements set forth in the Act of 20 July 2018 – Law on Higher Education and Science and the Regulations for Awarding the Doctoral Degree at the Silesian University of Technology. Therefore, I support the admission of the Candidate to the subsequent stages of the doctoral procedure and recommend the award of the degree of Doctor in the discipline of Materials Engineering.

Considering the scientific quality of the publications, the interdisciplinary character of the work, and its international visibility, the dissertation may also be considered for distinction, subject to fulfillment of the additional criteria applied by the Discipline Council.

Date: 01.07.2026

Dr. Hab. F. Javier Dominguez G.

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