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Review of

doctoral dissertation by Mr. Sachin Poudel, M.Sc. Eng., as a collection of thematically linked publications in scientific journals under the collective title - „SCALE Bridging Computational and Data-Driven Design of Microstructures in Multicomponent Alloys for Advanced Functional Materials”

This review was prepared at the request of Dr. hab. inż. Alicja Piasecka-Belkhat, Chair of the "Mechanical Engineering" Discipline Council at the Silesian University of Technology, dated July 15, 2026. The supervisor of the reviewed doctoral dissertation is Dr. hab. inż. Anna Timofiejczuk, and the co-supervisor is Dr. inż. Anil Kunwar.

1. Nature of the work

The ongoing development of industry drives the emergence of new structural methods and technologies. These advancements are inextricably linked to the materials available for use, prompting the creation of new materials and associated processing technologies. Such materials find applications across various scientific fields—extending well beyond mechanical structures alone. Materials analysis is a modern specialization utilized in the design of advanced structures; it encompasses the broad concept of computer-aided materials design. This approach is crucial for the optimal utilization of modern materials in contemporary engineering structures. However, knowledge in this area is not as well-established as it is for conventional materials. Consequently, undertaking an analysis of materials design addresses key contemporary issues regarding the strength of modern materials and their practical application. The doctoral thesis under review aligns perfectly with this subject matter and contributes to a deeper understanding of the issue. Thus, the topic addressed by the doctoral candidate, Mr.

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Sachin Poundel (MSc Eng.), fits ideally into this scope of research and analysis. The title of the thesis accurately reflects the scope of the work.

The doctoral thesis has been meticulously prepared and is distinguished by its high-quality layout, making it easy to read. The work consists of two parts: the first is the doctoral candidate's summary (written in English), and the second comprises two appendices—Appendix A, containing the seven publications that make up the collection, and Appendix B, containing signed co-author declarations. The entire document is preceded by eighteen pages of supplementary information, while the summary itself spans 42 pages.

The section preceding the summary includes information such as acknowledgments and abstracts in both English and Polish. Nowhere is the Polish title corresponding to the doctoral dissertation itself provided. Next, a list of seven publications forming the basis of the application for the doctoral degree is presented, along with two additional publications. The subsequent section outlines the author's contribution to the individual works and their scientific achievements. Additionally, a list of figures and tables is included, which is rather superfluous. It is positive, however, that a list of key abbreviations used in the summary is provided at the end of the document.

Following this section is the table of contents for the application, which lists parts that had already been presented earlier. This should have been placed after the title page (or possibly after the acknowledgments, which should not appear in the table of contents).

The self-report is divided into five numbered chapters. It concludes with an unnumbered "References" chapter, containing a list of 41 sources relevant to the subject matter. The aforementioned appendices follow the list of references.

The first chapter, titled "Introduction," presents the problem of designing microstructures in multicomponent alloys—based on calculations and data analysis—for advanced functional materials, and concludes by outlining the scope of the work. This scope is presented following two subsections that discuss advanced functional materials across various fields and large-scale computational methods based on data analysis; this is a sound scientific approach. This brief introduction references the specific studies that form the basis of the doctoral thesis. The second chapter outlines the scientific problem and formulates the hypotheses for the thesis. Here, key concepts used in the publications are defined, including computational design, data-driven design, multiscale integration, microstructure, and advanced functional materials. The chapter then reviews the state of knowledge and identifies research gaps in the subject area. Subsequently, the scientific problems are formulated, identifying five specific research issues. Based on this, one main hypothesis and four specific hypotheses are adopted; while hypotheses

are not mandatory in a doctoral thesis, they add value to the work. Chapter 3 describes the research objectives, detailing one general objective—the development and application of multiscale computational methods that combine physics-based modeling with data-driven techniques—along with three specific objectives. Chapter 4 summarizes the multiscale design of advanced functional materials. A table provides a concise overview of the specific materials, design methods, and key findings or design principles associated with the individual studies included in the thesis. Chapter 5 presents conclusions and directions for further research. Here, reference is made to the previously established research objectives and hypotheses.

Attachment A consists of copies of journal articles:

[P-I] **S. Poudel**, U. Subedi, M. O. Hamid, K. Gyanwali, N. Moelans, A. Timofiejczuk, and A. Kunwar, “Alloy ManufacturingNet for discovery and design of hardness-elongation synergy in multi-principal element alloys,” *Engineering Applications of Artificial Intelligence*, vol. 132, p. 107902, 2024.

[P-II] **S. Poudel**, R. Thapa, R. Basnet, A. Timofiejczuk, and A. Kunwar, “PiezoTensorNet: Crystallography informed multi-scale hierarchical machine learning model for rapid piezoelectric performance finetuning,” *Applied Energy*, vol. 361, p. 122901, 2024.

[P-III] **S. Poudel**, N. Moelans, R. Thapa, A. Timofiejczuk, D. Panthi, and A. Kunwar, “Unraveling elastochemical effects in microstructural evolution of Al–Cu–Ni system through DFT-informed multi-phase field simulations,” *International Journal of Solids and Structures*, vol. 300, p. 112894, 2024.

[P-IV] Y. Li, **S. Poudel**, S. Kumari, E. Azqadan, A. Kunwar, and N. Moelans, “Roadmaps for dendrite suppression in next generation lithium-ion batteries: Toward sustainable energy solutions,” *Energy Storage Materials*, vol. 86, p. 105000, 2026.

[P-V] **S. Poudel**, W. Smok, R. Thapa, A. Timofiejczuk, N. Moelans, and A. Kunwar, “Physics-guided machine learning for enhanced piezoelectric performance in electrospun PVDF/SnO₂ nanofibers,” *Sustainable Materials and Technologies*, p. e02008, 2026.

[P-VI] M. Dagnaw, **S. Poudel**, U. Subedi, R. Thapa, Ł. Reimann, A. N. S. Appiah, P. M. Nuckowski, M. Król, Z. Brytan, N. Moelans, et al., “Integrating experiments and phase field method through informatics for tailored corrosion performance of additively manufactured steel microstructures,” *Metals and Materials International*, 2026.

[P-VII] M. Dagnaw, **S. Poudel**, M. Król, and Z. Brytan, “Post-process heat treatment design for tunable strength and toughness in L-PBF 2507 super duplex stainless steel,” *Materialia*, p. 102799, 2026.

These papers are of high quality and have been published in reputable, internationally recognized journals. Additionally, statements from co-authors detailing their substantive contributions to the individual papers are provided in Appendix B. Based on these statements, it is possible to distinguish the doctoral candidate's specific contributions and, consequently, the body of work that forms the basis of his application for the doctoral degree. These papers demonstrate the candidate's contribution to the advancement of science—a contribution summarized, as previously mentioned, in the author's statement. The number of co-authors for the individual papers ranges from four to over ten.

2. Opinion on the work regarding compliance with statutory requirements

2.1. Assessment of general theoretical knowledge

The review of the state of the art—presented partly in the summary of professional accomplishments and in the candidate's co-authored papers—confirms the doctoral candidate's extensive understanding of microstructure design in multicomponent alloys (based on calculations and data analysis) for advanced functional materials. The literature review included in these works is comprehensive, even though the application of this approach to real-world structures is a relatively new development.

2.2. Assessment of the ability to conduct independent research

The doctoral candidate demonstrated independence in both the preparation and execution of the actual research on composite materials. Although the scientific publications forming the basis of the dissertation were not authored solely by the candidate, this does not call into question the independence of the research conducted; rather, it attests to an ability to work within a team. The only exception to this pattern is a paper with more than ten co-authors—an unusually high number—though, fortunately, there is only one such publication in the candidate's body of work. An analysis of the percentage contributions suggests that the share attributed to the doctoral candidate may be overstated; nevertheless, the candidate is the lead author on five of the seven papers.

2.3. Assessment of the original solution to a scientific problem

The achievements presented in the individual chapters demonstrate—as outlined in the summary of the work—the scientific contribution of this doctoral dissertation, its innovative nature, and the validity of the chosen topic. The candidate successfully addressed the challenge

of designing microstructures in multicomponent alloys—utilizing calculations and data analysis—for applications in advanced functional materials. Despite the highly positive review of the doctoral dissertation by Sachin Poudel, M.Sc. Eng.—as noted in the summary of the work and the description of the doctoral candidate's key achievements—I have raised a few points of doubt in the summary, as well as in the specific comments and questions regarding the thesis.

3. Comments and specific questions regarding the work

I have already addressed some points in the preceding sections. Below, I list other errors noted or questions raised:

- it is a pity that the Author did not make a greater effort to present their achievements in the summary report in a way that would avoid the need to search through individual papers and wonder what constituted the doctoral candidate's specific contribution;
- the reviewer feels that the contribution of co-authors to the individual papers appears disproportionately small. I understand that all parties agreed to this division of labor; however, it strikes me as understated. Nevertheless, the applicant's substantive contribution is the more important factor, and this appears sufficient;
- there is a relatively high proportion of materials engineering in the application compared to mechanical engineering, yet all the papers fall within—and are assigned to—both disciplines.

4. General observations and conclusions

The characterization of the work, along with the supplementary comments and questions, indicates that the dissertation demonstrates a profound understanding of the problem addressed—specifically, the integration of microstructure design in multicomponent alloys based on calculations and data analysis for advanced functional materials. Particular note should be taken of the knowledge and experience the doctoral candidate has gained in this field. The few comments included in the review may serve as a basis for the candidate's future research and publications, and may also prove useful when drafting subsequent scientific papers. It should be noted that a significant portion of these comments take the form of questions and suggestions for future consideration rather than direct criticism of the dissertation itself. The primary issue lies in the classification of the work under the discipline of Mechanical Engineering; however, the study frequently references mechanical engineering, and it is often difficult to draw a clear line between materials engineering and the mechanics of materials and structures made from various materials.

Key scientific and research achievements of the work include:

- computer-aided specification of multicomponent alloy composition and manufacturing routes to meet hardness–elongation requirements;
- selection, orientation, and evaluation of piezoelectric materials at the device level for sensors, actuators, and energy harvesting systems;
- temperature-consistent microstructure prediction for alloy process design;
- designing battery interface reliability through the analysis of dendrite formation and growth using the phase-field method and the synthesis of mitigation strategies.

An analysis of the work warrants a positive assessment regarding general theoretical knowledge, the ability to conduct independent research, and the development of an original solution to a scientific problem. Furthermore, it should be noted that the doctoral thesis under review is interdisciplinary in nature; as previously stated, it could be situated within two currently recognized disciplines: Mechanical Engineering and Materials Engineering. Given that material-related issues are addressed from the perspective of mechanics of materials, the thesis can be classified under the discipline of Mechanical Engineering, the category in which it was submitted for review.

5. Final conclusion

The overall assessment of the doctoral dissertation justifies the conclusion that the requirements set forth in the Act of 20 July 2018 – Law on Higher Education and Science (as amended) have been sufficiently met, and supports admitting the dissertation by Sachin Poudel, M.Sc. Eng., titled "SCALE Bridging Computational and Data-Driven Design of Microstructures in Multicomponent Alloys for Advanced Functional Materials," to the public defense procedure at the Silesian University of Technology in the discipline of Mechanical Engineering.

Kind regards

Tadeusz
Łagoda

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podpisany przez
Tadeusz Łagoda
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