

Grzegorz Klekot, PhD, DSc, Eng., University Professor
Warsaw University of Technology
Faculty of Automobiles and Heavy Machinery Engineering

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Review

of the doctoral dissertation of Sachin Poudel, MSc, Eng., "Scale Bridging Computational and Data-Driven Design of Microstructures in Multicomponent Alloys for Advanced Functional Materials"

Formal basis for the review:

The review of the doctoral thesis of Sachin Poudel, MSc, Eng., was prepared in accordance with the resolution of the Council of the Discipline of Mechanical Engineering of the Silesian University of Technology of July 15, 2026.

1. Notes on the choice of the subject matter

The vast array of machinery and technical equipment in the modern world facilitates work and enhances people's quality of life. Large-scale industrial production creates a need to optimize products with a focus on specific functional attributes. Modern structural materials are essential for creating products that are lightweight, durable, safe, and reliable; the requirement for reasonable manufacturing and operating costs is closely linked to material properties. Consequently, the role of tailoring the physical properties of engineering materials in the context of improving technical systems cannot be overstated.

I consider the subject matter of this work to be timely, and the research into modeling structural materials for specific components and structures to be of both scientific and practical significance.

2. Dissertation characteristics

The work submitted for evaluation comprises 216 pages. The main substantive component consists of a 37-page summary of accomplishments (text, figures, tables and bibliography), and a 143-page appendix containing a series of seven articles published in renowned scientific journals. The remaining elements are: a title page, a dedication, acknowledgments, abstracts in English and Polish, a list of the author's primary and supplementary publications, a description of the candidate's contribution to each publication, a list of scientific achievements, a table of contents, a list of figures, a list of tables, a list of abbreviations, and 19 declarations from co-authors.

In the first chapter of the summary of accomplishments entitled "Introduction", the author presents the philosophy of simulation design of structural materials with properties tailored to specific engineering applications, and outlines three directions of research (metal alloys, piezoelectric materials, lithium electrochemical cells).

The second chapter, based on a literature review, presents information on modelling methods for advanced functional materials applied to components and assemblies (multicomponent alloys, piezoelectric ceramics, polymers, and lithium-based battery interfaces).

In the third chapter, the PhD student presented as the aim of the work the development of a computational methodology combining the modeling of physical phenomena with data-based models in the task of supporting the design of elements and devices with assumed properties: mechanical (multi-component alloys), electromechanical (piezoelectric ceramics), electrochemical (battery durability and reliability).

The fourth chapter is dedicated to the design of advanced functional materials by synthesizing microstructural considerations (taking into account atomic bonding and intermolecular, thermal, and electromechanical interactions) with machine learning and finite element calculations. This chapter is a kind of guide to the co-authored scientific articles of the PhD student, containing the results of research.

The title "Conclusions and Future Work" reflects well the content of the final, fifth chapter. Here, the author presents a summary of the results obtained and directions for further research.

An important part of the dissertation consists of a series of seven thematically related articles prepared with the participation of the PhD student and published in reputable scientific journals (Appendix A), which document the scientific achievement. Four publications concern multicomponent alloys, two articles cover the issue of piezoelectric materials, while one article contains considerations on the role of dendrites in next generation lithium-ion batteries.

3. Evaluation of the thesis

The thesis is multidisciplinary in nature, covering issues in the fields of exact and natural sciences as well as engineering and technology. The qualification of the thesis to the discipline of mechanical engineering results from the use by the PhD student of methods and models typical for the field of mechanical engineering and from the possibility of using the results obtained in issues related to the construction of mechanical machines and devices.

I consider that the work falls within the discipline of mechanical engineering.

The layout of the dissertation is logical, particularly well-justified by documenting the results obtained at subsequent stages of work by research articles published between 2024 and 2026. Copies of these seven thematically related publications (Appendix A) emphatically highlight the spectacular outcomes of the research conducted.

The literature review presented reflects the current state of knowledge and draws upon existing research related to the dissertation's subject matter, conducted in foreign and domestic centers. The choice of literature presented by the Author as accurate, and the manner of citation as correct, proving the ability to use bibliographic material. The extensive bibliography accompanying all seven articles (Appendix A) also deserves to be highlighted.

The author identified the development and application of computational methods combining physics-based modelling with data-driven prediction as the main goal of the dissertation. Achieving this goal required devising a platform concept that

integrates spatiotemporal modelling, enabling operations across multiple scales – from the atomic level and material structure to the finished component or device. The PhD student employed various computational tools, including those based on density functional theory, the finite element method, and data-driven modelling, while also utilizing machine learning incorporating elements of artificial intelligence.

The summary of accomplishments was concluded with a correct recapitulation and indication of future development directions; it emphasizes the rationale for the integrated optimization of structural materials, components, devices, and structures.

The aim of the work has been achieved, and the developed methodology holds both scientific and practical significance, representing a contribution to the advancement of the discipline of mechanical engineering.

I evaluate the work's activities positively in terms of both substance and methodology. The author presented an interesting approach to the shaping of structural materials, and the results achieved open up new perspectives for researchers and design engineers.

The high quality of the work is further underscored by the appended articles, which, following positive peer reviews, were published in renowned scientific journals.

4. Detailed critical remarks

After reading the work, the following questions arise:

- Why is there no example to illustrate the subsequent operations carried out during the selection of a structural material for a specific application (step by step)?
- How can the correctness of the results obtained by computational and simulation methods be verified? Have the properties of real objects manufactured according to the developed methodology been tested?
- One of the articles (P-VI) is not available under the indicated DOI. What is the status of this publication?

5. Notes on the editing of the dissertation

The work has been carefully prepared from an editorial standpoint. The small font size in some of the figures slightly reduces their readability (e.g., Fig. 1.2a) but does not hinder the overall reception of the work.

6. Final conclusions

The doubts raised do not reduce the positive overall assessment of the work. I believe that the entire work presented for review is valuable from a cognitive and utilitarian perspective, and contains an innovative approach to shaping the properties of construction materials. The whole presented for review is valuable in cognitive and utilitarian terms and contains an innovative approach to tailoring the properties of structural materials.

Sachin Poudel, MSc, Eng., demonstrated the ability to formulate and independently solve a scientific problem: developing a coherent concept for tailoring the properties of structural materials using computational methods that combine multi-level spatiotemporal modelling of physical phenomena with data-driven inference. He properly planned and conducted simulation studies, and used the results obtained results to draw valid conclusions. The PhD student demonstrated that he possesses a sufficient level of knowledge and skills within the discipline of mechanical engineering.

I conclude that the reviewed dissertation by Sachin Poudel, MSc, Eng., "Scale Bridging Computational and Data-Driven Design of Microstructures in Multicomponent Alloys for Advanced Functional Materials" meets the requirements set for doctoral theses by Article 187(1) and (2) of the Act of 20 July 2018. Law on Higher Education and Science (Journal of Laws of 2024, item 1571) and may be admitted to public defense.

I also request that the reviewed doctoral dissertation be honored.

The justification is a **series of seven thematically related scientific articles** (total IF: **61.9**; a total of **970 points** of the Ministry of Science and Higher Education) in reputable journals. The PhD student is the first author of four publications with a share of more than 50% and the corresponding author of three subsequent ones.

Dr hab. inż. Grzegorz Klekot, prof. PW