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PhD Defense Jury Member Report

Candidate Name: Oleg V. Lebedev

Doctoral Program: Materials Science and Engineering

Thesis Title: Study of deformational behavior of electrical conductivity of polymer composites with different nanofiller distribution types

Supervisor: Sergey Abaimov

PhD Defense Chair: Alexei Buchachenko **Email:** a.buchachenko@skoltech.ru

PhD Defense Date: 02.10.2020

Name of Reviewer: Dmitrii Godovsky

I certify hereby that no conflict of interest (positive or negative) has been identified. *(Otherwise, the reviewer can describe a possible conflict.)*	**Signature:** **Date: 01-09-2020**

The purpose of this report is to obtain an independent review of the thesis from the PhD Defense Jury Members before the thesis defense. The PhD Defense Jury Members are asked to submit a completed copy of this report at least 30 (thirty) days prior to the thesis defense. The reviewers are asked to discuss the contents of each report with each other before the thesis defense.

If the reviewers have any queries about the thesis which they wish to raise in advance, they should contact the Chair of the Jury.

Reviewer's Report

The reviewer's report should contain the following items:

- *Brief evaluation of the thesis quality and overall structure.*
- *Consistency between the thesis topic and its actual content.*
- *Relevancy of the methods used in the thesis research.*
- *Scientific value of the results obtained and their conformity to the international standard and current state of the art.*
- *Usability of the obtained results in applications (if relevant.)*
- *Quality of the publications.*
- *Summary of the items to be addressed before/during the PhD thesis defense*

Dissertation of Lebedev Oleg Vladimirovich titled "Study of deformational behavior of electrical conductivity of polymer composites with different nanofiller distribution types" describes two approaches of multi-scale modelling of electrical conductivity changes prediction with deformation for composites filled with electroconductive nanoparticles. The topic is novel, and, in my opinion, the thesis meets all the requirements for a PhD degree on the Material Science and Engineering.

The structure of the thesis allows to understand easily the approaches used for multi scale

modeling, since the description of the modeling processes for each of the two described composite systems with segregated structure starts with investigation of the properties of a "building block" of the segregated structure, as numerically, as well as experimentally. This allows to use the results, obtained for the small scale, at the larger scale of the modeling, while also allowing to compare the results between different scales. This comparison helps to understand better how the segregation affects the changes of the electrical conductivity with the composite material deformation. The dissertation starts with introduction on the problem and literature review on the topic of electroconductive composites with segregated structure and studies of their piezoresistivity.

The literature review sufficiently represents current achievements in the scientific area at the current moment, while also demonstrating a clear gap in the knowledge, which the study of Lebedev Oleg tries to fill. Conclusions on the described in the thesis results demonstrate that it indeed was done with satisfactory success.

Finite element-based numerical modeling approach, as well as experimental methods used in this work to create digital twins of the representative volume elements for different scales of the composite structure are interesting and unique. The obtained numerically results for piezoresistivity studies were verified by experimental results for the same systems that were numerically investigated, which is state-of-the-art approach. Overall quality of the results is high, completely conforming with the international standards.

Lebedev Oleg published two papers (one in Q1 and second in Q2 journals) on the materials presented in the dissertation, while also submitting the third for publication. Quality of these articles are sufficient to consider Lebedev Oleg candidature for a PhD degree.

I advise to address the following issues in the Thesis before the Defense:

- Multi-scale modeling procedure for the second system investigated was separated in two chapter for easier comprehension of the material. In the first chapter, PP matrix filled with nanoparticles was studied, while in the second influence of the glass fibers presence was investigated. I think the same separation should be done for the first system as well (Chapter 3 in the dissertation): first chapter should describe the thin layer, while second will be dedicated to study of 3D segregated structure of modified UHMWPE.
- Specifications of the nanoparticles and polymers are better to be presented in tables in a designated Materials subsection for easier navigation.
- It is a good idea to add prediction accuracy (in relative terms) for each set of assumptions in the section 4.4. It can be done for each type of the filler, showing a relative deviation value averaged for all investigated concentration, and separately for each concentration as a plot of prediction accuracy vs. concentration.
- Errors are missing in table 2 (section 5.3., which is mistakenly named 4.3 in the text).

Provisional Recommendation

☒ *I recommend that the candidate defends the thesis by means of the PhD thesis defense.*

☐ *I recommend that the candidate defends the thesis by means of the PhD thesis defense subject to appropriate changes to be introduced in the thesis according to the recommendations of this report.*

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☐ *The thesis is not acceptable and I do not recommend that the candidate proceed to the PhD thesis defense.*

D. Godovsky 1.09.2020