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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: Stanislav Moshkalev

I certify hereby that no conflict of interest (positive or negative) has been identified. *(Otherwise, the reviewer can describe a possible conflict.)*	**Signature:**  **Date: 26-08-2020**

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*

In the Thesis titled "Study of deformational behavior of electrical conductivity of polymer composites with different nanofiller distribution types", Mr. Oleg Lebedev demonstrated his approach to solve a problem of prediction of electrical conductivity behavior with uniaxial deformation for composites with different nanofiller distributions.

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The Thesis begins with introduction on the problem, followed by Literature Review, describing recent research progress in the area, as well as different approaches currently under study in order to advance in development of the non-destructive testing of the complex polymer composites.

In the dissertation two kinds of systems are studied: i) composites with highly segregated structure based on UHMWPE (ultra-high molecular weight polyethylene) and ii) composites modified with nanoparticles and reinforced with glass fiber textile. To obtain the first system, UHMWPE is processed together with nanofiller particles of different types in a way that no particles can penetrate into the volume of polymer grains, thus allowing to form a well-defined segregated structure. In the second system, the electroconductive phase is represented by PP (polypropylene) filled with nanoparticles in an agglomerated state. The electroconductive phase is distributed in the composite non-uniformly due to the presence of insulating glass fibers.

To advance the understanding of the problems under study in the thesis, comprehensive experimental and numerical studies of the composites with segregated structures were conducted. By using different state of the art techniques and methods, such as the embedded element method for finite element analysis, or the advanced image processing of electron microscopy data, obtained for slices of experimentally obtained composite samples, the response of the electrical conductivity of the composite materials to deformations was investigated both numerically and experimentally. It was done for different scales separately, in order to understand how the segregation of fillers affects the final results. In the case of UHMWPE-based composites, first a thin layer of filler particles was investigated, after which the obtained results were used in the scale of several polymer grains in the composite. In the case of glass-fiber reinforced composites, the PP filled with agglomerated particles was studied first, followed by investigation of the properties of modified PP reinforced with textile glass fibers.

As the result of the study, two novel multi-scale modeling approaches were proposed for two types of segregated structures, qualitative differences between which are described in the conclusions of the dissertation. Verification of the consistency of numerical models by experimental studies demonstrated reliability of the proposed approaches, while also showing ways for possible future improvements. The conclusions of the thesis also correspond to the gap in the current knowledge indicated in the literature, demonstrating the valuable contribution of the research performed by Mr. Lebedev.

The obtained results have a clear practical value for future developments of constructions based on the materials modified by electroconductive nanoparticles, particularly for non-destructive evaluation of deformational state of the constructions.

The results were published in two papers in prestigious journals, and also one paper was submitted for a future publication.

Overall, it is clear for me that Mr. Lebedev fulfills all the requirements necessary for a successful PhD thesis defense.

Although the text of the Thesis is of a high quality in the current form, I recommend to make the following corrections and additions to the dissertation before the PhD thesis Defense:

- The electrical resistance of the MWCNT network depends mostly on resistances of contacts between individual nanotubes. The contact conditions may change strongly for the networks fabricated with and without polymer matrix, how this is considered in the simulations?
- For electrical measurements, 4 probes method was employed and only brief description of the method was done, more details on the method are needed.
- Equation 1 seems to be wrong, the weight must be proportional to the material density.

- Based on comparison of large amount of experimental and simulation results, the final conclusions were done in very general terms: “it was concluded, that contrast of mechanical properties between insulating regions and electroconductive phase in composite materials with segregated structure plays a significant role”. The differences in mechanical and electrical properties of the fillers and matrix used in the study are very large. So, it would be useful to provide more specific conclusions regarding the effects of fillers and matrix on the properties of the composite and the response to deformations.
- Throughout the text, many sentences are too long (5-7 lines or even more) and difficult to understand (example: in the page 30 - only 4 sentences, one of them has 9 lines), they should be broken in shorter phrases for easier reading;
- Chapters 1 and 2 have no Figures/Tables, I recommend to include some figures and tables for better presentation of the material.
- The English is good, however, several grammar or style corrections need to be done, for example:
  - P. 18: “electrostatic discharge” – should be substituted by “electrostatic protection”,
  - P. 27: “more thousands of articles” – should be “several thousands of articles” or “more than one thousand of articles”,
  - P. 34: “dielectric polymer matrix %” – should be “dielectric polymer matrix percentage” ,
  - P. 47: “The results of these test demonstrated…” – should be “The results of these tests demonstrated…”
  - P. 52: “(COD ~ 0.993)”- what is COD? The abbreviation should be explained first time it appears in the text,
  - P. 83: “…have high value of properties contrast between ...,” - should be “…have high contrast in values of parameters between …”,
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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.*

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