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Doctoral study program: Advanced Materials and Nanosciences

Field of study: Advanced nanotechnologies and microtechnologies

Supervisor: prof. Ing. Jozef Kaiser, Ph.D.

Reviewer: Univ. Prof. Dr. Hans Lohninger

PhD thesis title: Development of a device and methodology for Laser-Induced Breakdown Spectroscopy (LIBS)

Topicality of doctoral thesis:

The dissertation deals with a rapidly developing field, especially with regard to different approaches to create the LIBS plasma and the pressing questions of data analysis in the field of LIBS and universally usable spectral libraries for LIBS.

Meeting the goals set:

The dissertation takes a relatively broad approach to the analysis of LIBS spectra. On the one hand, an attempt is made to characterize the plasma especially for non-orthogonal ablation and orthogonal double-pulse LIBS. On the other hand, different approaches for the preparation and interpretation of the spectral data are pursued. The goals set were achieved and documented by nine peer reviewed papers, six of which the doctoral candidate is the first author. In addition a few papers are submitted or in preparation.
Problem solving and dissertation results:

The essence of the contributions of the doctoral candidate to the state of the art can be summarized as follows:

1) Tomographic characterisation of asymmetric plasmas: the characterisation of LIBS plasmas under non-orthogonal ablation conditions is certainly an interesting and important contribution to understand LIBS plasmas and possibly trigger practical applications in the future. Further the study of orthogonal double-pulse LIBS contributes to this general understanding, as well.

2) Bootstrapping as a sampling technique: this is a quite interesting approach, given that bootstrapping gained heavy attention during the rise of certain machine learning approaches.

3) Background subtraction: the question when to acquire the LIBS spectra after the laser pulse is quite important in the light of the continuum background radiation. The author showed that the common paradigm to measure spectra after the decay of the background radiation does not improve the LODs. Conversely, the author showed that measuring early after the laser pulse and subtracting the background by mathematical means results in considerably better LODs.

4) Dimensionality reduction beyond PCA: the discussion in the thesis addresses several interesting aspects, especially some approaches which deliver results similar to the classical PCA whilst being much faster. The findings have been reported in a peer-reviewed paper. Non-linear dimensionality reduction however is not discussed in detail, a paper is announced but not yet submitted (nor is it part of the thesis) and therefore cannot be judged.

5) Choosing the right classification model based on a benchmark dataset: the approach chosen by the author is quite valuable as this could be the starting point for further research on classifiers especially suitable for the interpretation of LIBS spectra.

6) Understanding black-box multivariate models: SVCs used to find important features of a dataset is certainly an interesting approach (paper under peer review). The discussion of CNNs is more like an outlook as the respective publication is not yet available as peer reviewed paper.

Importance for practice or development of the discipline:

While it is generally difficult to assess the future effect of basic research, in my opinion the inputs in this thesis will make a significant contribution to the further development as the goals and results of the thesis are highly relevant both for the future development of LIBS and the processing of the acquired spectra.
Formal adjustment of the thesis and language level:

(4) The study is duly completed by a state doctoral examination and the defense of a dissertation, which proves the ability and readiness for independent activity in research or development or for independent theoretical and creative artistic activity. The dissertation must include original and published results or results accepted for publication.

The impressive list of the doctoral candidate's publications shows his high level of expertise. The thesis is well written, regarding both the structure and the language level.

Questions and comments:

1) I find the title of the thesis a little bit too general. A more specific title would certainly attract more readers (assuming that the thesis will be publicly available and accessible via search engines).
2) The summaries of the individual papers are very well done!
3) Question: Fig 14-1 of the thesis does not match Fig. 1 of the paper [465] – despite the doctoral candidate claims this figure to be taken from [465] – why?

Conclusion:

*The dissertation is an excellent piece of work in terms of both form and content.*

In my opinion, the reviewed thesis fulfills all requirements posed on theses aimed for obtaining a PhD degree. This thesis is ready to be defended orally, in front of the respective committee.

Vienna, Jan-10, 2022

Univ. Prof. Dr. Hans Lohninger