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Annex No. 10 to the MU Directive on Habilitation Procedures and Professor Appointment Procedures

HABILITATION THESIS REVIEWER'S REPORT

Masaryk University	
Applicant	Mgr. Ondřej Zobač, Ph.D.
Habilitation thesis	Experimental and theoretical study of phase diagrams
Reviewer	Dr hab. inż. Przemysław Fima, assoc. prof.
Reviewer's home unit, institution	Institute of Metallurgy and Materials Science, Polish Academy of Sciences, Kraków (Poland)

Habilitation thesis of Ondřej Zobač, entitled "Experimental and theoretical study of phase diagrams", presents and overview of his main research activities and the most important results after obtaining a Ph.D. degree. These are related to the analysis and better understanding of binary and ternary alloys, where either phase equilibria were unknown or uncertain due to discrepancies in the literature.

Although at first the title of the thesis gives the impression of being very general, the scope of diverse materials systems studied is wide. In the thesis, the applicant presented the results of his investigations of two groups of materials i.e. binary and ternary aluminium-based alloys and selenium-based alloys. The materials from the first group e.g. Al-Cu, Al-Cu-Si are of great importance in automotive and other high-strength applications, alloys from the system Al-Cu-Zn were studied for phase memory applications, Al-Ge-Mg alloys are interesting for light-weight applications, while Al-Si-Zn alloys are important from the viewpoint of precision casting. The materials from the second group: Ni-Se, Ag-Se-Sn, Pb-Se-Sn, Ni-Se-Sn are interesting for the development of advanced photovoltaic, semiconductor and thermoelectric materials.

Modern technologies often rely on multicomponent and multiphase materials, which should possess required microstructure and resulting, well defined properties. Equilibrium phase diagrams are the key source of information on the coexistence and stability of phases. Phase diagrams can be studied experimentally and calculated by the CALPHAD method. Reliable theoretical descriptions of binary and ternary systems allow to predict higher order, multicomponent systems by extrapolation, even without additional data. While development of new materials is time consuming and costly, experimental work is now more and more supported by computational methods. Hence, the combination of experimental studies of phase diagrams with CALPHAD approach can substantially reduce the effort needed to develop new materials.

The reviewed habilitation thesis is composed of general introduction, followed by a brief introduction of the systems studied (chapter 1), two useful chapters with author's achievements in experimental investigation of phase diagrams (chapter 2) and CALPHAD assessment of phase diagrams (chapter 3). Conclusions are presented in chapter 4, references in chapter 5, and chapter 6 contains the reprints of papers included in the thesis. From the formal point of view the thesis is well written with good quality figures and multiple external references, which reflects on the applicant's pedagogical qualities.

In chapter 2, after briefly introducing the methods of synthesis and materials characterization, the author presented an extract of the results from papers [P1,P3,P4,P7,P9,P10] and

underlined their significance. Experimental investigation of phase diagrams requires good planning as it often involves preparation of multiple samples which are subsequently studied by multiple advanced methods. From chapter 2 the applicant's expertise in different experimental methods, such as thermal analysis (DTA and DSC), scanning electron microscopy and x-ray diffraction, and his skill to combine them to reveal true nature of phase equilibria in studied materials and solve out disagreements in literature is evident. In chapter 3, before the author's main contributions [P2,P5,P6,P8,P11,P12] are discussed, the author recapitulated the basics of the CALPHAD method. On the examples of Al-Cu [P1,P5] and Al-Cu-Si [P4,P11] systems the applicant demonstrated how his expertise in experimental studies and theoretical assessments of phase diagrams complement each other. Another important aspect of applicant's achievements in CALPHAD method is his contribution to the development of so-called third generation models [P2,P11]. The latter was possible thanks to the applicant's membership in an international collaboration specifically focused on this purpose.

In chapter 5, along the list of twelve papers selected for the habilitation thesis, the applicant provided his declaration of how he contributed to the results published in these papers. The author's contribution, divided into: scientific work (experimental and theoretical), supervision of students, manuscript writing and research motivation is presented as a share in %. Although it would be more informative if the contributions to the scientific work were described in detail, it is clear that the applicant contributed significantly to the creation of these papers. Chapter 6 contains the reprints of the above-mentioned papers, which were published in the years 2019-2024 in renowned Web of Science-indexed journals, including the journals specialised in phase diagram studies: *Metal. Mater. Trans. A*, *CALPHAD*, *J. Mater. Sci.* and *J. Phase Equilib. Diff.* The applicant is the first author of nine and the corresponding author of ten, out of the papers included in the thesis. It is particularly commendable that one of these papers [P1] received numerous citations (over one hundred) since its publication date, which further underlines the importance of applicant's research to the scientific community.

The applicant collaborated with several leading scientists over the years, and all the papers selected for the thesis have three or four co-authors. In some of the papers young researchers were involved under the direction of the applicant. The applicant carried out his research activities at his home unit i.e. Institute of Physics of Materials, Czech Academy of Sciences as well as abroad. In particular, the results in papers [P1,P3,P4,P5] result directly from the applicant's two years long postdoctoral position at the University of Vienna in Austria. Research, and extensive experimental work in particular, would hardly be possible without funding. The applicant was successful in securing funding for his research. The prestigious Lise Meitner grant funded by the Austrian Science Fund (FWF), which is mentioned in the funding or acknowledgment sections of six papers, is commendable.

Reviewer's questions for the habilitation thesis defence

The papers included in the thesis underwent robust peer review procedure prior publication, which attests to their high scientific quality. I would appreciate answers to the below questions, which may give some outlook of the future:

1. It is noted in the thesis that currently only a fraction of scientific community supports transition to the third-generation data. Do you expect the third-generation data to be more broadly used for phase diagram assessments in foreseeable future?
2. Since 1980 over 1200 different binary systems SGTE-compliant thermodynamic datasets were published (B. Hallstedt, CALPHAD 2025,59:102833). Commercial thermodynamic database producers invested a lot in their existing products. What incentives they may have to move towards the third-generation data?
3. In the case of Al-Zn [P2], Al-Si and Si-Zn [P12] systems a conversion method of interaction parameters was presented as a tool to obtain a starting point for reassessment of thermodynamic data of each system. These three are fairly simple

systems only with solution phases, and it is easy to understand that more complex binaries would require more work to convert to third generation data. Do you expect Large Language Models could effectively be used as an assist in transition from existing datasets to third generation data?

Conclusion

The reviewed habilitation thesis summarizes the basics and new findings in the experimental and computational studies of phase diagrams. From its content it can be stated that the applicant achieved original results which demonstrate his expert knowledge and contribute to the field of physical chemistry. He carried out his studies at home unit and abroad, applied for highly-competitive external funding with success, and published the results in renowned peer reviewed journals.

As a reviewer I conclude that the habilitation thesis entitled "Experimental and theoretical study of phase diagrams" by Ondřej Zobač **fulfils** requirements expected of a habilitation thesis in the field of physical chemistry.

Date: 26.02.2026 Signature: