

HABILITATION THESIS REVIEWER'S REPORT

Masaryk University

Applicant

Mgr. Ondřej Zobač, PhD.

Habilitation thesis

Experimental and theoretical study of phase diagrams

Reviewer

RNDr. Viera Homolová, PhD.

**Reviewer's home unit,
institution**

Institute of Materials Research, Slovak Academy of Sciences

The habilitation thesis provides an overview of the main results of the applicant's research focused on the experimental and theoretical investigation of phase diagrams for two significant groups of materials: Al-based systems and Se-based systems. I consider this work to be highly topical. Both types of material systems have significant application potential: aluminium-based alloys are interesting for using in the automotive and aerospace technology applications, while selenium-based materials are promising materials for photovoltaics, superconductors and thermoelectric applications. The scope of these applications clearly demonstrates the topicality, and practical importance of the applicant's research.

The thesis brings many new results in the field of phase diagrams for three binary systems (Al-Cu, Al-Zn, Ni-Se) and seven ternary systems (Al-Cu-Zn, Al-Cu-Si, Al-Si-Zn, Al-Ge-Mg, Ag-Se-Sn, Pb-Se-Sn, Ni-Se-Sn). The achieved results significantly extend the current knowledge of these systems through the determination of phase transition temperatures, the characterization of invariant reactions, the identification of phase fields, and the discovery of new ternary phases. The results are more detailed described in attached papers that were published in high-quality journals. And I must also highlight the publication impact of the work on the Al-Cu system, which has reached a number of citations significantly exceeding one hundred — a clear indication of its relevance and visibility within scientific community. I also consider the thermodynamic datasets developed for these systems to be significant results, since as part of multicomponent databases they can expand the possibilities of designing new materials with specific properties using computational methods. It remains an important fact that computational approaches offer considerable savings in both time and cost.

From a formal standpoint, the thesis contains several typographical and technical inaccuracies. However, these inaccuracies do not affect the scientific content of the work and do not reduce its overall quality.

- the caption of Figure 13 mistakenly repeats the description of Figure 12;
- the left-hand side of equation (1) is missing;
- there are several incorrect references to the author's publications in the text (for instance: on page 13 there should be P5 instead of P6, P9 instead of P10, on page 19 there should be P9 instead of P10 etc.);
- on page 8 in in the third sentence it should be 'stavů' instead of 'stvů' (in Czech language)

Reviewer's questions for the habilitation thesis defence

1. The phases Al_4Cu_9 (γ') and Cu_5Zn_8 (γ), are modelled using the four-sublattice model. I would be interested to know whether you also considered using a simpler model.
2. How do you envision the future direction of your research in the field of CALPHAD modelling?
 - A. In particular, which material systems do you consider most promising for your next research?
 - B. In the field of thermodynamic descriptions of systems, do you plan to focus only on the development of third-generation thermodynamic datasets or do you also plan to continue developing earlier generation CALPHAD datasets?

Conclusion

The habilitation thesis entitled "Experimental and theoretical study of phase diagrams" by Mgr. Ondřej Zobač, PhD. **fulfils** requirements expected of a habilitation thesis in the field of Physical chemistry.

Date: 27.2.2026

Signature: