M U N I

COMMENTARY TO HABILITATION THESIS[1]

Experimental and theoretical study of phase diagrams

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The idea of equilibrium phase diagrams dates back to the second half of the 19th century to J. W. Gibbs and his study of thermodynamics and phase equilibria. A phase diagram is a graphical representation of the state of a system in thermodynamic equilibrium as a function of selected state variables. Phase diagrams are directly related to the rules of thermodynamics and thermodynamic quantities. They differ from property diagrams, because they carry a different type of information. Each point in a phase diagram has its own meaning and carries some information about phase equilibria.

The equilibrium phase diagram is an essential source of information for the design of new materials. Detailed knowledge of the coexistence and stability of phases in stable or metastable equilibrium significantly rationalises the development of material research.

For the experimental phase diagram investigation, a combination of dynamic and static analytical methods can be used. The overall and phase chemical composition is measured by scanning electron microscopy with an energy/wave dispersive X-ray spectroscopy detector (SEM-EDX/WDX) or transmission electron microscopy (sTEM-EDX) in specific cases. Identification of phase structure is done by powder X-ray diffraction (XRD) or electron diffraction analysis in TEM. Temperatures of phase transitions are evaluated by methods of thermal analysis - differential scanning calorimetry (DSC) or differential thermal analysis (DTA).

Phase diagrams can be predicted by a semiempirical thermodynamic method known as a CALPHAD approach (CALculation of the PHAse Diagram). This approach is based on the sequential modelling of multicomponent systems, starting from the simplest - modelling the temperature dependence of the Gibbs energy of the pure elements, followed by modelling more complex binary and ternary systems, which include solid solutions and intermetallic phases. The robust theoretical description of simpler (binary and ternary) systems consequently allows us to predict the behaviour of complex multicomponent systems by extrapolation without additional model parameters. The knowledge of the Gibbs energy dependence on composition, temperature and pressure for all phases which might occur in the system (stable and even metastable) is crucial. Unfortunately, this information is usually experimentally inaccessible for metastable phases. The lack of experimental data can be compensated by first-principles calculations, which, based on quantum mechanics, can determine thermodynamic quantities such as enthalpy of formation even for metastable or unstable phases at temperature T = 0 K. Using phonon spectra modelling, the calculations can be extended to the high-temperature region and used to calculate e.g. the specific heat capacity for a given phase.

Over the last decade, an international collaborative activity has started towards the development of a new generation of data for the pure elements based on the conclusions of a series of workshops held at Schloß Ringberg. This progress is motivated by the suggestion that the thermodynamic functions for elements should be described by models accounting for different physical phenomena rather than simple mathematical polynomials.

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[1] The commentary must correspond to standard expectations in the field and must include a brief characteristic of the investigated matter, objectives of the work, employed methodologies, obtained results and, in case of co-authored works, a passage characterising the applicant's contribution in terms of both quality and content.

The author's contributions to the results published in the selected twelve papers included in this habilitation thesis are summarised below. The author's contribution is divided into the following topics: scientific work (experimental and theoretical work), supervision of students, manuscript writing and research motivation.

[P1] **Zobač, O.**, Kroupa, A., Zemanová, A., Richter, K.W., *Experimental description of the Al-Cu binary phase diagram*, Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2019, 50(8), pp. 3805-3815 doi: 10.1007/s11661-019-05286-x (IF 2.050)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
80	0	80	100

[P2] Dinsdale A., **Zobač O.**, Kroupa A., Khvan A., *Use of third generation data for the elements to model the thermodynamics of binary alloy systems: Part 1 - The critical assessment of data for the Al-Zn system*, CALPHAD, 2019, 65, pp. 86-92, doi: 10.1016/j.calphad.2019.02.007 (IF 1.947)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
20	0	30	60

[P3] **Zobač, O.**, Kroupa, A., Richter, K.W., *Experimental study of the Al-Cu-Zn ternary phase diagram*, Journal of Materials Science, 2020, 55(24), pp. 10796-10810, doi: 10.1007/s10853-020-04686-4 (IF 4.220)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
80	0	90	100

[P4] **Zobač, O.**, Kroupa, A., Richter, K.W., *Experimental isothermal sections of the ternary phase diagram Al-Cu-Si at 600 °C and 800 °C*, Journal of Materials Science, 2020, 55(31), pp. 15322-15333, doi: 10.1007/s10853-020-05077-5 (IF 4.220)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
80	0	90	100

[P5] Kroupa, A., **Zobač, O.**, Richter, K.W., *The thermodynamic reassessment of the binary Al-Cu system*, Journal of Materials Science, 2021, 56, pp. 3430-3443, doi: 10.1007/s10853-020-05423-7 (IF 4.682)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
25	0	30	80

[P6] **Zobač, O.**, Buchlovská, K., Pavlů, J., Kroupa, A., *A thermodynamic description of binary system nickel-selenium,* Journal of Phase Equilibria and Diffusion, 2021, 42(4), pp. 468-478, doi: 10.1007/s11669-021-00906-9 (IF 1.284)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
50	80	70	80

[P7] **Zobač, O.**, Richter, K.W., Kroupa, A., *Experimental phase diagram of the Ag-Se-Sn system at 250, 400 and 550 °C*, Journal of Phase Equilibria and Diffusion, 2022, 43, pp. 32-42, doi: 10.1007/s11669-022-00937-w (IF 1.4)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
80	0	80	40

[P8] **Zobač, O.**, Zemanová, A., Chen, S.W., Kroupa, A., *CALPHAD-type assessment of the Pb-Se-Sn system*, Journal of Phase Equilibria and Diffusion., 2022, 43, pp. 243-255, doi: 10.1007/s11669-022-00956-7 (IF 1.4)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
40	0	60	40

[P9] **Zobač, O.**, Karpíšková, L., Kroupa, A., *Experimental study of the ternary phase diagram Al-Ge-Mg*, Journal of Phase Equilibria and Diffusion, 2022, 44, pp. 127-136, doi: 10.1007/s11669-023-01025-3 (IF 1.4)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
50	80	70	80

[P10] **Zobač, O.**, Žižka, R., Roupcová, P., Kroupa, A., *Experimental study of the Ni-Se-Sn phase diagram isothermal sections at 800 K, 1000 K and 1100 K*, Journal of Phase Equilibria and Diffusion, 2023, 44, pp. 594-605, doi: 10.1007/s11669-023-01058-8. (IF 1.4)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
50	100	80	80

[P11] Kroupa A., **Zobač O.**, Zemanová A., Richter K.W., *CALPHAD-Type Reassessment of Cu-Si and Full Assessment of the Al-Cu-Si Systems*, Journal of Phase Equilibria and Diffusion, 2024, doi: 10.1007/s11669-024-01160-5. (IF 1.4)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
30	50	40	80

[P12] **Zobač O.**, Kroupa A., Dinsdale A., Use of third generation data for the pure elements to model the thermodynamics of binary alloy systems: Part 3 – The theoretical prediction of the Al–Si–Zn system, CALPHAD, 2024, 87, 102742. doi: 10.1007/s11669-024-01160-5. (IF 1.947)

Scientific work [%]	Supervision [%]	Manuscript [%]	Research direction [%]
30	0	40	80