Automated CALPHAD assessment of Cu-Mg system with ESPEI and segmented regression model from 0K

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Thermodynamic modeling using the CALPHAD (=CALculation of PHAse Diagram) method is one of the key component for a successful and robust design of new materials. Recent implementation of the CALPHAD method, however, is lacking strategies and tools for straightforward implementation of the new models and new experimental and DFT data into existing databases. The development of data repositories and automation tools together with robust mathematical models are three main components to improve the efficiency of existing CALPHAD modeling approach, especially for updating multicomponent databases.

In this work, an approach for automated assessment will be demonstrated on the Cu-Mg binary system (Figure 1). The proposed solution is based on combination of open-source software ESPEI (= Extensible Self-optimizing Phase Equilibria Infrastructure) [1, 2] and newly proposed physically-based segmented regression (SR) model [3], which allows to perform thermodynamic calculations from 0K.

ESPEI is an open-source Python-based software for automated thermodynamic database development within the CALPHAD method. It uses the pycalphad software package [4] for calculating Gibbs free energies of thermodynamic models to rapidly develop and modify databases using a combination of first-principles and experimental thermochemical and phase equilibria data. Unlike traditional database development, ESPEI uses Markov chain Monte Carlo (MCMC) to optimize and quantify the uncertainty for all model parameters simultaneously.

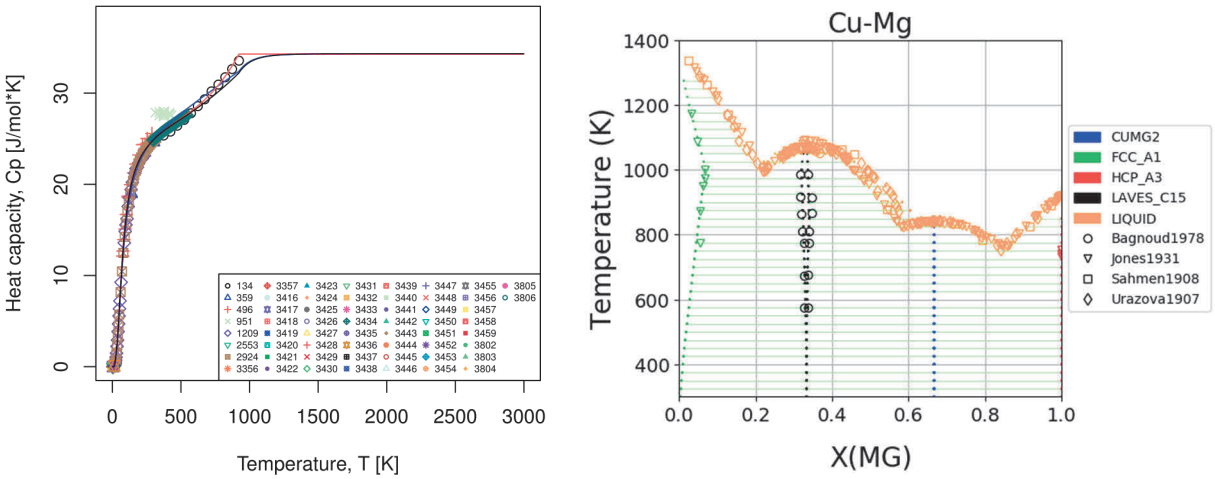

Figure 1. (left) Heat capacities of pure Mg for hcp_a3, liquid and fcc_a1 phases using SR model, (right) Cu-Mg phase diagram calculated using ESPEI software. Parameters are selected from single phase thermochemical data and fit to phase equilibria data with uncertainty quantification using Markov Chain Monte Carlo. Squares are experimental phase equilibria data.

References

[1] Shang, S. L., Wang, Y., & Liu, Z. K. ESPEI: Extensible, self-optimizing phase equilibrium infrastructure for magnesium alloys. In Magnesium Technology (2010) pp. 617-622

[2] www.espei.org

[3] I. Roslyakova, B. Sundman, H. Dette, L. Zhang, and I. Steinbach. Modeling of Gibbs energies of pure elements down to 0 K using segmented regression. CALPHAD Journal, 55, 2016.

[4] Otis, R. and Liu, Z.-K. "pycalphad: CALPHAD-based Computational Thermodynamics in Python", J. Open Res. Softw. 5 (2017)