

An Open Source Software and Database Structure for Thermodynamic and other Materials Properties

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Thermodynamic data are important in many fields of science and the compilation of consistent thermodynamic databases for these has been an important scientific project for many decades. However, most of these databases are proprietary and so is the software one must use to obtain practical results using these databases. A new open source software, called Open Calphad (OC), based on the Calphad approach [1] including sophisticated models for temperature, pressure and composition dependence has now been launched by a group of scientists with long experience in the field [2]. In the project the relations between the thermodynamic properties and their physical origin are included and a large effort is being made to make the software easy to use in applications like phase field simulation software. At present single equilibrium calculations for the well established Compound Energy Formalism (CEF) have been implemented for multicomponent systems. However several models are under test in order to be added later on. New models to include results from DFT calculations and the inclusion of low temperature data are in development [3]. The software and database structure has been designed to make it possible to store model parameters for the composition dependence of properties like lattice parameters, mobilities, magnetic transitions, elastic constants, etc. A module to assess experimental and theoretical data in terms of model parameters will also be included and a prototype for unaries is already available. Software for phase transformations and phase field simulations are outside the scope of this project but collaborations are ongoing to make sure that the new software can fulfill the requirements of such applications. The source code will be free with a GNU license available for any scientist to use as a basis to develop and test new models without the cumbersome efforts to develop also a minimizer and graphics packages. A database with published assessments will be provided with the intention that this can be a start of a truly public thermodynamic database.

[1] H L Lukas, S G Fries and B Sundman, Computational Thermodynamics, Cambridge University Press, Cambridge, 2007

[2] U. R. Kattner, B. Sundman, M. Palumbo, S. G. Fries, "Open Calphad Software and Databases", presented at CALPHAD XL, 22-27th May 2011, Rio, Brazil[3] M. Palumbo et al., to be presented in this symposium