

SAPIENS Thermophysical Database for Pure Elements: DFT and Experiments

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Thermodynamic models used in the so called CALPHAD databases describe the temperature dependence of Gibbs energy of pure elements and its derivatives from room temperature to the melting point. Thermodynamic properties calculated using density functional theory (DFT) are often limited to 0 K. Our aim is to connect these ranges, not only incorporating the first-principles energetics at 0 K, but also taking into account different contributions to the heat capacity such as phonons, electronic excitations, magnons, etc. In this way, physical meaning is attributed to the coefficients that are nowadays used in CALPHAD to express the temperature dependence of the heat capacity [1]. Furthermore, such properties as volume, thermal expansion, and bulk modulus are also consistently calculated as a function of temperature. The goal is to model unary and binary systems, starting with those relevant to steels. DFT data and experimental data are being kept independently, stored in a database to allow versatile updates and testing of new models. The methodology is also being applied to complex phases, testing new models, which can be compared to measurements accessing well documented experimental databases. We envisage having versatile and more predictive models. The Open Calphad, OC, software for calculations and optimization handling the new models is presented in the symposium [2]. The results of the work are public and can be accessed interactively. The name of this work is SAPIENS, and it calls for international cooperation. We present a preliminary set containing five elements to illustrate the method, its potentialities and difficulties.

[1] A. T. Dinsdale, CALPHAD, 15, 4 (1991) p. 317

[2] B. Sundman, U. R. Kattner, S. G. Fries, M. Palumbo, "An Open Source Software and Database Structure for Thermodynamic and other Materials Properties", to be presented in this symposium