Progress on Sapiens thermophysical database for unaries

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We report the continuation of the Sapiens project on thermodynamic descriptionsalready announced and detailed in previous CALPHAD meetings [1,2]. Our approach is based as far as possible on first-principles calculations, supplemented by an extensive experimental database. First-principles calculations are essential to firmly understand the physical origin of the different contributions to properties such as the heat capacity, i.e. to evaluate the effect of vibrational, electronic and magnetic excitations.

We present here a first-principles and experimental database for the pure elements. Based on this database, we propose a parametric modeling of thermophysical properties such as heat capacity and thermal expansion. Our approach is based on the Helmholtzenergy for ease of coupling with first-principles calculations. The methodology has been demonstrated for four technologically important pure elements (Fe,Cr,Ni,Al)and will be subsequently extended to more elements.

A new code, Open Unary, developed in C++ as part of the Open Calphadsoftware (see lecture of B. Sundman), was developed for the unaries. The code allows us to easily derive thermophysical properties using the results of first-principles calculations (performed using,for example, Quantum Espresso) and to determine the values of fitting parameters using least-squares minimization of the errors.

Finally we report some first attempts to extend the Sapiens methodology to binary systems, taking the Cr-Ni system as an example.

We understand the enormous advantage that the use of the SGTE unary database [3] has brought to the CALPHAD community, as without these universally accepted standards the construction of multicomponent databases would not be possible. We hope with the present work to contribute to a better understanding of the physical background of theseunary descriptions, to the enlargement of the community involved in this effort and to the discussion ofpossible new standards.

Keywords: unaries, first principles, experimental database, Open Calphad

References:
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