

The Development of Databases for Open Calphad,

a free thermodynamic software

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ABSTRACT

Thermodynamic data are essential for the understanding, developing, and processing of materials. The CALPHAD (Calculation of Phase Diagrams) technique has made it possible to calculate properties of multicomponent systems using databases of thermodynamic descriptions with models that were assessed from experimental data. A large variety of data, such as phase diagram and solubility data, including consistent thermodynamic values of chemical potentials, enthalpies, entropies, thermal expansions, heats of transformations, and heat capacities, can be obtained from these databases. CALPHAD calculations can be carried out as stand-alone calculations or can be carried out coupled with simulation codes using the result from these calculations as input. A number of CALPHAD software are available for the calculation of properties of multicomponent systems, and the majority are commercial products.

The Open Calphad (OC) initiative to develop a free software to calculate equilibria and thermodynamic and related properties for materials and processes is an important contribution to ICME. The third version is now available on the web site <http://openalphad.org> and it had an application software interface to handle parallel calculations of equilibria in multicomponent systems. On the web site there are extensive documentation and examples a few applications are available on the website.

The OC software can handle all types of data for materials that depend on temperature, pressure and phase composition for example Gibbs energy, heat capacities, thermal expansion, mobility data, elastic constants (that are not very constant), resistivity, viscosity etc. It can calculate the equilibrium state and also provide essential information on chemical potentials, diffusion coefficients, strain and stress properties etc. during phase transformations and processing. The OC software is open and has a GNU license, the user has access to the source code and can make modifications to adapt it to a specific application. The development of databases for different kinds of calculations is in progress.

REFERENCES

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