Computational Thermodynamics - Knowledge, Tools and Applications

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Computational thermodynamics is a very important tool in materials science. Although the fundamentals of materials thermodynamics are well known for the long time [1], only with increasing the computational power it became possible to calculate thermodynamic properties and phase equilibria in multi-component materials system [2]. To make the calculations the suitable software and related thermodynamic and mobility databases should be used. For example Thermo-Calc software [3] allows to calculate the state of the materials system to obtain the amounts and compositions of phases, transformation temperatures, solubility limits, driving forces for phase formation, activities and chemical potentials, phase diagrams and potential diagrams. These results can be used for prediction of materials property data, as thermophysical properties, kinetic properties and properties related to equilibrium and non-equilibrium solidification. All results can be exported e.g. to MATLAB software [4] and processed in complex models enabling the more detailed description and simulation of materials processes and properties of materials. This approach is considered as a part of "materials genome" [5] and is used for effective development of new materials and optimization of properties of existing materials.

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[3] https://thermocalc.com

[4] https://www.mathworks.com

[5] L. Kaufman, J. Agren: CALPHAD, first and second generation – Birth of the materials genome. Scripta Materialia 70 (2014), pp. 3 – 6