Thermodynamic calculations and modeling for ceramics

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Thermodynamic calculations are usually the starting point for materials design or synthesis process in materials science. They allow to predict phases at equilibrium under specific conditions, to plot property diagrams, and of course to compute phase diagrams. These calculations are achieved using a database, where the thermodynamic data are gathered using a specific formalism and various models. The accuracy of the calculations depends on the quality of the thermodynamic data. Since ceramics exhibit a wide range of properties (phase transitions, range of stoichiometry, high temperature, nature of bonds, ordering...), it's then of importance to take care of the selected models and to critically select the thermodynamic data. DFT calculations are increasingly used to extend or supplant experimental data.

We will depict here the models that we may use for ceramics modeling, and the problematic of thermodynamic data acquisition at high temperature. Different cases will be presented for different applications (nuclear materials, aeronautics and aerospace), mostly in harsh environment.

Until now, the thermodynamic data were assessed from 298K up to high temperature, and lower temperature values were extrapolated, violating the third law of thermodynamics. More recently, researchers started the design the third generation of database, from OK up to high temperature, coupling DFT calculations, new models, and experimental data.