

Advances in the Development of OpenCalphad Software and Databases

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Thermodynamics is at the core of materials science. The Calphad method, a powerful tool for materials design and engineering applications, has been shown to be an excellent platform for linking experiments and theoretical, quantum mechanics based results thereby greatly contributing to the understanding of materials and their properties. Most of today's databases and software are proprietary restricting expansion and development of new models and their integration into software tools for materials simulations. This presentation describes the progress made in development of the OpenCalphad software code and databases. The goal of OpenCalphad is to develop free high quality software for thermodynamic calculations and databases with parametric physical models of the pure elements as basis for multicomponent databases as well as conventional Calphad databases. OpenCalphad provides a highly structured tool that can be used, together with kinetic models, in microstructure and continuum simulations.