



High throughput CALPHAD modeling and the Materials Genome®

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CALPHAD modeling begins with the development of models and the evaluation of parameters of individual phases of unary and binary systems, followed by extension to ternary systems by combining the constitutive binary systems with ternary interactions. The self-consistent model parameters are collected in databases, covering the whole composition and temperature ranges and used for the extrapolation to multicomponent systems. The shortcoming of this hierarchical structure implies that any modification of a constitutive subsystem has a snowball effect on the description of a multicomponent system in that it affects every description of systems that includes this subsystem, i.e. data in high-order systems depends on data in lower-order systems. To address this issue, we have been developing a high throughput CALPHAD modeling software package named ESPEI (extensible, self-optimizing phase equilibrium computer program). ESPEI establishes a data infrastructure for storing input data used for thermodynamic modeling and output data for thermodynamic analysis.

It is evident that the CALPHAD modeling implies that the building blocks of materials are individual phases. In the Materials Genome Initiative (MGI) by the US government, the word genome, when applied in non-biological contexts, connotes a fundamental building block toward a larger purpose. This works well when the fluctuation of internal configurations of a phase is around its stable configuration, i.e. the phase behaves normally. On the other hand, when anomaly appears, such as negative thermal expansion, more detailed understanding of internal configurations of the phase is needed. It will be argued that when some internal configurations are no longer fluctuations of the stable configuration, anomaly occurs. It is further shown that anomaly can be predicted when relevant individual internal configurations are identified.

1. Liu ZK, et al. (2004) An integrated framework for multi-scale materials simulation and design. *Journal of Computer-Aided Materials Design* 11(2-3):183-199.
2. Liu ZK (2009) First-Principles Calculations and CALPHAD Modeling of Thermodynamics. *Journal of Phase Equilibria and Diffusion* 30(5):517-534.
3. Shang S, Wang Y, & Liu ZK (2010) ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure for Magnesium Alloys. *Magnesium Technology* 2010:617-622.
4. Liu ZK, Wang Y, & Shang SL (2011) Origin of negative thermal expansion phenomenon in solids. *Scripta Materialia* 65(8):664-667.
5. Campbell CE, Kattner UR, & Liu ZK (2014) File and data repositories for Next Generation CALPHAD. *Scripta Materialia* 70:7-11.