ALLOY THERMODYNAMICS: From *AB INITIO* to PHENOMENOLOGY

Patrice E. A. Turchi
LLNL (L-353), P. O. Box 808, Livermore CA 94551, USA
Turchi1@llnl.gov

Stability and chemical order are some of the fundamental properties that drive the design of new complex materials. Using methods based on a combination of quantum mechanics and statistical thermodynamics, the following question: "*Which ordered configuration, and to some extent which crystalline structure, an alloy will exhibit as a function of temperature, pressure, and concentration?*" can be addressed from an *ab initio* standpoint.

Despite the success of these approaches, thermodynamics of complex multicomponent alloys, as used in engineering applications, requires a more versatile approach presently afforded within the so-called CALPHAD framework. Hence, there is a need to take advantage of *ab initio* approaches when thermodynamic databases lack information on a specific alloy, and cast their output in a "CALPHAD format" for further analysis.

Following a brief overview of the advanced methodologies and the CALPHAD approach, applications to general stability trends and phase diagram predictions will be presented for various alloys. Some of the results will then be used in a "CALPHAD format" to predict ternary phase diagrams. Finally, validity of the overall approach and future prospect will be discussed.

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