CALPHAD Modeling of the Molar Volume

Ursula Kattner [C, S]
Materials Science and Engineering Division, NIST, Gaithersburg, MD, U.S.A.
ursula.kattner@nist.gov

The molar volume of phases is an important quantity for many materials simulations. For example, knowledge of the molar volume enables the calculation of the misfit of precipitates or the heat evolution per volume in casting processes. Despite its importance, few CALPHAD-type evaluations of the molar volume in multi-component systems have been published, and no model for describing the temperature and composition dependence has been generally accepted by the community. Different formalisms have been used to describe the temperature dependence of the molar volume of the pure elements, some of which can be used down to 0 K. Although it is generally agreed upon to use the same formalisms for the compositional dependence as for the description of the Gibbs energy, different ways can be implemented to describe the combination of temperature and composition dependence. At the same time, limitations imposed by the software or the goals of modeling using the CALPHAD method may impose restrictions on the model approach being used. The approaches taken for current development of databases and future opportunities for model improvement will be discussed.