CALPHAD-Type Modeling of the Molar Volume in the Al-Co-Ni-W System

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The CALPHAD method was originally used to model the thermochemical properties and phase diagrams of alloy systems. The approach taken by the CALPHAD method, describing the Gibbs energy functions of individual phases as function of temperature, pressure, and composition, is also well suited for the description of many kinds of other phase-based data. The list of properties described with the CALPHAD method has grown to include diffusion mobilities, molar volume and, in some instances, the bulk modulus. Although molar volume is a property that is needed for the simulation of numerous materials processes, it has been included only in a handful of proprietary CALPHAD databases. Most of the published literature discusses the CALPHAD modeling of the temperature and pressure dependence of the molar volume but not models for the composition dependence. It is a common assumption to apply the same relations, such as the Neumann-Kopp rule for the heat capacity, to the molar volume. These assumptions are tested in development of a molar volume database for the Al-Co-Ni-W, a system with phases of varying complexity.