Thermodynamic assessment of the Co–Mg system supported by ab-initio calculations

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Abstract

The objective of this work is the thermodynamic modeling of the Co-Mg binary system using two methods: The CALPHAD method (Calculation of Phase diagrams) and the ab-initio calculations.

CALPHAD is a very important method for modeling thermodynamic properties of phase diagrams for systems with several components. This method is based on a semi approach by modeling the free energies of the different phases existing in a system. Therefore reliable experimental data are necessary for the description of thermodynamic properties of phases.The basic principles of this method are to harmonize a set of this experimental and theoretical information.The theoretical thermodynamic data are obtained by the ab-initio calculation. The enthalpies of formation of defined compounds are obtained by a calculation based on the first principle quantum simulations also called ab-initio method that allow the theoretical determination of various properties (electronic, structural, energy, etc ..) of the material without using experimental tools.

The phase diagram of the Co-Mg system has a single defined compound which is Co_2Mg. its enthalpy of formation is calculated using the WIEN2k code based on the method "full-potential linearized augmented plane-wave"and the GGA approximation "Generalized gradient approximation". The liquid phase was modeled using the Redlich-Kister polynomial. The results obtained are in good agreement with experimental results.

Keywords: Phase diagram, Co-Mg system,thermodynamic assessments, Calphad, Ab-initio calculations