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Thermodynamic reassessment of the Neodymium-Gold binary system

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Abstract

Phase relationships in Nd–Au binary system have been thermodynamically assessed by means of the CALPHAD technique through Thermo–Calc software package based on the experiment information of phase equilibria and thermodynamic properties from the published literature data. The excess Gibbs energy functions of the solution phases including liquid, fcc_A1, bcc_A2, and dhcp were formulated with Redlich-Kister polynomial functions. The two–sublattice energy model was employed to describe the Nd₁₄Au₅₁ phase which exhibits a homogeneity range. The intermetallic compounds Nd₂Au, NdAu, Nd₃Au₄, Nd₁₇Au₃₆, and NdAu₆ were treated as stoichiometric phases. A set of self-consistent thermodynamic parameters formulating the Gibbs energy of various phases in the Nd–Au binary system were then obtained. A much better agreement was achieved between the calculated results and the reported experimental data.

Keywords: Nd–Au phase diagram; Thermodynamic assessment; CALPHAD method;

1. Introduction

Gold–Rare Earth Elements (REEs) alloys have widely been used during recent years in the fabrication of modern electronic devices, because of their great properties [1–3]. REEs are potential candidate to replace Au or at least to reduce its use in the eutectic Au–20 wt. % Sn solders broadly used in the electronics industry in order to avoid the scarce resources and high price of Au as well as the poor mechanical properties of the Au–Sn intermetallic compounds. Furthermore, REEs can refine the mechanical properties and improve the wettability of solders [4]. By reducing the oxidization of solder and cleaning the grain boundaries, the REEs improve the fatigue performance under slow deformation [5–7].

The use of REEs in corrosion protection as inhibitors is very attractive because of their non-toxicity, as compared to the common chromate inhibitors [8]. A brief analysis of literature indicates that a protective effect can be provided by small amounts of REEs [8, 9] which become increasingly important in the transition to a green economy, due to their crucial role in

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