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Thermodynamic description of the Palladium-Ytterbium binary system

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Phase diagrams are the maps for materials and process development. Traditionally, they have been determined purely by experimental approach that is costly, meticulous and time-consuming. In principle, they can be determined experimentally, but the time required to do so can be significantly longer. This is where the computer simulation and the CALPHAD (an acronym for Calculation of Phase Diagrams) method comes in and plays an important role. The CALPHAD method is based on the description of the Gibbs free energies of the different phases present in a system. These are evaluated in simple systems by least-square fitting of model parameters in order to describe as well as the possible available experimental data (phase diagram and thermodynamic data) on a given system. One of the merits of the technique is its ability to describe metastable equilibrium since the phases are most often described out of their temperature and composition stability ranges. The intermetallic compounds formed by Rare Earth Elements and Transition Metals are of particular interest regarding their potential usage as high value functional materials, such as permanent magnets and hydrogen storage materials. In this context, the Pd-Yb binary system attracts much attention in recent years. To understand the physical properties and the technological applications of these compounds, it is necessary to obtain a better knowledge of the thermodynamic properties of this system. The phase diagram of the Pd-Yb system assessed by Okamoto contains 11 intermediate phases: Pd₇Yb, Pd_{2.13}Yb, Pd₂Yb, α- and β-Pd_{1.63}Yb, Pd₄Yb₃, α- and β-PdYb, α- and β-Pd₂Yb₅, PdYb₃. Most of these phases were characterized by Iandelli and Palenzona; these two authors, ascertained the exact stoichiometry of the Pd_{1.63}Yb and Pd_{2.13}Yb phases, which could now be more correctly indicated as Pd₃Yb₃ and Pd₂₁Yb₁₀, respectively. Recently, Ciccioli et al. studied the vaporization behavior and thermodynamics of the Pd-Yb intermediate phases in the Pd-rich part of the phase diagram. This work deals with an assessment of the thermodynamic description of the Pd-Yb system by means of the CALPHAD method. A set of self-consistent thermodynamic parameters of the Pd-Yb system was obtained.

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