THERMODYNAMIC DATABES FOR PLATINUM GROUP METALS: THEORY MEETS PRACTICE

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Multicomponent metallic materials containing platinum group metals (PGM) and rhenium are widely used in industrial applications as high-temperature materials, in superalloys and as catalysts. In particular, bimetallic PGM—Re and PGM—Os compositions are used in high-temperature thermocouples, as coatings with a high thermal, mechanical and chemical stability [1]. Rhenium has a specific role in constructional materials science due to its remarkable effect on improving the room-temperature ductility of multicomponent alloys known as "*Rhenium effect*". Nevertheless, the information available for several PGM—Re, PGM—Ru and PGM—Os binary metallic systems is poor and contradictory as well as not all phase diagrams are correct and known in details especially in the *liquidus* part due to the difficulties that arise during the preparation of equilibrium solid solutions and melting [2]. Critical topological and thermodynamic analysis of known experimental data (12 binary *hcp—fcc* and *hcp—hcp* phase diagrams) shows numerous unlike thermodynamic futures and a need for partial re-investigation of the existing phase diagrams. This, together with the high cost of the materials, limits the practical applications of PGM alloys and composites. Construction of the correct equilibrium phase diagrams would provide a solid basis for future investigations of chemical, physical and material properties of composite systems based on PGM and Re solid solutions and could enable their usefulness to be extended. Comprehensive knowledge of two-component systems is also essential for the prediction and construction of accurate ternary and quaternary phase diagrams [3, 4].

CALPHAD (CALculation of PHAse Diagrams [5]) approach makes possible to analyse experimental data of various nature (phase composition, free energy, diffusion coefficients *etc*) at the same time to find concordant thermodynamic parameters characterized particular phase diagram in a whole range of concentration and temperature. The corresponding mixing parameters depend on the model chosen for the solution description. The set of parameters for all possible phases presented in the particular system can be regarded as thermodynamic database. Parameters characterized the binary system can be directly transferred to ternary and higher order systems, which makes *CALPHAD* a suitable technique for the rough estimation of phase boundaries in complex systems. The information about binaries, such as their thermodynamic behaviour in *solidus* and *liquidus* parts and mixing parameters, can be applied for the ternary systems. Calculated phase diagrams can be further used as starting models to be improved in terms of correction of mixing parameters and drawing of boundaries.

The actual status of PGM phase diagrams and their thermodynamic database will be discussed hereby. Collection of correct experimental data and strategies for redetermination of PGM phase diagrams will be discussed to achieve the construction of the complete database for materials chemistry and metallurgy, improve properties of existing constructional materials and develop novel application frontiers.

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