BOOK OF ABSTRACTS

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Application Of CALPHAD Method For Materials Design

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In the frameworks of CALPHAD (Calculation of Phase Diagrams) method, the experimental information on the thermodynamic properties of phases and phase equilibria in the system is converted into optimized parameters of Gibbs energy models of the phases. The term “thermodynamic assessment of the system” indicates that the parameters of thermodynamic models of phases of the system obtained in such way that the thermodynamic properties of phases and the phase diagram of the system can be calculated simultaneously. CALPHAD method allows to summarize and clarify in the one model the data on phase equilibria and thermodynamics of phases and is a powerful tool for theoretical research and establishing of the most accurate information. The model parameters can be summarized in self-consistent databases for multicomponent systems and can be applied for the development of new materials. Different problems associated with equilibrium transitions in multicomponent materials such as the temperature-composition boundaries of phase range, the determination of the optimal concentration of additives, or analysis of the dependence of the phase composition on temperature, for example, can be solved. Also, the questions associated with the occurrence of metastable transformations in the systems leading to the formation of amorphous alloys, supersaturated solid solutions based on pure components and intermediate phases. This report covers a wide range of issues, such as examples of thermodynamic descriptions of binary and ternary systems, development of the databases for the quinary Cu–Ni–(Fe, Co)–Ti–(Zr, Hf) and Co–Cu–Cr–Fe–Ni systems. We will also consider examples related to the prediction of concentration regions for obtaining materials with different morphological structural features, and crystalline and amorphous high-entropy alloys.

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