NATIONAL THERMODYNAMIC DATABASE FOR MODELING OF PHASE EQUILIBRIA OF OXIDE SYSTEMS AT HIGH TEMPERATURES

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Progress in high temperature technologies such as microelectronics, the nuclear, space, aviation and optical industries as well as metallurgy requires of development of advanced materials which have to be stable under operation during long high-temperature impacts up to the temperature 3000 K. During increasing the temperature, as a rule, the complex changes of physicochemical properties of materials may be observed as the result of processes available in the condensed and gaseous phases. At present the thermodynamic data bases for modeling of phase diagrams of multicomponent systems at high temperatures are widely used abroad in the frame of CalPhad (Calculation of Phase Diagram) approach. However the similar thermodynamic data bases are absent in Russia. Development and approbation of new additional thermodynamic semi-empirical and statistical thermodynamic approaches for calculation of thermodynamic properties and phase equilibria in multicomponent oxide systems containing hafnium, zirconium and rare earth oxides were illustrated and recommended for the application in the National thermodynamic data base. The availability of such National data base will allowed to predict and to prevent the ecological accidents at high temperatures with the participation of inorganic materials as well as to develop and to apply in industry ultra high-temperature materials for ensuring of national interests in the variety of the high-temperature adaption areas [1, 2].

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