PHASE STABILITY OF $A_2B_2O_7$-TYPE ULTRAHIGH-ENTROPY COMPOUNDS

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The research is aimed at the synthesis and investigation of the structure, stability, and properties of novel oxide ultrahigh-entropy phases, whose compositions correspond to the formulas $A_2Zr_2O_7$, $A_2Hf_2O_7$, $A_2Ti_2O_7$, $A_2Ce_2O_7$, $A_2Pr_2O_7$, and $A_2Sn_2O_7$, where A represents a high-entropy sublattice composed of 12–13 rare-earth elements (excluding Ce, Pr, and Pm).

Experimental samples are synthesized using solid-state sintering at temperatures of 1500–1600 °C, as well as via a modified Pechini method. The composition and structure are characterized using SEM, EDS, and XRD. The results demonstrate various fluorite-type structures (fluorite, defect fluorite, pyrochlore). The coefficients of thermal expansion and thermal conductivity of the obtained materials are studied. Additionally, electrochemical properties are investigated due to their potential relevance for the use of these substances as catalysts in various chemical processes.

Special attention is given to the study of the phase stability of the synthesized materials over a wide temperature range using differential thermal analysis. The obtained results indicate that the studied phases exhibit high structural stability.

As part of the research, a thermodynamic description of the new high-entropy oxide phases is developed, based on the analysis of literature data and our own experimental results (primarily data on the temperature and concentration stability limits of solid solutions in the studied systems). Expressions correlating the Gibbs energy of such phases with their composition and temperature have been derived.

These studies employ modern thermodynamic modeling techniques implemented in contemporary specialized software (the FactSage 8.0 software package, in which a proprietary user database has been developed based on the results of this work).

The analysis of the obtained experimental data will allow the formulation of general trends governing the formation of high-entropy oxide phases, which should include criteria for the structural stability of such phases.

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