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Phase complex model of ternary reciprocal system $Na^+,Sr^{2+}||WO_4^{2-},MoO_4^{2-}$

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Abstract

The paper presents the results of a theoretical study of the phase complex of a three-component reciprocal system consisting of sodium and strontium tungstates and molybdates. Previously, a literature review was conducted on data on phase equilibria in the condensed state of individual salts, binary faceting systems. In two Na_2MoO_4 – $SrMoO_4$ and Na_2WO_4 – $SrWO_4$ binary systems, a eutetic equilibrium is observed with the formation of solid phases corresponding to the system components, and in two other Na_2MoO_4 – Na_2WO_4 and $SrMoO_4$ – $SrWO_4$ binary systems, one phase of a continuous series of solid solutions crystallizes. Based on the mathematical model of the molar balance, one can uniquely determine the quantities of reaction products, the molecular formulas of solid solutions, and the equations of chemical reactions for an arbitrary mixture of system components. This model represents a set of algebraic equations by which the balance is calculated. To build a 3D computer model, the paper presents the equations for the conversion of coordinates from barycentric to Cartesian. The model is implemented in concentration-temperature coordinates using the KOMPAS-3D program using experimental data on the system. The model is built in two interpretations: based on data on the faceting elements and on the basis of all available data about the system. Comparison of the two models makes it possible to evaluate the predictive ability carried out using 3D modeling. From this comparison, it was found that using the 3D model it is possible to conduct a preliminary a priori forecast of phase equilibria in order to identify the structure of phase diagrams at the qualitative and quantitative levels. The projection of the crystallization polytherm onto the square of the compositions is represented by two fields of solid solutions – $Na_2Mo_xW_{1-x}O_4$ and $SrMo_xW_{1-x}O_4$. Isothermal and polythermal sections were constructed. The system implements di- and monovariant equilibria.

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