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Forecasting of phase equilibria in the system $NaCl-Na_2MoO_4-Na_2WO_4$ at the liquid-solid interface

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Abstract

The paper presents the results of a theoretical study of the phase complex of a three-component system consisting of tungstates, molybdates and sodium chlorides for equilibrium "liquid - solid". Previously, a literature review was conducted on data on phase equilibria in the condensed state of individual salts, binary faceting systems. In two $NaCl-Na_2MoO_4$ and $NaCl-Na_2WO_4$ binary systems, a eutetic equilibrium is observed with the formation of solid phases corresponding to the system components and Na_3ClMoO_4 and Na_3ClWO_4, and in binary faceting system Na_2MoO_4 – Na_2WO_4, 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. With 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 three fields of solid solutions – NaCl, $Na_3ClMo_xW_{1-x}O_4$ and $Na_2Mo_xW_{1-x}O_4$. Isothermal and polythermal sections were constructed. The system implements di- and monovariant equilibria. A diagram of the material balance of crystallizing phases is constructed. The paper presents the calculation of the ratio of equilibrium phases, as well as their qualitative and quantitative composition for the two-phase and three-phase regions according to the coordinates of the points - the vertices of the conode segments and conode triangles, which are extracted from the 3D model. The calculation is implemented for a given composition and temperature.

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