3D Model of Phase Diagram for System $MgO-SiO_2-Al_2O_3$ and its Application

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Systems $CaO(MgO)-SiO_2-Al_2O_3$ have a great practical importance, and their phase diagrams (PD) are used not only for the description of properties of advanced and building materials, but for the characterization of geological objects too. Data for invariant processes in the binary and ternary systems (with taking into account the existence and type of binary and ternary compounds) is the base for creation of schema of mono- and invariant equilibria. At the first stage for construction of 3D model, the invariant horizontal complexes at the temperatures of ternary points are reconstructed. Then they are completed by the ruled and unruled surfaces, and the phase regions are formed [1-3].

The system $MgO-SiO_2-Al_2O_3$ has a rather complex geometric structure. It includes four binary compounds and two ternary compounds. It's characterized by 11 invariant transformations: three eutectics, one peritectic, five quasiperitectic equilibria and two four-phase regroupings of phases with polymorphous modifications of silicon oxide (cristobalite and tridymite). Obtained computer model of phase diagram for system $MgO-SiO_2-Al_2O_3$ includes liquid immiscibility surface, 10 liquidus surfaces, 78 ruled surfaces, 11 horizontal complexes at the temperatures of invariant points, 21 two-phase regions and 29 three-phase regions. Projection of PD is divided into 100 two-, 170 one- and 71 zero-dimensional concentration field.

The diagrams of vertical mass balance have been calculated for each concentration field. They permit to obtain the lists of intersected phase regions and the crystallization stages for given mass center over the entire temperature range. In addition, the list of microconstituents for each field is obtained on the base of this investigation. As a result, we can identify the concentration fields with coinciding sets of crystallization scheme and microconstituents and the fields with individual characteristics [4]. However, some concentration fields can differ by the crystallization stages but coincide by the microconstituents with neighboring fields.

There are a large number of concentration fields with coinciding microconstituents in the SiO_2 angle, unlike other parts of PD. The reason is the presence of phase regions with liquids immiscibility and two polymorphous modifications of SiO_2. Processes occurring in the phase regions L_1+L_1, $L_1+L_1+B_1$, $L+B_1$ (B_1 - cristobalite) not influence on the final set of microconstituents, because the products of reactions for these fields are fully expended. Other parts of PD have the similar influence on the microstructure.

Therefore, analysis of concentration fields using the model of phase diagram is a tool to design the microconstituents sets of the heterogeneous material. All possible crystallization schemas of considered system and the content of each microstructural constituents taking into account its origin are analyzed by means of PD model.

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[1] V. Lutsyk, A. Zelenaya, Építőanyag - *Journal of Silicate Based and Composite Materials* **65** (2013) 34-38.
[2] V. Lutsyk, A. Zelenaya, *Solid State Phenomena* **200** (2013) 73-78.
[3] V.I. Lutsyk, A.E. Zelenaya, E.R. Nasrulin, E.S. Bimbaev, *Melts* **3** (2016) 206-215.
[4] V.I. Lutsyk, A.E. Zelenaya, E.R. Nasrulin, A.M. Zyrianov, *Melts* **3** (2016) 216-225.