Analysis of the geometric features of T-x-y diagrams with melt immiscibility for silicate systems

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Abstract. Analysis of the geometric structure of phase diagrams for ternary systems with the two immiscible liquids has been carried out. T-x-y diagrams with the both types of the monotectic equilibriums (univariant and invariant ones) have been analyzed. Three-dimensional computer models of T-x-y diagrams for the four silicate systems with mono- and invariant equilibriums and different variants of the immiscibility surfaces location have been built. T-x-y diagram of the ZrO2-SiO2-Al2O3 system includes one immiscibility cupola, located in the ZrO2 crystallization field, which adjoins the ZrO2-SiO2 side. The 3D model of T-x-y diagram includes four invariant transformations: peritectic P: L→ZrO2+SiO2→R2, quasi-peritectic Q: L→ZrO2→R1+R2, two eutectic E1: L→ZrO2+Al2O3+R1, E2: L→SiO2→R1+R2. Five surfaces of liquidus, which correspond to the beginning of primary crystallization of three initial components and two binary compounds R1=3Al2O3·2SiO2 and (congruently melting) and R2=ZrO2·SiO2 (decomposed without liquid) are formed in the system. T-x-y diagram TiO2-ZrO2-SiO2 is characterized by one eutectic E: L→TiO2+SiO2+ZrO2·TiO2 and one quasi-peritectic Q: L→ZrO2→SiO2+ZrO2·TiO2 transformations and includes two immiscibility surfaces from the sides of TiO2-SiO2 and ZrO2·SiO2 binary systems. FeO-SiO2-Fe2O3 system with common immiscibility cupola, that prolongs from the system FeO-SiO2 to the system SiO2-Fe2O3, is characterized by three invariant transformations of eutectic type, and one metatectic transformation V: B1→L+B2+C, which corresponds to the transfer from high-temperature allotropy of silica (B1 - cristobalite) to the low-temperature one (B2 – tridymite). T-x-y diagram KAlSi2O6-Fe2SiO4-SiO2 has two immiscibility surfaces: one of them adjoins to the Fe2SiO4-SiO2 binary system and the second one is located on the Fe2SiO4 and tridymite liquidus surfaces, dividing the univariant curve on their boundary into two parts, and has three points of the maximum and three points of the minimum. Using of the computer models of T-x-y diagrams allows you to take into account different variants of the geometric structure of the investigated silicate systems.

1. Introduction
Silicate systems are quite often characterized by the presence of one or more regions of two immiscible liquids [1]. The location of the immiscibility dome relative to other elements of the phase diagram significantly affects its geometric structure. The most common are the ternary silicate systems, in the formation of which the binary monotectic system participates. At the same time, the immiscibility dome is in the crystallization field of one component, and the system is characterized by a monovariant monotectic equilibrium. These include, for example, systems CaO-BaO-SiO2, MgO-Al2O3-SiO2, CaO-Al2O3-SiO2, Y2O3-Al2O3-SiO2, FeO-Al2O3-SiO2, CoO-Al2O3-SiO2.

If two monotectic binary systems are involved in the formation of the ternary system, the regions of immiscibility may be located in different fields of liquidus, without touching each other or crossing the monovariant curves of the liquidus, as in the systems TiO2-ZrO2-SiO2, MgO-ZrO2-SiO2 [2-3].
Another common option in a similar situation is a combination of two binary monotectics into one immiscibility dome. In this case, as a rule, the immiscibility region divides the field of Cristobalite (high-temperature allotropy of SiO₂) into two parts, not crossing the monovariant curve of the liquidus. This version of the immiscibility region structure is found in the systems MgO-CaO-SiO₂, MgO-ZnO-SiO₂, CaO-ZnO-SiO₂, MgO-MnO-SiO₂, CaO-MnO-SiO₂, MgO-FeO-SiO₂, CaO-FeO-SiO₂ [2-4]. A variation of a diagram with two binary monotectic systems is the CaO-TiO₂-SiO₂ system with two regions of immiscibility, that intersect each other [3].

A more complex version of the diagram structure is obtained when the immiscibility dome crosses the curve of the joint crystallization of two phases. The presence of invariant monotectic equilibrium significantly complicates the structure of the phase diagram. As an example, we can mention the system BaO-B₂O₃-SiO₂ [3].

In addition, it is possible to build a T-x-y diagram, in which the immiscibility dome appears inside the ternary system, despite the fact, that there is no immiscibility in the binary systems, forming it. At the same time, the immiscibility surface can be located within the same surface of liquidus (Na₂O-MnO-SiO₂) or cross one (K₂Si₂O₆-Fe₂SiO₄-SiO₂), two or all three monovariate curves of liquidus [3, 5, 6].

Using spatial (three-dimensional - 3D) computer models T-x-y diagrams allows you to take into account different variants of the geometric structure of the silicate systems studied [7]. 3D computer models of T-x-y diagrams are built on the basis of their assembly from phase regions [8-15].

The technology of spatial (three-dimensional - 3D) models of T-x-y diagrams creating from geometric elements [7] is implemented in the author's program Constructor of Phase Diagrams (Constructor of PD). T-x-y diagrams assembling from surfaces and phase regions to build a 3D computer model is done in several steps: 1) scheme of mono- and invariant states; 2) 3D computer model of T-x-y diagram prototype; 3) 3D model of the T-x-y diagram for the real system [15].

The scheme of mono- and invariant states is a normal scheme of phase reactions supplemented by trajectories of changes in the compositions of the three phases in monovariant transformations [7, 15]. It allows: – determine the number and type of surfaces (non-ruled or ruled surface, plane, dome, etc.); – find out the number of phase regions; - clarify the degeneration of the surface or phase region, indicating which solid-phase participants of the three-phase transformations do not have the limited solubility; – translate the table scheme of mono- and invariant states into three-dimensional one, receiving a phase diagram frame - a mock-up of the future T-x-y diagram; – get a compact description and explanation of the geometric structure of the phase diagram; – formalize the description of phase diagram; – restore the missing (supposed) geometric elements and prepare for the construction of its geometric model.

The prototype is a kind of perfect geometric structure, which then you need to get closer to the real one. To do this, it first introduces the real coordinates of all base points and "degenerates" those surfaces that merge with the diagram boundaries – the edges and faces of the prism. Then begins the struggle for the accuracy of the model and adequate display of the available experimental material (or obtained from different sources, including thermodynamic calculations). To do this, the curvature of curves, surfaces is specified, and, as a result, a spatial computer model of a specific T-x-y diagram is obtained. The process of the perfect model getting can be long, it may require additional refining experiments. However, we can be sure that there are no methodological errors in the computer model built in this way, caused by the misinterpretation of the experiment and which are found in the construction of phase diagrams by conventional traditional methods.

From the prototypes of 3D computer models of spatial phase diagrams of the main topological types a special Handbook is collected [8]. It includes the models of phase diagrams of ternary systems, formed by I-V types of binary systems by the classification of Roseboom, with the formation of compounds of varying degrees of congruence and conditions of existence, with allotropy of components in different temperature intervals, immiscibility of liquid and decay of solid solutions. Using the Handbook, diagrams of real systems are reconstructed to build the computer models, the
quality of which ultimately depends on the completeness and correctness of the original experimental information.

Figure 1. T-x-y diagram includes one (a,c), two (b,d), three (g) monotectic binary systems,
when the immiscibility cupola is in one liquidus field (a,b) or intersects curves of co-crystallization of phases (c,d,g,h) (shape od immiscibility surfaces (e,g) are shown in detail for T-x-y diagrams d and f)

2. 3D computer models of T-x-y diagrams with melt immiscibility

Most complete overview of T-x-y diagrams with immiscibility was given in the monograph [16]. This work presented the examples of nine T-x-y diagrams of the eutectic type, among which five are formed with the participation of one, two or three binary systems with monotectics. There are different variants of the immiscibility cupola location relative to the liquidus surfaces and other immiscibility surfaces. For example, the immiscibility cupola occupies a part of one liquidus field; it passes through the entire liquidus field and crosses the immiscibility curve of the second binary system; it can crosses two liquidus fields; it exists in all three liquidus fields, forming a complex structure of three liquids immiscibility. Four more examples are given for a eutectic system, in which the immiscibility cupola is not adjoined with binary systems, but exists in one, two, three liquidus fields and crosses one, two or three lines eE, respectively. The diagrams with liquid immiscibility were considered in [17-21], in addition the diagrams with liquid immiscibility coexisting with vapor are discussed in [22-24]. Article [18] shows the invariant equilibrium of four liquid phases. Notice that the authors of [25] cite the work [26], in which is excluded such interaction.

Our reference book of 3D computer models includes five T-x-y diagrams with liquid immiscibility formed by binary systems with monotectics, four T-x-y diagrams with the ternary cupola of immiscibility without monotectics in binary systems, four diagrams with immiscibility of three liquids based on data from [16], as well as T-x-y diagrams with syntectic uni- or invariant transformation.

2.1. T-x-y diagram with univariant monotectic equilibrium

If the cupola of immiscibility mknK is located in the liquidus field of component A (Figure 1a), then it is important to understand that the solidus A corresponding to it has a fold A mAK conjugated with the mK, nK lines [27]. These three lines (mn, mK, nK) are the directing lines of the ruled surfaces that form the region of monotectic transformation L1 L2+A.

2.2. T-x-y diagram with invariant monotectic equilibrium

T-x-y diagram with invariant monotectic transformation (Figure 1c) was considered in [29], with the immiscibility cupola divides line eBCE, as well as in monographs [16, 25, 30]. Unlike the works [16] and [25], the author of [30] analyzed this diagram without taking into account the solid-phase solubility and showed the trajectories of changes of melts. In [16], the surfaces under the liquidus are indicated indistinctly, and the schema of phase transformations show only the trajectories of composition changes for melts.

By virtue of the fact that the immiscibility of two liquids L1+L2 takes place under the cupula mknNKM crossing the line eAC E, then it is necessary to distinguish which of the two liquids L1 or L2 coexist with crystals A, B, C on the schema of uni- and invariant states (Table 1).

Since the monotectic reaction in the binary system A-B is performed in the form L1 L2+A, then in the upper part of the two-phase region L+A should be L1+A (from the fold A mAM on the solidus sA). The surfaces of liquidus qA and solidus sA are divided into two parts. It is also required to rename the three-phase region L+A+B and two-phase region L+B as L2+A+B and L2+B accordingly. The phase region L2+B+C is arranged on other side of the region L2+B, which does not violate the rule on contiguous phases [28] (this rule is formulated in the monograph [28, p. 212-221] and is cited in [25, p. 230]). Three-phase regions L2+A+B and L1+A+C adjoining to the corresponding binary systems border on two-phase regions L2+A and L1+C. Due to immiscibility the crystals A and C interact with both L1 and L2, and also together after the finish of the monotectic invariant transformation L1(M)→L2(N)+A+C in the region L2+A+C, therefore an additional 3 three-phase regions appear: L1+L2+A, L1+L2+C, L2+A+C.

Thus, the phase diagram includes: by 3 phase regions I and I + J, 7 three-phase regions L2+A+B, L1+A+C, L2+A+C, L2+B+C, L1+L2+A, L1+L2+C, A+B+C, 6 two-phase regions L1+L2, L1+A,
L2+A, L1+C, L2+C, L2+B and 21 ruled surface, 4 liquidus, 4 solidus, 6 solvuses, immiscibility cupola, 8 horizontal simplex, and a total of 19 phase regions and 44 surfaces.

The immiscibility cupola mMKNNk adjoining to the binary system A-B divides the liquidus field A into two parts along the line $e_{AC}E$. If the cupola divides this surface along the line $e_{BC}E$ adjoining to the binary system BC (as in [29]), then formally the scheme of uni- and invariant states will not change, and two invariant transformations of the eutectic type will also be represented. However, participation in monovariant transformations of phase A will be replaced by B.

Since the liquidus contour C is given by 6 points: $e_{AC}$, M, K, N, E, $e_{BC}$, then the conjugated solidus $s_C$ has 6 corresponding points: $C_A$, $C_M$, $C_K$, $C_N$, $C_E$, $C_B$. The main innovation in this kind of computer models is the presence of a pseudo-fold $C_KC_M$ on the solidus $s_C$. It is a directing line of two ruled surfaces and does not affect the smoothness of the solidus C. The upper point of the $C_K$ has the temperature of critical point K at the intersection of the immiscibility cupola with the liquidus surface $q_C$. Due to the fold starting at the point $C_K$, the liquidus and solidus become topologically equivalent, because the curve $C_KC_M$ is conjugate with two parts of the arc NKM.

In [25], the surfaces of the solvus are constructed so that the lines of its contour $I_J-I_0J$, $I_E-I_0E$ are vertical. Therefore, the x-y projections of the points $I_J$ and $I_0J$, as well as $I_E$ and $I_0E$ are combined, and the solvus contour $C_AC_MC_E^0C_A^0$ is not closed, since there is no line $C_0AC_E^0$ [31].

Table 1. Schema of uni- and invariant states of the T-x-y diagram with invariant monotectic transformation, $A>\kappa>m(n)>B>C>e_{AB}>K>e_{AC}>M(N)>e_{BC}>E$ (Figure 1c)

| A-B | A-B-C | B-C | A-C |
|-----|-------|-----|-----|
| L2→A+B | L1→L2+A | L1→A+C | L1→A+C |
| $e_{AB}E$, $A_BE$, $B_AE$ | mM, nN, $A_MA_C$ | $e_{AC}M$, $A_CA_M$, $C_AE$ | $e_{AC}M$, $A_CA_M$, $C_AE$ |
| L1→L2+C | KM, KN, $C_KC_M$ | L2→B+C | $e_{BC}E$, $B_AB_E$, $C_BE$ |
| M(N): L1→L2+A+C | $L1→A+C$ | | |
| M(N)E, $A_MA_E$, $C_MC_E$ | $e_{BC}E$, $B_AB_E$, $C_BE$ | |
| E: L2→A+B+C | $A+BE$, $C_EE$, $B_BE^0$ | |
| $A_EA^0_E$, $C_EE$, $B_BE^0$ | |

The use of such model-prototypes makes it possible to understand, as the formation of the immiscibility regions influences on the T-x-y diagram geometric structure and, naturally, helps investigations of the real silicate systems.

3. 3D models of T-x-y diagrams of silicate systems with the immiscibility regions

T-x-y diagram of the $\text{ZrO}_2$-$\text{SiO}_2$-$\text{Al}_2O_3$ system includes one immiscibility cupola, located in the $\text{ZrO}_2$ crystallization region, which adjoins the $\text{ZrO}_2$-$\text{SiO}_2$ side (Figure 2a), and relates to the topological type, corresponding to the Figure 1a. Two binary compounds are formed in the system: congruently melting $R_1=3\text{Al}_2O_3$-$2\text{SiO}_2$ and $R_2=\text{ZrO}_2$-$\text{SiO}_2$, which is decomposed without liquid in the $\text{ZrO}_2$-$\text{SiO}_2$ binary system. The $e_{\text{max}}$ maximum points located on the QE$_1$ univariant curve; it is simultaneously the eutectic of the $R_1$-$R_2$ quasi-binary section. The T-x-y diagram 3D model has been designed by data [2, 3], and according to them, there are four invariant transformations: peritectic P: $L+\text{ZrO}_2+\text{SiO}_2\rightarrow R_2$, $R_1$. 

...
quasi-peritectic Q: L+ZrO₂→R₁+R₂, two eutectic E₁: L→ZrO₂+Al₂O₃+R₁, E₂: L→SiO₂+R₁+R₂.

Five surfaces of liquidus, which correspond to the beginning of primary crystallization of three initial components and two binary compounds R₁ and R₂, and the immiscibility cupola are formed in the system.

Figure 2. X-Y projections of 3D models of ZrO₂-SiO₂-Al₂O₃ (a), TiO₂-ZrO₂-SiO₂ (b), FeO-SiO₂-Fe₂O₃ (c), KAISi₂O₆-Fe₂SiO₄-SiO₂ (d) liquidus and immiscibility surfaces

The TiO₂-ZrO₂-SiO₂ T-x-y diagram includes two immiscibility surfaces from the sides of TiO₂-SiO₂ and ZrO₂-SiO₂ binary systems (Figure 2b). One of them is located in the TiO₂ crystallization field, the second - inside the ZrO₂ crystallization field. Both these surfaces do not intersect liquidus univariant curves. Design of the 3D model takes into account the formation of two binary compounds: the incongruently melting R₁=ZrO₂/g₁₁₁ TiO₂ and R₂=ZrO₂/g₁₅₂ SiO₂, which decomposes in the binary system. The model was constructed on the assumption that the system is characterized by one eutectic E: L→TiO₂+SiO₂+R₁ and one quasi-peritectic Q: L→ZrO₂→SiO₂+R₁ transformations; and its T-x-y diagram includes four liquidus surfaces of initial components and the compound R₁. The compound R₂ has not its liquidus surface, because it is decomposed without the participation of liquid.

The FeO-SiO₂-Fe₂O₃ system is also formed with the participation of FeO-SiO₂ and Fe₂O₃-SiO₂ two binary systems with the liquid immiscibility (Figure 2c). However, one common immiscibility cupola is formed in the ternary system; it unites them and occupies the large part of the diagram. This
topological type is presented in the Figure 1b. The immiscibility surface is located in the cristobalite crystallization field and divides it into two parts.

This system is characterized by four invariant transformations: three eutectic $E_1$: $L \rightarrow R_1 + R_2 + R_3$, $E_2$: $L \rightarrow B + R_1 + R_3$, $E_3$: $L \rightarrow B + C + R_3$ and one metatectic $V$: $B_1 \rightarrow L + B_2 + C$, which corresponds to the transfer from high-temperature polymorphous modification of silica ($B_1$ - cristobalite) to the low-temperature one ($B_2$ – tridymite). More detail about the contradictions in the description of the FeO-SiO$_2$-Fe$_2$O$_3$ system and the construction of its 3D computer model it can see in [14].

Liquidus of the KAlSi$_2$O$_6$-Fe$_2$SiO$_4$-SiO$_2$ T-x-y diagram is the combination of two immiscibility surfaces (Figure 2d) [5, 6]. One of them adjoins the Fe$_2$SiO$_4$-SiO$_2$ binary system and is in the cristobalite crystallization region. The second surface is located inside the T-x-y diagram and borders on the Fe$_2$SiO$_4$ and tridymite liquidus surfaces, dividing the univariant curve on their boundary into two parts (according topological type is presented in the Figure 1c). It is necessary to take into account, that the contour of the second immiscibility surface $k_1 N k_2 k_3 k_4 M$ contains three points of the maximum ($k_1$, $M$, $N$) and three points of the minimum ($k_2$, $k_3$, $k_4$). One binary incongruently compound $R = $KAlSi$_3$O$_8$ is formed in the KAlSi$_2$O$_6$-Fe$_2$SiO$_4$-SiO$_2$ system. This system is characterized by eutectic $E$: $L \rightarrow B + C + R$ and quasi-peritectic $Q$: $L + A \rightarrow B + R$ invariant transformations. There are five liquidus surfaces, corresponding to primary crystallization of initial components (KAlSi$_2$O$_6$, Fe$_2$SiO$_4$), two polymorphous modifications of SiO$_2$ and the compound $R$.

4. Summary

Design of the three-dimensional computer model of phase diagram gives the possibility to understand and to dismantle in detail its geometric structure, and also to construct isothermal sections and isopleths and to calculate the paths of crystallization. The special feature of this method is the possibility to obtain the complete data about the stages of crystallization and the phase and microstructural composition of sample without taking into account diffusion processes for each crystallization field. If to project all elements of phase diagram, the concentration triangle is divided into two-dimensional, one-dimensional (lines) and zero-dimensional (points) concentration fields. The stages of crystallization (with the enumeration of phase reactions) are examined for each field and the paths of crystallization are formed (with the tracing of the liquid trajectory). Fields both types, as with the individual set of microstructural elements, as with sets of microstructure, which coincide with the adjacent fields of the larger dimensionality [32, 33], are revealed on the basis of these data.

The approach in consider, based on assembling of the phase diagram model from the phase regions, in the case of incomplete information about the binary systems either liquidus surfaces or with contradicted data, gives the possibility to design the prototype of the studied system or several its alternatives, which can be modified and be refined with the appearance of new information.

The main advantage of the space models, designed by assembling from the phase regions, are excellent possibilities for: – the visualization of phase diagrams in the three-dimensional space through any projections and sections, in the form of individual phase regions and/or the border surfaces; – the comparison of model sections with sections, obtained from experiments; – verification and the search for disagreements in the data according to the phase diagram, constructed by different researchers; – the construction of the different versions of one and the same phase diagram in the case of fundamental divergences according to the data, obtained from the different sources; – the construction of the T-x-y diagram even in the absence some data, i.e., by prediction of the diagram elements (it is impossible in the thermodynamic models).

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