

# Crystallization paths in $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO}$ system as a genotype of silicate materials

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## Abstract

The phases trajectories in the fields of primary crystallization of cristobalite ( $\text{SiO}_2^{\text{cr}}$ ), tridymite ( $\text{SiO}_2^{\text{tr}}$ ), mullite ( $3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$ ) and in a field of liquid immiscibility are analyzed on a basis of computer model for T-x-y diagram of  $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO}$  system. The concentration fields with unique set of microconstituents and the fields without individual crystallization schemes and microconstituents are revealed.

Keywords: phase diagram, crystallisation path,  $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO}$  system, computer model

## 1. Introduction

A phase diagram of system  $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO}$  (S-A-C) has wide applications and can be used in the cement industry to describe the properties of Portland and aluminous cements [1-3], and in studies of refractories and alkali-free glass [4]. To extend the capabilities of research and examine the processes of crystallization for S-A-C system allows its computer model [5-6]. Analysis of concentration fields obtained by the projection of phase regions onto Gibbs triangle allows to establish the boundaries of phase regions (located above the considered fields), the sequence of phase transformations and microstructural elements in crystallized initial melt at the equilibrium condition. Based on this technology, the research identifies fields with coinciding sets of crystallization scheme and microconstituents and the fields with individual characteristics.

## 2. T-x-y diagram model for $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO}$ (S-A-C) system

The experimental data about the structure of S-A-C presented in the literature is usually confined to the surface of the primary crystallization (figure 1a) and triangles of coexistent phases [1-2, 7-9]. The spatial scheme of mono and invariant equilibria permits to restore the full construction of phase diagram. In the first stage a position of invariant planes are reproduced (figure 1b). Then the ruled surfaces of three-phase region borders are formed.

Let's consider the fragment of scheme adjoining to the component  $\text{SiO}_2$  (figure 1c). The plane of four-phase regrouping of phases  $\text{L}_U + \text{SiO}_2^{\text{cr}} \rightleftharpoons \text{R}_5 + \text{SiO}_2^{\text{tr}}$  has a degenerated structure  $\text{U-R}_5\text{-S}_1\text{-S}_2$  ( $\text{S}_1 = \text{SiO}_2^{\text{cr}}$  and  $\text{S}_2 = \text{SiO}_2^{\text{tr}}$ ,  $\text{cr}$  – cristobalite,  $\text{tr}$  – tridymite), because the points  $\text{S}_1\text{U}$  and  $\text{S}_2\text{U}$  coincide together. Two ruled surfaces  $\text{S}_1\text{E}_4\text{-E}_4\text{-U-S}_1\text{U}$  and  $\text{R}_5\text{E}_4\text{-E}_4\text{-U-R}_5\text{U}$  bounding the phase region  $\text{L+S}_1+\text{R}_5$  fit to the plane. The plane of ternary eutectic point  $\text{E}_4$ :  $\text{L}^{\text{E}_4} \rightarrow \text{S}_2^{\text{E}_4} + \text{R}_5^{\text{E}_4} + \text{R}_12^{\text{E}_4}$  ( $\text{S}_2^{\text{E}_4} = \text{R}_5^{\text{E}_4} = \text{R}_12^{\text{E}_4}$ ) is arranged below. Three pairs of ruled surfaces ( $\text{S}_2\text{U-U-E}_5\text{-S}_2^{\text{E}_5}$ ,  $\text{R}_5\text{U-U-E}_5\text{-R}_5^{\text{E}_5}$ ;  $\text{S}_2\text{E}_4\text{-E}_4\text{-[E}_4\text{,E}_5\text{]-S}_2^{\text{E}_4\text{E}_5}$ ,  $\text{R}_12\text{E}_4\text{-E}_4\text{-[E}_4\text{,E}_5\text{]-R}_12^{\text{E}_4\text{E}_5}$ ) are bounded

the phase regions  $\text{L+S}_2+\text{R}_5$ ,  $\text{L+S}_2+\text{R}_12$ ,  $\text{L+R}_5+\text{R}_12$ . The ruled surfaces  $\text{S}_2\text{E}_4\text{-E}_4\text{-[E}_4\text{,E}_5\text{]-S}_2^{\text{E}_4\text{E}_5}$ ,  $\text{R}_12\text{E}_4\text{-E}_4\text{-[E}_4\text{,E}_5\text{]-R}_12^{\text{E}_4\text{E}_5}$  are formed from the maximum point  $[\text{E}_4\text{,E}_5]$  on monovariant curve  $\text{E}_4\text{E}_5$ . Three-phase region  $\text{S}_2+\text{R}_5+\text{R}_12$  situates below the simplex  $\text{S}_2^{\text{E}_5}\text{-R}_5^{\text{E}_5}\text{-R}_12^{\text{E}_5}$ .

Step-by-step restoring of phase regions boundaries permits to obtain the complete model of phase diagram (figure 1d).

The projection of phase regions of system S-A-C divides the Gibbs triangle onto 117 two-dimensional, 163 one-dimensional and 45 zero-dimensional concentration fields. It is previously found that the projection of primary crystallization fields  $\text{CaO}$ ,  $\text{C}_3\text{S}$  and  $\text{C}_3\text{A}$  are divided onto 52 concentration fields (19 two-, 21 one- and 12 zero-dimensional), among which 18 fields (12 one- and 6 zero-dimensional) haven't unique set of microconstituents [10].

Let's consider the fragment of phase diagram adjoining to component  $\text{SiO}_2$  and carry out the analysis of concentration fields under the surfaces of primary crystallization cristobalite ( $\text{SiO}_2^{\text{cr}}$ ), tridymite ( $\text{SiO}_2^{\text{tr}}$ ), mullite ( $\text{A}_3\text{S}_2$ ) and a cupola of melt immiscibility (i).

## 3. Structure of phase diagram adjacent to component $\text{SiO}_2$

There are 18 ruled surfaces, 4 horizontal planes at the temperatures of invariant points ( $\text{E}_4$ ,  $\text{E}_5$ ,  $\text{Q}_8$ ,  $\text{U}$ ), 4 vertical triangulation planes under the fields of primary crystallization  $\text{SiO}_2^{\text{cr}}$  (surface  $\text{Q}_{\text{S}_1}$  with the contour  $\text{mkn}_3\text{Ue}_4\text{S}$ ),  $\text{SiO}_2^{\text{tr}}$  ( $\text{Q}_{\text{S}_2} = \text{e}_3\text{E}_4[\text{E}_4\text{,E}_5]\text{E}_5\text{Up}_3$ ),  $\text{A}_3\text{S}_2$  ( $\text{Q}_{\text{A}_3\text{S}_2} = \text{e}_4\text{UE}_5\text{Q}_8\text{e}_5\text{R}_5$ ) and the surface of immiscibility melt ( $i = \text{k}^0\text{nk}_m$ ) (figure 2, table 1). The following designations are used: e and p – binary eutectic and peritectic points, m and n – binary points of monotectic segment, E and Q – ternary eutectic and quasiperitectic points, U – point of the four-phase regrouping with participation of two polymorphous modifications  $\text{SiO}_2^{\text{cr}}$  and  $\text{SiO}_2^{\text{tr}}$ ,  $[\text{E}_4\text{,E}_5]$  – maximum point on the monovariant curve  $\text{E}_4\text{E}_5$ .

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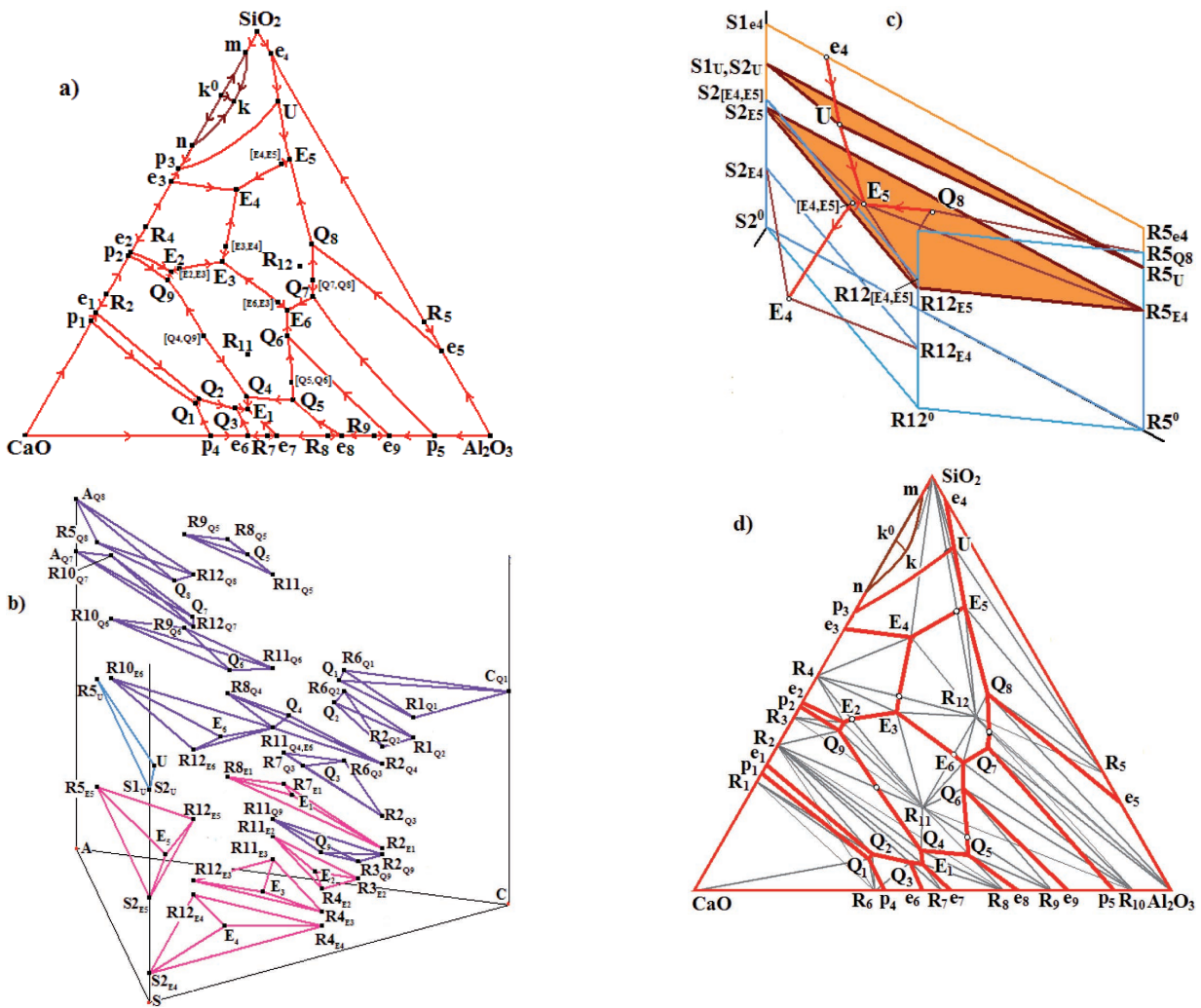


Fig. 1. XY projection of primary crystallization surfaces (a); 3D scheme of invariant planes arrangement (b) and three-phase regions of diagram fragment adjoining to the component S (c); XY projection of all phase regions (d) ( $R_1=C_3S$ ,  $R_2=C_2S$ ,  $R_3=C_3S_2$ ,  $R_4=CS$ ,  $R_5=A_3S_2$ ,  $R_6=C_2A$ ,  $R_7=C_{12}A_7$ ,  $R_8=CA$ ,  $R_9=CA_2$ ,  $R_{10}=CA_6$ ,  $R_{11}=C_2AS$ ,  $R_{12}=CAS_2$ )

1. ábra Elsődleges kristályosodási felületek XY vetülete (a); invariáns síkok elhelyezkedésének 3D sémája (b); háromfázisú diagramszakaszok az S-fázishoz tartozóan (c); az összes fázisrész XY vetülete (d) ( $R_1=C_3S$ ,  $R_2=C_2S$ ,  $R_3=C_3S_2$ ,  $R_4=CS$ ,  $R_5=A_3S_2$ ,  $R_6=C_2A$ ,  $R_7=C_{12}A_7$ ,  $R_8=CA$ ,  $R_9=CA_2$ ,  $R_{10}=CA_6$ ,  $R_{11}=C_2AS$ ,  $R_{12}=CAS_2$ )

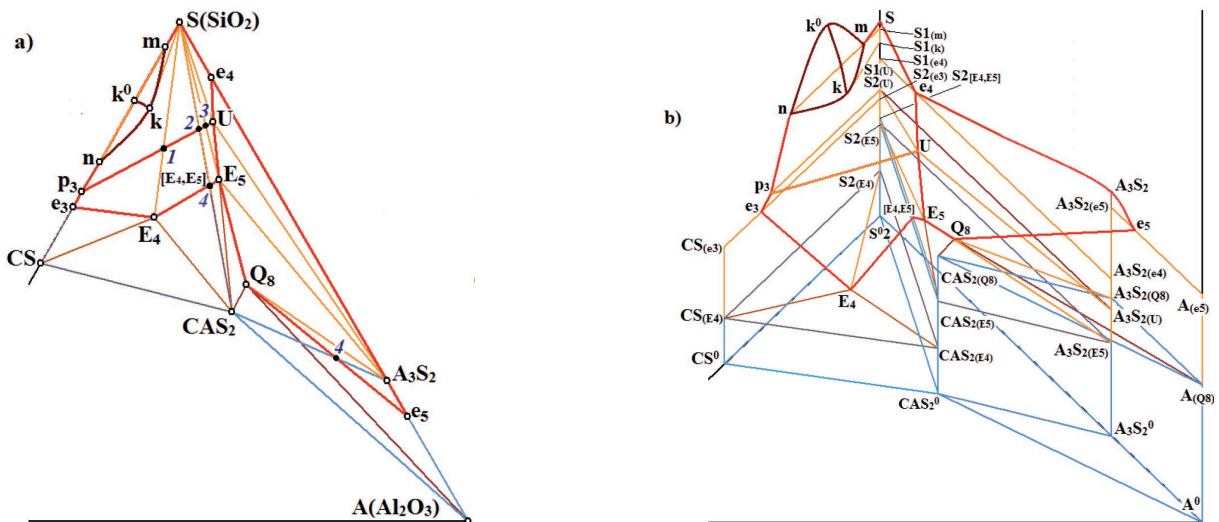


Fig. 2. XY projection (a) and 3D model (b) of fragment of system S-A-C phase diagram

2. ábra Az S-A-C fázisdiagram egy töredékének XY vetülete (a) és 3D modellje (b)

16 phase regions are located under the considered fields of primary crystallization:  $L_1+L_2$ ,  $L+S1$ ,  $L+S2$ ,  $L+A_3S_2$ ,  $S+CAS_2$ ,  $A+CAS_2$ ,  $CS+CAS_2$ ,  $A_3S_2+CAS_2$ ,  $L_1+L_2+S1$ ,  $L+S1+S2$ ,  $L+S2+CS$ ,  $L+S2+CAS_2$ ,  $L+A_3S_2+CAS_2$ ,  $S_2+CS+CAS_2$ ,  $A+A_3S_2+CAS_2$ ,  $S+A_3S_2+CAS_2$  (table 2). The phase region  $L+S1+S2$  is degenerated into line and the corresponding phase reaction proceeds at one temperature.

Symbol	Contour	Symbol	Contour
$Q_{e4\_A3S2}^r$	$A_3S_{2(e4)}-e_4-U-A_3S_{2(U)}$	$Q_{E4E5\_R12}^r$	$CAS_{2(E4)}-E_4-[E_4^+,E_5^-]-CAS_{2(E4,E5)}$
$Q_{E5U\_A3S2}^r$	$A_3S_{2(U)}-U-E_5-A_3S_{2(E5)}$	$Q_{E5E4\_R12}^r$	$CAS_{2(E5)}-E_5-[E_4^+,E_5^-]-CAS_{2(E4,E5)}$
$Q_{Q8E5\_A3S2}^r$	$A_3S_{2(Q8)}-Q_8-E_5-A_3S_{2(E5)}$	$i^r$	m-k-n
$Q_{e5\_A3S2}^r$	$A_3S_{2(e5)}-e_5-Q_8-A_3S_{2(Q8)}$	$i_m^r$	$S1_{(mn)}$ -m-k-S1 <sub>(k)</sub>
$Q_{e4\_S}^r$	$S1_{(e4)}-e_4-U-S1_{(U)}$	$i_n^r$	$S1_{(mn)}$ -n-k-S1 <sub>(k)</sub>
$Q_{E5U\_S}^r$	$S2_{(U)}-U-E_5-S2_{(E5)}$	$H_{E4}$	$S2_{(E4)}$ - $CS_{E4}$ - $CAS_{2(E4)}$
$Q_{e5\_A}^r$	$A_{(e5)}-e_5-Q_8-A_{(Q8)}$	$H_{E5}$	$S2_{E5}$ - $A_3S_{2(E5)}$ - $CAS_{2(E5)}$
$Q_{Q8E5\_CAS2}^r$	$CAS_{2(Q8)}-Q_8-E_5-CAS_{2(E5)}$	$H_{Q8}$	$Q_8-A_3S_{2(Q8)}$ - $A-CAS_{2(Q8)}$
$Q_{e3\_S}^r$	$S2_{(e3)}-e_3-E_4-S2_{(E4)}$	$H_U$	$U-A_3S_{2(U)}$ - $S1_{(U)}$ - $S2_{(U)}$
$Q_{p3\_S}^r$	$S1_{(U)}-p_3-U$	$V_{S-CAS2}$	$S2_{[E4,E5]}$ - $CAS_{2[E4,E5]}$ - $CAS_2^0S_2^0$
$Q_{E4E5\_S}^r$	$S2_{(E4)}-E_4-[E_4^+,E_5^-]-S2_{[E4,E5]}$	$V_{A-CAS2}$	$A_{Q8}$ - $CAS_{2(Q8)}$ - $CAS_2^0A_3S_2^0$
$Q_{E5E4\_S}^r$	$S2_{(E5)}-E_5-[E_4^+,E_5^-]-S2_{[E4,E5]}$	$V_{R5-CAS2}$	$A_3S_{2(Q8)}$ - $CAS_{2(Q8)}$ - $CAS_2^0A_3S_2^0$
$Q_{e3\_CS}^r$	$E_3-E_4-CS_{E4}-CS_{e3}$	$V_{R4-CAS2}$	$CS_{(E4)}$ - $CAS_{2(E4)}$ - $CAS_2^0CS^0$

Table 1. Contours of ruled surfaces ( $Q_r$ ,  $i_r$ ), horizontal ( $H$ ) and vertical ( $V$ ) planes  
1. táblázat Az irányított felületek ( $Q_r$ ,  $i_r$ ) kontúrjai, vízszintes ( $H$ ) és függőleges ( $V$ ) síkok

### 4. Analysis of the concentration fields

At projection the surfaces  $Q_{S1}$ ,  $Q_{S2}$ ,  $Q_{A3S2}$  and  $i$  are divided onto 15 two-, 28 one- and 9 zero-dimensional concentration fields. Thirteen (2 two-, 8 one- and 3 zero-dimensional) fields coincide with neighbouring fields by the set of microconstituents.

The microconstituents of concentration fields corresponding to the regions of immiscibility melt (m-n-k,  $SiO_2$ -m-k,  $SiO_2$ -k, n-k, m-k, k) coincide with the of field  $p_3$ -1- $SiO_2$ -k-n. Meanwhile the fields m-n-k,  $SiO_2$ -m-k and m-k differ from field  $p_3$ -1- $SiO_2$ -k-n by intersected surfaces, phase regions and crystallization scheme (table 3). The phase region  $L+S_1$  and phase region of immiscibility melt  $L+S_1+S_2$  are located under the field  $SiO_2$ -m-k. At the phase region  $L+S_1$  is twice crossed for this field. So the field is characterized by two primary

crystallization reactions  $L^1 \rightarrow S_1^1$  between which the monotectic reaction  $L_1^m \rightarrow L_2^m + S_1^m$  takes place. Field m-n-k arranges under the surface of immiscibility melt (i) and intersects the phase regions  $L_1+L_2$  и  $L_1+L_2+S_1$ , where the phase reaction  $L_1^1 \rightarrow L_2^1$  и  $L_1^m \rightarrow L_2^m + S_1^m$  occur.

Since the process of melt immiscibility ends in the phase region  $L_1+L_2+B_1$ , then the reaction products  $L_2^1$  and  $L_2^m$  doesn't influence on the microconstituents forming. The crystals  $B_1$  are not present in the microconstituents, because they are fully disappeared in the reactions  $L^p, B_1 \rightarrow B_2^p$  and  $L^u, S_1 \rightarrow S_2^u + A_3S_2^u$  and in the subsequent phase transformations there are only  $B_2$  crystals. The reactions  $L^p, S_1 \rightarrow S_2^p$  and  $L^u, S_1 \rightarrow S_2^u + A_3S_2^u$  have degenerated form as the result of degeneration of phase regions  $L+S_1+S_2$  in horizontal line and four-phase plane in the triangle  $U-A_3S_{2(U)}-S1_{(U)}-S2_{2(U)}$  [11].

The fields  $SiO_2$ -k, n-k and k coincide with field  $p_3$ -1- $SiO_2$ -k-n by the list of phase reactions and the microconstituents.

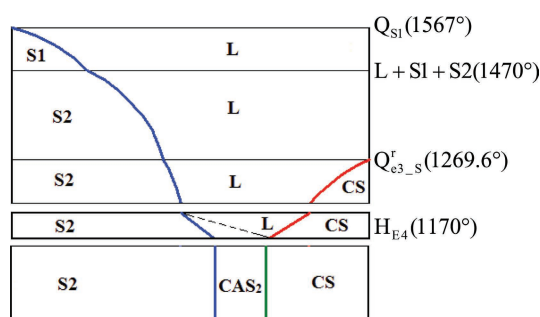


Fig. 3. Diagram of material balance for the concentration field  $p_3$ -1- $SiO_2$ -k-n  
3. ábra  $p_3$ -1- $SiO_2$ -k-n koncentráció mező anyag egyensúlyi diagramja

Let's consider the diagram of mass balances for composition given in the field  $p_3$ -1- $SiO_2$ -k-n (figure 3). After the reaction of primary crystallization  $L^1 \rightarrow S_1^1$  in the phase region  $L+S1$  the composition falls into phase region  $L+S_1+S_2$  (degenerated into line) where the crystals  $S_1$  is fully disappeared as the result of reactions  $L^p, S_1 \rightarrow S_2^p$  and  $L^u, S_1 \rightarrow S_2^u + A_3S_2^u$ . Then the composition moves into the phase region  $L+S_2$  where the post-peritectical primary crystallization  $L^{1p} \rightarrow S_2^{1p}$  takes place with the increasing of phase part  $S_2$ . In the phase region  $L+S_2+CS$  the part of phase L is decreased and parts of phases  $S_2$  and CS are increased: ( $L^{ep} \rightarrow S_2^{ep(CS)} + CS^{ep(B2)}$ ). The phase L is fully disappeared as the result of reaction  $L^{E4} \rightarrow S_2^{E4} + CS^{E4} + CAS_2^{E4}$

Symbol	Bounding surfaces	Symbol	Bounding surfaces
$L_1+L_2$	$i, i^r$	$L+A_3S_2+CAS_2$	$Q_{Q8E5\_A3S2}^r, Q_{Q8E5\_CAS2}^r, H_{Q8}, H_{E5}, V_{A3S2-CAS2}$
$L+S1$	$Q_{S1}^r, i^r, Q_{e4\_S}^r, Q_{p3\_S}^r$	$S2+CS+CAS_2$	$V_{S-CAS2}, V_{CS-CAS2}, H_{E4}$
$L+S2$	$Q_{S2}^r, Q_{e3\_S}^r, Q_{p3\_S}^r, Q_{E5U\_S}^r, Q_{E4E5\_S}^r, Q_{E5E4\_S}^r$	$A_3S_2+CAS_2+A$	$H_{Q8}, V_{A-CAS2}, V_{A3S2-CAS2}$
$L+A_3S_2$	$Q_{A3S2}^r, Q_{e4\_A3S2}^r, Q_{E5U\_A3S2}^r, Q_{Q8E5\_A3S2}^r, Q_{e5\_A3S2}^r$	$S2+A_3S_2+CAS_2$	$V_{A3S2-CAS2}, V_{S-CAS2}, H_{E5}$
$L_1+L_2+S1$	$i^r, i_n^r, i_m^r$	$S2+CAS_2$	$V_{S-CAS2}$
$L+S1+S2$	$Q_{p3\_S}^r$	$A+CAS_2$	$V_{A-CAS2}$
$L+S2+CS$	$Q_{e3\_CS}^r, Q_{e3\_S}^r, H_{E4}$	$A_3S_2+CAS_2$	$V_{A3S2-CAS2}$
$L+S2+CAS_2$	$Q_{E4E5\_S}^r, Q_{E5E4\_S}^r, Q_{E5E4\_CAS2}^r, Q_{E4E5\_CAS2}^r, H_{E4}, H_{E5}, V_{S-CAS2}$	$CS+CAS_2$	$V_{CS-CAS2}$

Table 2. Phase regions structure  
2. táblázat Fázis területek szerkezete

Concentration fields	Intersected surfaces	Intersected phase regions	Crystallization scheme	Microconstituents
<b>p<sub>3</sub>-1-SiO<sub>2</sub>-k-n</b>	Q <sub>S1'</sub> Q <sup>r</sup> <sub>p3-S'</sub> Q <sup>r</sup> <sub>e3-S'</sub> H <sub>E4</sub>	L+S <sub>1'</sub> L+S <sub>1</sub> +S <sub>2'</sub> L+S <sub>2'</sub> L+S <sub>2</sub> +CS, B <sub>2</sub> +CS+CAS <sub>2</sub>	L <sup>1</sup> →S <sub>1</sub> <sup>1</sup> , L <sup>p</sup> +S <sub>1</sub> <sup>1</sup> →S <sub>2</sub> <sup>p</sup> , L <sup>1p</sup> →S <sub>2</sub> <sup>1p</sup> , L <sup>ep</sup> →S <sub>2</sub> <sup>ep(CS)</sup> +CS <sup>ep(B2)</sup> L <sup>E4</sup> →S <sub>2</sub> <sup>E4</sup> +CS <sub>4</sub> <sup>E4</sup> +CAS <sub>2</sub> <sup>E4</sup>	S <sub>2</sub> <sup>p</sup> , S <sub>2</sub> <sup>1p</sup> , S <sub>2</sub> <sup>ep(CS)</sup> , CS <sup>ep(B2)</sup> S <sub>2</sub> <sup>E4</sup> , CS <sup>E4</sup> , CAS <sub>2</sub> <sup>E4</sup>
<b>SiO<sub>2</sub>-m-k</b>	Q <sub>S1'</sub> i <sup>r</sup> <sub>m'</sub> i <sup>r</sup> <sub>n'</sub> Q <sup>r</sup> <sub>p3-S'</sub> Q <sup>r</sup> <sub>e3-S'</sub> H <sub>E4</sub>	L+S <sub>1'</sub> L <sub>1</sub> +L <sub>2</sub> +S <sub>1'</sub> L+S <sub>1'</sub> L+S <sub>1</sub> +S <sub>2'</sub> L+S <sub>2'</sub> L+S <sub>2</sub> +CS, S <sub>2</sub> +R <sub>4</sub> +CAS <sub>2</sub>	L <sup>1</sup> →S <sub>1</sub> <sup>1</sup> , L <sub>1</sub> <sup>m</sup> →L <sub>2</sub> <sup>m</sup> +S <sub>1</sub> <sup>m</sup> , L <sup>1</sup> →S <sub>1</sub> <sup>1</sup> , L <sup>p</sup> +S <sub>1</sub> <sup>1,1p</sup> →S <sub>2</sub> <sup>p</sup> , L <sup>1p</sup> →S <sub>2</sub> <sup>1p</sup> , L <sup>ep</sup> →S <sub>2</sub> <sup>ep(CS)</sup> +CS <sup>ep(B2)</sup> L <sup>E4</sup> →S <sub>2</sub> <sup>E4</sup> +CS <sup>E4</sup> +CAS <sub>2</sub> <sup>E4</sup>	S <sub>2</sub> <sup>p</sup> , S <sub>2</sub> <sup>1p</sup> , S <sub>2</sub> <sup>ep(CS)</sup> , CS <sup>ep(B2)</sup> S <sub>2</sub> <sup>E4</sup> , CS <sup>E4</sup> , CAS <sub>2</sub> <sup>E4</sup>
<b>m-n-k</b>	i, i <sup>r</sup> , i <sup>r</sup> <sub>n'</sub> Q <sup>r</sup> <sub>p3-S'</sub> Q <sup>r</sup> <sub>e3-S'</sub> H <sub>E4</sub>	L <sub>1</sub> +L <sub>2'</sub> , L <sub>1</sub> +L <sub>2</sub> +S <sub>1'</sub> , L+S <sub>1'</sub> , L+S <sub>1</sub> +S <sub>2'</sub> , L+S <sub>2'</sub> , L+S <sub>2</sub> +CS, S <sub>2</sub> +CS+CAS <sub>2</sub>	L <sub>1</sub> <sup>1</sup> →L <sub>2</sub> <sup>1</sup> , L <sub>1</sub> <sup>m</sup> →L <sub>2</sub> <sup>m</sup> +S <sub>1</sub> <sup>m</sup> , L <sup>1</sup> →S <sub>1</sub> <sup>1</sup> , L <sup>p</sup> +S <sub>1</sub> <sup>1</sup> →S <sub>2</sub> <sup>p</sup> , L <sup>1p</sup> →S <sub>2</sub> <sup>1p</sup> , L <sup>ep</sup> →S <sub>2</sub> <sup>ep(CS)</sup> +CS <sup>ep(B2)</sup> L <sup>E4</sup> →S <sub>2</sub> <sup>E4</sup> +CS <sup>E4</sup> +CAS <sub>2</sub> <sup>E4</sup>	S <sub>2</sub> <sup>p</sup> , S <sub>2</sub> <sup>1p</sup> , S <sub>2</sub> <sup>ep(CS)</sup> , CS <sup>ep(B2)</sup> S <sub>2</sub> <sup>E4</sup> , CS <sup>E4</sup> , CAS <sub>2</sub> <sup>E4</sup>
<b>SiO<sub>2</sub>-k</b>	Q <sub>S1'</sub> Q <sup>r</sup> <sub>p3-S'</sub> Q <sup>r</sup> <sub>e3-S'</sub> H <sub>E4</sub>	L+S <sub>1'</sub> , L+S <sub>1</sub> +S <sub>2'</sub> , L+S <sub>2'</sub> , L+S <sub>2</sub> +CS, S <sub>2</sub> +R <sub>4</sub> +CAS <sub>2</sub>	L <sup>1</sup> →S <sub>1</sub> <sup>1</sup> , L <sup>p</sup> +S <sub>1</sub> <sup>1</sup> →S <sub>2</sub> <sup>p</sup> , L <sup>1p</sup> →S <sub>2</sub> <sup>1p</sup> , L <sup>ep</sup> →S <sub>2</sub> <sup>ep(CS)</sup> +CS <sup>ep(B2)</sup> L <sup>E4</sup> →S <sub>2</sub> <sup>E4</sup> +CS <sup>E4</sup> +CAS <sub>2</sub> <sup>E4</sup>	S <sub>2</sub> <sup>p</sup> , S <sub>2</sub> <sup>1p</sup> , S <sub>2</sub> <sup>ep(CS)</sup> , CS <sup>ep(B2)</sup> S <sub>2</sub> <sup>E4</sup> , CS <sup>E4</sup> , CAS <sub>2</sub> <sup>E4</sup>
<b>n-k</b>	Q <sub>S1'</sub> Q <sup>r</sup> <sub>p3-S'</sub> Q <sup>r</sup> <sub>e3-S'</sub> H <sub>E4</sub>	L+S <sub>1'</sub> , L+S <sub>1</sub> +S <sub>2'</sub> , L+S <sub>2'</sub> , L+S <sub>2</sub> +CS, B <sub>2</sub> +R <sub>4</sub> +CAS <sub>2</sub>	L <sup>1</sup> →S <sub>1</sub> <sup>1</sup> , L <sup>p</sup> +S <sub>1</sub> <sup>1</sup> →S <sub>2</sub> <sup>p</sup> , L <sup>1p</sup> →S <sub>2</sub> <sup>1p</sup> , L <sup>ep</sup> →S <sub>2</sub> <sup>ep(CS)</sup> +CS <sup>ep(B2)</sup> L <sup>E4</sup> →S <sub>2</sub> <sup>E4</sup> +CS <sup>E4</sup> +CAS <sub>2</sub> <sup>E4</sup>	S <sub>2</sub> <sup>p</sup> , S <sub>2</sub> <sup>1p</sup> , S <sub>2</sub> <sup>ep(CS)</sup> , CS <sup>ep(B2)</sup> S <sub>2</sub> <sup>E4</sup> , CS <sup>E4</sup> , CAS <sub>2</sub> <sup>E4</sup>
<b>m-k</b>	Q <sub>S1'</sub> i <sup>r</sup> <sub>m'</sub> i <sup>r</sup> <sub>n'</sub> Q <sup>r</sup> <sub>p3-B'</sub> Q <sup>r</sup> <sub>e3-B'</sub> H <sub>E4</sub>	L+S <sub>1'</sub> , L <sub>1</sub> +L <sub>2</sub> +S <sub>1'</sub> , L+S <sub>1'</sub> , L+S <sub>1</sub> +S <sub>2'</sub> , L+S <sub>2'</sub> , L+S <sub>2</sub> +CS, S <sub>2</sub> +R <sub>4</sub> +CAS <sub>2</sub>	L <sup>1</sup> →S <sub>1</sub> <sup>1</sup> , L <sub>1</sub> <sup>m</sup> →L <sub>2</sub> <sup>m</sup> +S <sub>1</sub> <sup>m</sup> , L <sub>1</sub> <sup>1</sup> →S <sub>1</sub> <sup>1</sup> , L <sup>p</sup> +S <sub>1</sub> <sup>1,1p</sup> →S <sub>2</sub> <sup>p</sup> , L <sup>1p</sup> →S <sub>2</sub> <sup>1p</sup> , L <sup>ep</sup> →S <sub>2</sub> <sup>ep(CS)</sup> +CS <sup>ep(B2)</sup> L <sup>E4</sup> →S <sub>2</sub> <sup>E4</sup> +CS <sup>E4</sup> +CAS <sub>2</sub> <sup>E4</sup>	S <sub>2</sub> <sup>p</sup> , S <sub>2</sub> <sup>1p</sup> , S <sub>2</sub> <sup>ep(CS)</sup> , CS <sup>ep(B2)</sup> S <sub>2</sub> <sup>E4</sup> , CS <sup>E4</sup> , CAS <sub>2</sub> <sup>E4</sup>

\* 1 – primary crystallization L<sup>1</sup>→I<sup>1</sup>; e – monovariant eutectic reaction L<sup>e</sup>→I<sup>e</sup>+J<sup>e</sup>; p – monovariant peritectic reaction L<sup>p</sup>+A<sup>p</sup>→R<sup>p</sup>; m – monovariant monotectic reaction L<sub>1</sub><sup>m</sup>→L<sub>2</sub><sup>m</sup>+R<sup>m</sup>; E – invariant eutectic crystallization L<sup>E</sup>→B<sup>E</sup>+C<sup>E</sup>+R<sup>E</sup>; Q – invariant quasiperitectic regrouping of masses L<sup>Q</sup>+A<sup>Q</sup>→B<sup>Q</sup>+R<sup>Q</sup>; 1<sup>p</sup> – post-peritectic primary crystallization L<sup>1p</sup>→R<sup>1p</sup>; ep – post-peritectic monovariant crystallization L<sup>ep</sup>→R<sup>ep</sup>+J<sup>ep</sup> (J=B, C)

Table 3. Crystallization scheme and microconstituents for surface of immiscibility *i* and the fragment of primary crystallization surface Q<sub>S1</sub> of high-temperature modification SiO<sub>2</sub> (S1)\*  
3. táblázat Kristályosodási séma és mikro-összetevők az *i* oldhatatlansági felülethez és a Q<sub>S1</sub> elsődleges kristályosodási felület töredéke a SiO<sub>2</sub> (S1)\* módosulására magas hőmérsékleten

on the plane at the temperature of ternary eutectic points E<sub>4</sub>. Below the plane the composition gets to the solid-phase region S<sub>2</sub>+CS+CAS<sub>2</sub>.

The concentration fields e<sub>4</sub>-U and U coincide with fields SiO<sub>2</sub>-U-e<sub>4</sub> и SiO<sub>2</sub>-U by the microconstituents, but differ the crystallization scheme. Fields e<sub>4</sub>-U and U haven't the reaction of primary crystallization L<sup>1</sup>→B<sub>1</sub><sup>1</sup>. The concentration fields p<sub>3</sub>-1 and 2 differ from fields e<sub>3</sub>-E<sub>4</sub>-1-p<sub>3</sub> and 2-4 by intersected surfaces. The fields E<sub>5</sub>-3, A<sub>3</sub>S<sub>2</sub>-U и A<sub>3</sub>S<sub>2</sub>-Q<sub>8</sub> are identical with E<sub>5</sub>-U-3, U-E<sub>5</sub>- A<sub>3</sub>S<sub>2</sub> and E<sub>5</sub>-Q<sub>8</sub>-A<sub>3</sub>S<sub>2</sub> by the microconstituents and crystallization scheme correspondently.

## 5. Conclusion

Computer model of PD gives the possibility to analyze the crystallization stages for any composition and to find the concentration fields both with individual set of microstructure elements and the fields at which the crystallization scheme and microconstituents of phases assemblage coincide with those in the adjoining fields. It is used as an important tool to investigate

multicomponent system, to correct its constitutional diagram, to design the microstructures of heterogeneous material, to decipher the genotype of heterogeneous material [12]. One more reason for the microstructures variety is the competition of crystals with different dispersity, when a field of invariant reaction is divided into the fragments with the tiny eutectical crystals, with more large primary crystals and with the both type of these crystals [13].

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**Kristályosodási folyamatok a SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub>-CaO anyagrendszerben, mint a szilikát anyagok genotípusában**

A SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub>-CaO anyagrendszerben a nem elegyedő folyadékfázisok mezőjéből kiindulva a krisztobalit (SiO<sub>2</sub> cr), a tridimit (SiO<sub>2</sub> tr) és a mullit (3Al<sub>2</sub>O<sub>3</sub> x 2SiO<sub>2</sub>) fázisátalakulása – kristályosodása – kerül a szerzők által bemutatásra a T-x-y koordináta rendszerben számítógépes modellezés segítségével. Az elvégzett számítógépes modellezés és elemzés eredményeként feltárulnak azok a hőmérséklettől és összetételtől függő unikális mikro-szerkezettel bíró terek és mezők, amelyekben a szilikát anyagok genotípusát alkotó anyagrendszerben az egyes komponensek kristályosodási folyamata nem önállóan megy végbe.

Kulcsszavak: fázisdiagram, kristályosodás, SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub>-CaO rendszer, számítógépes modellezés

**NIISK, the Ukrainian state agency “Research Institute of Building Constructions” celebrates its 70<sup>th</sup> anniversary in 2013**



The Institute was founded in 1943 by the Council of People’s Commissars of the USSR on October 26, 1943 and received the name “Ukrainian Research Institute facilities (UkrNDIS)” from the temporary location of the Institute in Moscow. The main purpose of the institute was the development and implementation of advanced building science and technology, conduct research on housing and civil engineering and technical assistance to construction companies. The main activity of the Institute was to address a number of issues in the construction industry, contributing to the implementation of the program of construction of recovery in short term construction projects destroyed during the 2<sup>nd</sup> World War and find the most efficient design, saving in building materials and replacement techniques. The UkrNDIS was transferred to Kyiv in March 1944.

During the years of its history NIISK solve complex scientific and technical issues concerning the construction of many buildings in Ukraine and other former Soviet republics. Numerous research and development institute were used in our country and abroad. Scientists and engineers have created a unique institute of technology and building construction in the Ukraine and other former Soviet republics and make several housing estates in difficult

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