PHASE COMPOSITION OF FOUR COMPONENT OXIDE SYSTEMS IN CHOSEN PLANE SECTIONS

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The procedure to compute Phase Field's Maps (PFM) representing interceptions of phase tetrahedra with chosen planes in four component oxide systems is described briefly and illustrated with examples. It can be exploited in phase equilibria studies, or in technologies in which polyphase products are analysed or received.

INTRODUCTION

Polycomponent oxide systems ($n \geq 4$) are usually known in their basic features. In most cases, only the identity of phases is known, together with their subsolidus compatibility, as shown in Fig. 1 [1].

Because of lack of sufficient equilibrium data the phases of polycomponent oxide systems are considered as being stochiometric at all temperatures, and the composition of phases is taken as corresponding to their formulae.

In spite of this serious simplification phase diagrams similar to the one shown in Fig. 1, when adequately excerpted, can be the source of additional useful information.

In our previous contribution, it was shown that the phase (compatibility) diagram can be converted into a corresponding phase compatibility matrix and consequently used for an algotirithmised computation of the phase composition of systems from their given chemical compositions [2].

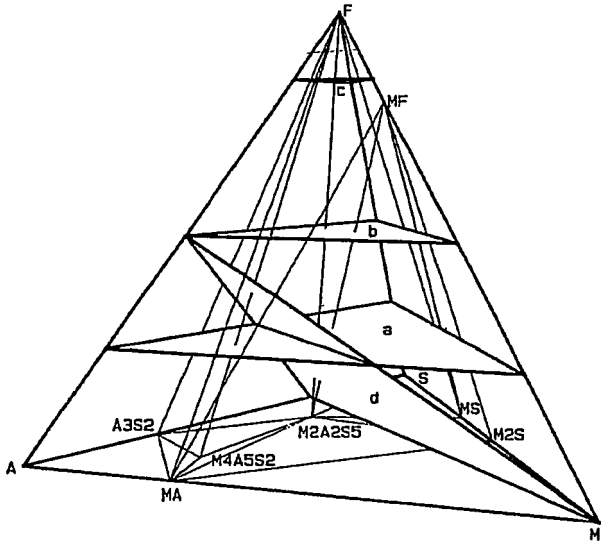

Fig. 1. The Phase Compatibility Diagram of the System M-S-A-F with Position of Section Planes.

In this contribution, the phase compatibility matrix (Table I) is a starting point again, this time to identify the specific phase regions (so called phase field's maps) in arbitrarily defined section planes.

The most general use of this procedure is seen in the prompt establishment of phase fields relevant to equilibriated mixtures of given three components or raw components respectively.

THE PRINCIPLE OF PFM COMPUTATION

The phase compatibility diagram in Fig. 1 shows also the position of four inserted planes for which phase field's maps were computed. The phase compatibility matrix of the system (PCM) is shown in Table I. The "zero" matrix elements geometrically (in correspondence to Fig. 1) represent individual conodes of the system.

So when the section plane of interest is defined in the system the "single step" in PFM computation is to determine the point of interception of the plane with the given conode. This is a standard problem of analytical geometry.

Let the plane and the conode be given by points $(x_i,\ y_i,\ z_i)$ with $i = 1, 2, 3$ and $i = 4, 5$ respectively. The procedure is then as follows:

1. The coefficients A, B, C, D in the equation of the plane are computed

$$A = (y_3 - y_1)(z_1 - z_2) - (y_1 - y_2)(z_3 - z_1)$$

$$B = (z_3 - z_1)(x_1 - x_2) - (z_1 - z_2)(x_3 - x_4)$$

$$C = (x_3 - x_1)(y_1 - y_2) - (x_1 - x_2)(y_3 - y_1)$$

$$D = -Ax_1 - By_1 - Cz_1$$

2. $R = A(x_5 - x_4) + B(y_5 - y_4) + C(z_5 - z_4)$

If $R = 0$ then the conode is parallel with the plane and no intercept exist

3. $t = -\dfrac{Ax_4 + By_4 + Cz_4 + D}{R}$

Table I

Phase Compatibility Matrix of the System M-S-A-F[+]

	M_2S	S	MA	A	A_3S_2	MF	F	$M_2A_2S_5$	$M_4A_5S_2$	MS
M	0	1	0	1	1	0	1	1	1	1
M_2S	-	1	0	1	1	0	1	0	1	0
S	-	-	1	1	0	1	0	0	1	0
MA	-	-	-	0	0	0	0	0	0	1
A	-	-	-	-	0	1	0	1	1	1
A_3S_2	-	-	-	-	-	1	0	0	0	1
MF	-	-	-	-	-	-	0	0	1	0
F	-	-	-	-	-	-	-	0	0	0
$M_2A_2S_5$	-	-	-	-	-	-	-	-	0	0
$M_4A_5S_2$	-	-	-	-	-	-	-	-	-	1

0 – compatible phases
1 – incompatible phases
[+]M=MgO, S=SiO_2, A=Al_2O_3, F=Fe_2O_3, M_2S=2MgO.SiO_2 (forsterite), etc.

Table II

Phase Assemblages of the System M-S-A-F

	Assemblages	V_i	$\sum V_i$
I	M – M_2S – MA – MF	0.2436	0.2436
II	M_2S – MA – MF – $M_2A_2S_5$	0.1678	0.4114
III	M_2S – MF – $M_2A_2S_5$ – MS	0.0476	0.4590
IV	S – A_3S_2 – F – $M_2A_2S_5$	0.0989	0.5579
V	S – F – $M_2A_2S_5$ – MS	0.1400	0.6979
VI	MA – A – A_3S_2 – F	0.0799	0.7778
VII	MA – A_3S_2 – F – $M_4A_5S_2$	0.0206	0.7984
VIII	MA – MF – F – $M_2A_2S_5$	0.0752	0.8736
IX	MA – F– $M_2A_2S_5$ – $M_4A_5S_2$	0.0187	0.8923
X	A_3S_2 – F – $M_2A_2S_5$ – $M_4A_5S_2$	0.0651	0.9574
XI	MF – F – $M_2A_2S_5$ – MS	0.0426	1.0000

V_i – the volume of corresponding tetrahedron

The coordinates of the intercept are:

$$x_0 = x_4 + t\,(x_5 - x_4)$$

$$y_0 = y_4 + t\,(y_5 - y_4)$$

$$z_0 = z_4 + t\,(z_5 - z_4)$$

The computation is finished when the "single step" procedure is repeated for all conodes given in PCM. The phase field map is established when the individual points of interception are joined into a set of triangles and tetragons. The joining of two points of interception is permisible when they both belong to the same face of an elementary tetrahedron.

The list of phase assemblages of the system M-S-A-F (of elementary tetrahedrons) generated from the given phase compatibility matrix is shown in Table II.

EXAMPLES OF PHASE FIELD'S MAPS

The phase field's map shown in Fig. 2 was established from computed results given in Table III. This table lists individual conodes (phase1–phase2), their identification numbers and x, y coordinates of their

Table III

Characteristics of points in the plane *a* (Fig. 2)

Ident. number	Point position		Phase composition (mass %)	
	x	*y*	phase *1*	phase *2*
1	0.0	0.0	70.0 A	30.0 F
2	14.1	24.4	70.0 A_3S_2	30.0 F
3	27.9	13.1	30.0 F	70.0 $M_4A_5S_2$
4	28.3	0.0	70.0 MA	30.0 F
5	36.2	0.0	62.3 MA	37.7 MF
6	39.4	44.5	30.0 F	70.0 $M_2A_2S_5$
7	46.1	39.6	37.7 MF	62.3 $M_2A_2S_5$
8	50.0	86.6	70.0 S	30.0 F
9	70.0	51.8	30.0 F	70.0 MS
10	73.4	46.1	37.7 MF	62.3 MS
11	81.0	32.9	62.3 M_2S	37.7 MF
12	100.0	0.0	62.3 M	37.7 MF

points of interceptions with the given plane a. The table also includes the quantitative phase composition of the system corresponding to points of interception. The identification numbers from Table III are used also to denote the corresponding points of interception in Fig. 2. Numbering of points of interception is similarly used also in next figures.

The individual phase fields in Figs. 2–5 (four phase regions) are denoted by Roman numerals in correspondence to the list of equilibrium phase assemblages given in Table II.

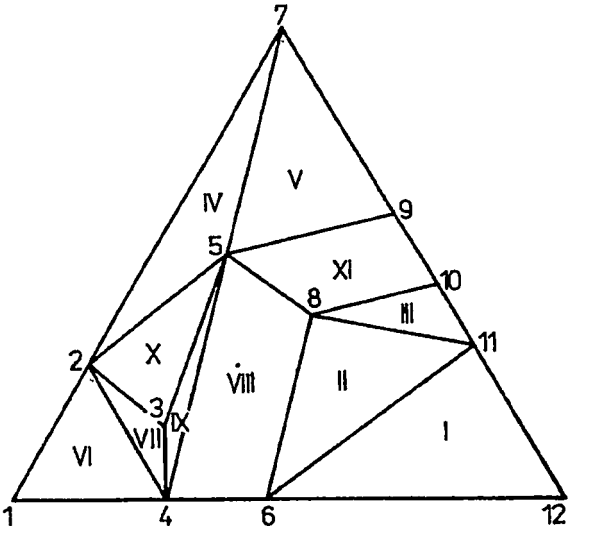

Fig. 3. The Phase Field's Map in the Section b of the System.

IMPLICATIONS

Sections planes in the four component oxide systems are most usually taken in such a way as to create the quasi-ternary subsystems. In such cases the endpoints of section planes (triangles) coinside with the figurative points of phases of the system.

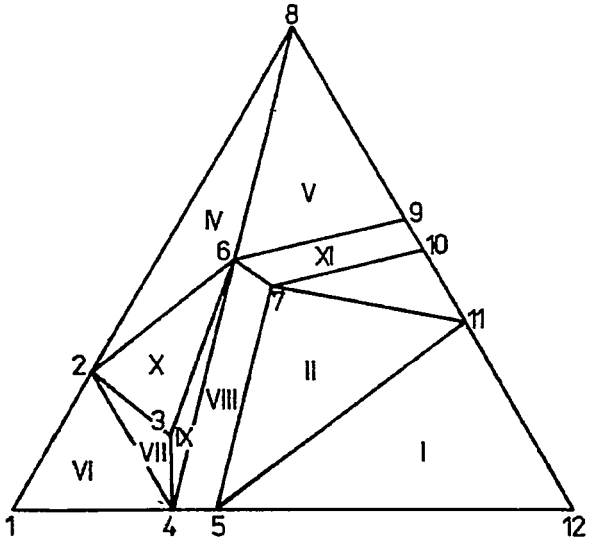

Fig. 2. The Phase Field's Map in the Section a of the System.

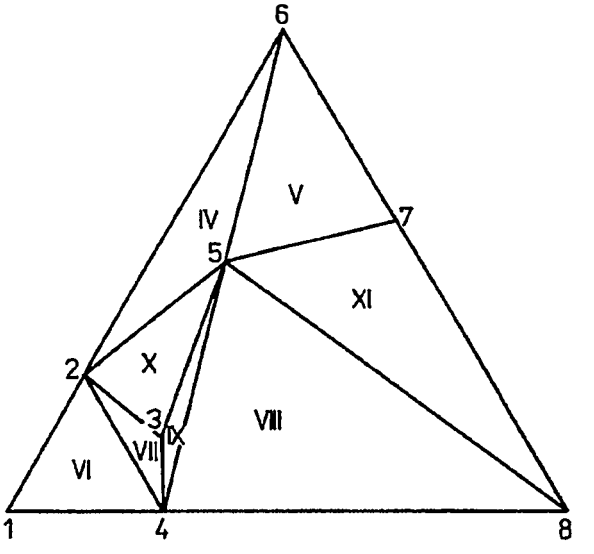

Fig. 4. The Phase Field's Map in the Section c of the System.

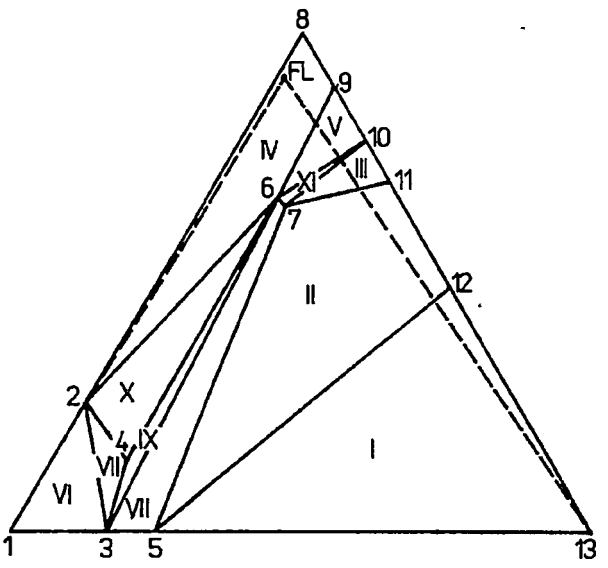

Fig. 5. The Phase Field's Map in the Section d of the System.

The positions of planes a, b, c were taken as parallel to the face A-M-S of the basic tetrahedron but arbitrarily in their altitude from this face.

In the case of plane d only one end point (apex) of the triangle was taken arbitrarily (the point at the conode A-F in Fig. 1.).

The second point is taken to represent "pure" MgO (MgO say as the potential raw mix component). The third endpoint is calculated with respect to the previous two apexes of the triangle and with respect to the chemical composition of a power plant fly ash taken into account (Fly ash *1* in [2]).

The third apex of the triangle is adjusted then to such a position as to keep the figurative point of the fly ash and of the too previously defined apexes in a common plane (d).

The phase field map in Fig. 5 is relevant then to phase composition of the three component "raw" mix system: "ferroaluminate component" – MgO – "alumosilicate component" which can, when necesary, be transformed to the "raw" mix system Fly ash – MgO – "ferroaluminate" component.

In such case, when the plane of a section is defined by three points, each of them representing the raw component, the PFM attained gives a survey of equilibrium phase compositions achievable within given raw components.

References

[1] Berezhnoy A.S.: *Multicomponent Oxide Systems* (in Russian), Izd. Naukova Dumka, Kiev 1970.

[2] Majling J., Jesenák V., Roy Della M., Roy R.: J. Mater. Res. *4*, [2] 447 (1989).

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FÁZOVÉ ZLOŽENIE ŠTVORZLOŽKOVÝCH SÚSTAV V ZVOLENÝCH ROVINNÝCH REZOCH

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Rovinné rezy v štvorzložkových sústavách sa obyčajne volia tak, aby zodpovedali zloženiu kváziternárnych systémov.

V tomto príspevku sa predkladá postup výpočtu, pomocou ktorého možno identifikovať fázové oblasti v obecných rezoch sústav. Východiskom výpočtu je matica koexistencie fáz sústavy a jeho základnou operáciou určenie priesečíka konódy (spojnice dvoch fáz sústavy s príslušnou rovinnou rezu.

V prípade, ak sa rovina rezu definuje pomocou „surovinových" zložiek, vypočítaná mapa fázových oblastí potom koreluje surovinové zloženie zmesí a mineralogické zloženie produktov keramickej technológie.

Obr. 1. Diagram koexistencie fáz sústavy M-S-A-F s polohami rovín rezu
Obr. 2. Mapa fázových oblastí v reze a.
Obr. 3. Mapa fázových oblastí v reze b.
Obr. 4. Mapa fázových oblastí v reze c.
Obr. 5. Mapa fázových oblastí v reze d.