Material Balances Design in the Al$_2$Yb-Al-Al$_4$Sr Subsystem

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Abstract. The vertical mass balances - for the given center of masses, and the horizontal ones - for the isothermal state of isopleth, have been analyzed. These results are used for the different purposes: microstructures characterization, solidification paths confirmation, phase regions 3D-prototyping for the exploded diagram. It is once more showed, that a computer assembled model of the T-x-y diagram is a useful tool to solve different fundamental and applied tasks of the materials science.

1. Introduction

Like the purpose of the work “Phase Diagrams: The Beginning of Wisdom” [1] is to present a primer on “How to Read and Apply Phase Diagrams” in the current environment of powerful software packages, this paper illustrates the new opportunities, that have been arrived with the spacious computer models of the T-x-y and more complex diagrams for the multicomponent systems invention.

“Phase diagrams are the perfect road map to understand the conditions for phase formation or transformation in any material system caused by variation of temperature, composition, pressure or any other viable state variable. That is why one can use phase diagrams as the starting point for materials design and process optimization by manipulating composition and processing variables to achieve the desired microstructures. That applies to all sorts of materials, such as alloys, ceramics, semiconductors, cement, concrete etc., and to a multitude of processes, such as melting, casting, crystal growth, joining, solid-state reaction, heat treatment/phase transformation, oxidation, vapor deposition, and so on” [1]. Computer model of T-x-y diagram adds many new applications, thanks to the two kinds of material balances: the vertical ones - for the given center of masses, and the horizontal ones - for the isothermal states on the isopleth.

On the road to assemble a T-x-y diagram there are some obstacles. One of them is the initial description of the phase diagram. Let’s discuss it in the next section of this paper.

2. Graphics correction within T-x-y diagrams with melt immiscibility.

In some cases the errors in the phase diagrams description prohibit a right understanding of their graphics. First example (Fig. 1, a-b) corresponds to the series of phase diagrams with the melt immiscibility in [2, p. 119-222]. One-type error is present in the description of some T-x-y diagrams: for the surface of solvus with 5 dots on its contour $a_0a_0^0a_0^0a_0^0E$ (Fig. 1, a) a line $a_0^0a_0^0$ is lost (Fig. 1, b). As a result, a contour projection of this surface isn’t closed. At the same time, the solvus surfaces are supposed to be of cylindrical type with the orthogonal position of their originating segment and project into a curve. Such description adds the difficulties in understanding of the diagrams structure. Surely a computer model of phase diagram permits to image all possible variants of degeneration for the surfaces.

In [3, p. 368], while imaging a T-x-y diagram (Fig. 1, c) with a complex structure of the immiscibility dome (nQkMm), a tie-line $k_0$ has been lost, that conjugates a critical dot of immiscibility $k$ and the end dot $a_0$ of the fold $a_0$ on the solidus surface $a_0A^0C^0a_0$. This misleading
was overcome only when the right picture has been found in the original monograph [3] in English (Rhines F. N. Phase Diagrams in Metallurgy. Their Development and Application. N.Y.-Toronto-London. 1956).

More often are the situations with the concentration coordinates correction for the subsystems of the more large system, like in this paper.

![Figure 1. Fragment of diagram with a solvus surface $v_{AB}$, projecting into a line [2] (a, b); projection of diagram with a dome of liquid immiscibility crossing a eutectic curve $e_{AB}e_{BC}$ [3] (c).](image)

3. 3D computer models of T-x-y diagrams for subsystem $\text{Al}_2\text{Yb}-\text{Al}-\text{Al}_4\text{Sr}$

The sub system $\text{Al}_2\text{Yb}-\text{Al}-\text{Al}_4\text{Sr}$ was obtained by the dividing of ternary system Yb-Al-Sr with the quasi-binary section $\text{Al}_2\text{Yb}-\text{Al}_4\text{Sr}$.

As the initial data for simulation of model, we used information about the structure of binary systems concerning the coordinates of binary points and the resulting compounds. Systems Al-Sr and Al-Yb are presented in the reference book [4].

In this case, the subsystem Al-Al$_4$Sr contains one binary eutectic, the subsystem Al-$\text{Al}_2$Yb includes the eutectic, the peritectic and the incongruently melting compound Al$_3$Yb. The work [5] presents data on the quasi-binary section $\text{Al}_2\text{Yb}-\text{Al}_4\text{Sr}$ (this subsystem is a simple eutectic), and also shows the liquidus of the subsystem $\text{Al}_2\text{Yb}-\text{Al}_4\text{Sr}$, and two invariant points are defined: eutectic (L$_E$→Al+SrAl$_2$+$\text{YbAl}_3$) and quasiperitectic (L$_Q$+$\text{YbAl}_2$→SrAl$_4$+$\text{YbAl}_3$) [5].

For the correct simulation of model, it is necessary to transform the coordinates of binary points from the systems Al-Sr and Al-Yb to the subsystems Al-Al$_4$Sr and Al-$\text{Al}_2$Yb using the matrix transformations: $Z=M\cdot x$, where $Z$ – vector column of point coordinates in the global system, $M$ - matrix of coordinates of subsystem points in the global system, $x$ - vector column of point coordinates in the subsystem [6-7].

So the eutectic point in the system Al-Sr near Al ($e_{BC}$) has coordinates (0.99; 0.01), and the compound Al$_4$Sr owns (0.8; 0.2). To convert its coordinates from the system Al-Sr to the subsystem Al-Al$_4$Sr, a matrix transformation is compiled:

$$e_{BC} : \begin{pmatrix} 0.99 \\ 0.01 \end{pmatrix} = \begin{pmatrix} 1 & 0.8 \\ 0 & 0.2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 & 0.8 \\ 0 & 0.2 \end{pmatrix}^{-1} \begin{pmatrix} 0.99 \\ 0.01 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0.95 \\ 0.05 \end{pmatrix}.$$  

Thus, the coordinates of binary eutectic $e_{BC}$ in the subsystem Al-Al$_4$Sr is $\begin{pmatrix} 0.95 \\ 0.05 \end{pmatrix}$.

Similarly, the coordinates of eutectic ($e_{BR}$), peritectic ($p_{AR}$) and compound $\text{R}=$Al$_3$Yb are converted from the system Al-Yb to the subsystem Al-$\text{Al}_2$Yb:

$$e_{BR} : \begin{pmatrix} 0.96 \\ 0.04 \end{pmatrix} = \begin{pmatrix} 1 & 0.67 \\ 0 & 0.33 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 & 0.67 \\ 0 & 0.33 \end{pmatrix}^{-1} \begin{pmatrix} 0.96 \\ 0.04 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0.879 \\ 0.121 \end{pmatrix}.$$  

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\[
\begin{align*}
\mathbf{p}_{AR} & : (0.87, 0.13) = (1.067, 0.33) \ \mathbf{x}_1 \rightarrow (x_1, x_2) = \begin{pmatrix} 1.067 \\ 0.33 \end{pmatrix}^{-1} \begin{pmatrix} 0.87 \\ 0.13 \end{pmatrix} \rightarrow (x_1, x_2) = (0.61, 0.39). \\
R & : (0.75, 0.25) = (1.067, 0.33) \ \mathbf{x}_1 \rightarrow (x_1, x_2) = \begin{pmatrix} 1.067 \\ 0.33 \end{pmatrix}^{-1} \begin{pmatrix} 0.75 \\ 0.25 \end{pmatrix} \rightarrow (x_1, x_2) = (0.24, 0.76).
\end{align*}
\]

It should be noted that in work [5], preliminary transformation of the binary points coordinates was not done at the studying of ternary subsystem \(\text{Al}_2\text{Yb}-\text{Al}-\text{Al}_3\text{Sr}\). And the obtained ternary subsystem \(\text{Al}_2\text{Yb}-\text{Al}-\text{Al}_3\text{Sr}\) uses the coordinates of the Al-Sr and Al-Yb systems on the one side and the quasibinary system \(\text{Al}_2\text{Yb}-\text{Al}_3\text{Sr}\) on the other. In this regard, for the correct model construction, the coordinates of ternary points were recalculated through the compositions of the local simplex \(\text{Al}_2\text{Yb}-\text{Al}-\text{Al}_3\text{Sr}\):

\[
\begin{align*}
\mathbf{Q} & : (0.043, 0.84) = (0.33, 0, 0) \ \mathbf{x}_1 \rightarrow (x_1, x_2) = \begin{pmatrix} 0.33 \\ 0.84 \end{pmatrix} \rightarrow (x_1, x_2) = (0.13, 0.285), \\
\mathbf{E} & : (0.032, 0.95) = (0.33, 0, 0) \ \mathbf{x}_1 \rightarrow (x_1, x_2) = \begin{pmatrix} 0.33 \\ 0.95 \end{pmatrix} \rightarrow (x_1, x_2) = (0.1, 0.81).
\end{align*}
\]

Thus, the coordinates of points on the surfaces contour were transformed from the system Yb-Al-Sr to the subsystem Al-Al\(_2\)Yb-Al\(_3\)Sr (Table 1) and used for the construction of T-x-y diagram model. To simplify the model, the solid-phase solubility was not taken into account. The model was developed by the assembly method from phase regions [8-9] using the author’s software [10].

The obtained computer model of T-x-y diagram for subsystem \(\text{Al}_2\text{Yb}-\text{Al}-\text{Al}_3\text{Sr}\) (A-B-C) contains four liquidus surfaces corresponding to the components \(\text{Al}_2\text{Yb}\) (A), Al (B), Al\(_3\)Sr (C) and compound R=Al\(_3\)Yb; ten ruled surfaces associated with them; four ruled surfaces at the boundary of the two-phase region R+C; two horizontal complexes at the temperatures of invariant points E and Q (Table 2); five two-phase regions (L+A, L+B, L+C, L+R, R+C) and seven three-phase regions (L+A+C, L+A+R, L+B+R, L+B+C, L+C+R, A+C+R, B+C+R) (Table 3, Fig. 2). The R+C phase region has a degenerate structure in the form of a vertical plane.

### Table 1. Coordinates of initial points on the surfaces contour.

|   |   |   |   |
|---|---|---|---|
|  | z1 | z2 | z3 | T   |
| A=\(\text{Al}_2\text{Yb}\) | 1  | 0  | 0  | 1360 |
| B=Al | 0  | 1  | 0  | 660,425 |
| C=\(\text{Al}_3\text{Sr}\) | 0  | 0  | 1  | 1040 |
| \(\epsilon_{AC}\) | 0.13 | 0 | 0.87 | 1025 |
| \(\epsilon_{BC}\) | 0  | 0.95 | 0.05 | 654 |
| \(\rho_{AR}\) | 0.39 | 0.61 | 0 | 980 |
| \(\epsilon_{BR}\) | 0.121 | 0.879 | 0 | 625 |
| E | 0.1 | 0.81 | 0.09 | 620 |
| Q | 0.13 | 0.285 | 0.585 | 800 |
| R=\(\text{Al}_2\text{Yb}\) | 0.76 | 0.24 | 0 | 800 |
| \(\epsilon_c\) | 0.6 | 0 | 0.4 | 1025 |
| \(\epsilon_A\) | 0.03 | 0 | 0.907 | 1025 |

### Table 2. Surfaces contours.

| \(\mathbb{N}\) | Name | Contour | \(\mathbb{N}\) | Name | Contour |
|---|---|---|---|---|---|
| 1 | \(q_A\) | \(A\rho_{AR}Q\epsilon_{AC}\) | 3 | \(q_C\) | \(C\epsilon_{AC}Q\epsilon_{BC}\) |
| 2 | \(q_B\) | \(B\epsilon_{BC}E\epsilon_{BR}\) | 4 | \(q_R\) | \(\rho_{AR}Q\epsilon_{BR}\) |
### Table 3. Structure of phase regions.

| №  | Phase region | Boundary surfaces | №  | Phase region | Boundary surfaces |
|----|--------------|-------------------|----|--------------|-------------------|
| 1  | L+A          | q_A, q'_AC, q'_AR| 6  | L+B+R        | q'_BR, q'_KB, h^[h:BBR] |
| 2  | L+C          | q_C, q'_CA, q'_CR, q'_CB | 7  | L+B+C        | q'_BC, q'_CB, h^[h:BBE] |
| 3  | L+B          | q_B, q'_BR, q'_BC | 8  | L+C+R        | q'_CR, q'_RC, h^[h:CRE], h^[h:CRE], s^[s:CR] |
| 4  | L+A+C        | q'_AC, q'_CA, h^[h:ACQ] | 9  | A+C+R        | h^[h:ACR], h^[h:AC], h^[h:AR], h^[h:CRE(Q)] |
| 5  | L+A+R        | q'_AR, q'_RA, h^[h:ARQ] | 10 | B+C+R        | h^[h:CRE], h^[h:BR], h^[h:BC], h^[h:CRE(E)] |

Figure 2. 3D computer model (a) and x-y projection (b) of T-x-y diagram Al₂Yb-Al-Al₄Sr.
4. Calculation of mass balances and analysis of concentration fields

At the projecting of all elements of T-x-y diagram into concentration simplex, it is divided on two-dimensional, one-dimensional and zero-dimensional concentration fields. The particularities of occurring processes in this fields are studied using the diagrams of vertical mass balance, which show an increase or decrease of phase portion for each phase region. [11-12]. They also make it possible to compare the processes taking place in different concentration fields and qualitatively show the concentrations fields with different by phase schemes, but with similar microstructure [11-12].

So the projection of studied subsystem is divided into 14 two-dimensional fields (1-14), 18 one-dimensional (eACQ, Q, pARER, E, Q, eBC, eER, Q, CE, RQ, Q, Q, A, A, Q, RQ, E, E, RQ, Q) and 5 zero-dimensional (Q, E, Q, E, Q) concentration fields (Fig. 3a). Using diagrams of vertical mass balance, it was revealed that five concentration fields coincide by the crystallization stages and microstructural sets with neighboring fields of higher dimension (12, 13, 14, 5, 10). One more one-dimensional field Qe coincides with field 12 by the microstructural set, but differs in the crystallization stages [13-14].

Let’s consider in more detail the diagrams of vertical mass balance calculated for fields 12 and Qe.

\[
\begin{align*}
\text{Al} = \text{B} &
\end{align*}
\]

\[
\text{Al} \text{Yb} = \text{A} &
\]

\[
\text{Al} \text{Sr} = \text{C} &
\]

Figure 3. x-y projection of T-x-y diagram Al-Al2Yb-Al4Sr with dividing into concentration fields (a); diagrams of vertical mass balance for mass centers G1∈12 (b) and G2∈Q-Qe (c).
The mass center $G_1$ (0.213; 0.173; 0.386) giving in field 12 (Fig. 3b) intersects the liquidus surface $q_A$ at 946.6°C and falls in two-phase region $L+A$, where the portion of phase A increases and the portion L decreases, which corresponds to primary crystallization $L^1\rightarrow A^1$. Then it crosses the ruled surface $q''_{AC}$ on the boundary of three-phase region $L+A+C$, in which, along with an increase of portion of phase A, the phase C appears and grows, while the content of $L$ decreases, i.e. monovariant eutectic crystallization occurs $L^1\rightarrow A^1+C^1$. Further, on the horizontal complex at the temperature of the invariant quasiperitectic point Q, a four-phase regrouping of the masses occurs $L_Q+A\rightarrow C_Q+R_Q$ at 800°C, as a result of which the crystals $A^1$ and $A^2$ are completely replaced by crystals R. Then the mass center falls into the three-phase region $L+C+R$, where the growth of phases C and R corresponds to the postperitectic secondary eutectic reaction $L^p\rightarrow C^p+R^p$. On the horizontal complex at the temperature of ternary eutectic E, the invariant eutectic reaction $L_E\rightarrow B_E+C_E+R_E$ at 620°C ends with the deficiency of melt and crystals B, C and R remain below. Thus, the field 12 is characterized by the following set of microstructural components: $C^1$, $C_Q$, $R_Q$, $C^p$, $R^p$, $B_E$, $C_E$, $R_E$. Crystals $A^1$ and $A^2$ are not included in this set, because completely consumed at invariant quasiperitectic reaction.

The diagram of vertical mass balance for center of mass $G_2$ (0.13; 0.161; 0.709) giving for neighboring field $Q_1Q$ does not include the primary crystallization reaction (Fig. 3c), since this one-dimensional field is the part of a monovariant liquidus line $e_{AC}Q$. The mass center for this field will immediately fall into the three-phase region $L+A+C$. Otherwise, the crystallization stages coincide with field 12. Therefore, fields 12 and $Q_1Q$ differ in the crystallization stages, but coincide with set of microstructural components.

The analysis of all concentration fields for the subsystem Al$_2$Yb-Al-Al$_2$Sr was carried out in a similar way.

5. Summary

Frederick N. Rhines gave some useful advices [3] to master the language of phase diagrams: “Each phase region is modeled separately in clay of different colour, and the various pieces are fitted into the completed diagrams. When finished, the model may be cut horizontally or vertically to obtain the isotherms and isoplets. Another very satisfactory method of making a model of a ternary diagram is by the use of wires to represent all the lines in the diagram. Cardboard may be used and coloured threads strung horizontally around the wires bounding the three edges of each three-phase region will serve to produce tie-triangles. This kind of models cannot be sectioned, of course, but it has the advantage, that the structure can be “seen through” and each phase region observed”.

In our days, thanks to the computer models of T-x-y diagrams, this task (to master the language of phase diagrams) may be solved by means of a 3D printer. After the prototyping, the phase regions will be used to puzzle the so-called exploded phase diagrams.

One more application of the T-x-y diagrams computer models is connected with the opinion of William Hume-Rothery [15]. He has estimated, that experimental building of a T-x-y diagram with medium-complexity will require the collaboration of two experienced researchers over a period of 5-10 years.

Computer models of the phase diagrams will help to do it in more short time. Thanks to the information on material balances, it is possible to generate the DTA spectrum prototype for any composition. The peak height of the DTA signal represents the phase with the maximal increase or decrease of mass portion in the corresponding temperature interval. Not gear but rectangular peak corresponds to the invariant regrouping of masses on the horizontal plane. The melt presence is showed by the elevated level of electrical conductivity. For generation of X-ray spectra the training software has been fitted by the data base with characteristics of initial components A, B, C and corresponding binary and ternary compounds (with their allotropies).

Main destination of PD computer model – to solve practical problems, beginning from correct and compact representation of the experimental information and finishing the calculation of formed in the system microconstituents of the phase assemblages. Diagram of vertical mass balances give a possibility to follow the changing of phase’s mass fraction for any composition within the temperature.
interval. Horizontal mass balances help to show the phases portions on the isopleth at the given temperature.

When the phase regions are projecting on the concentration simplex, the latter is dividing into the concentration fields with the individual sets of phase reactions and appropriate microstructures. Then the fields, which belong to the 3-phase regions, are dividing additionally by the surfaces of 2-phase reaction into the fragments with the different dynamics of phase masses increment. 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 eutectic crystals, with more large primary crystals and with the both types of these crystals.

Thus a kind of the training software will allow to create the PD computer model and then to construct vertical and horizontal sections with the decoding of intersected surfaces and phase regions, to calculate the mass balances, to generate the spectra of thermal and X-ray phase analyses for given composition. A user will assume the PD topology by means of the binary systems information, and then will determine all geometrical elements by means of minimal number of experiments.

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