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Florentina Cziple

The Prognosis of the Phase Equilibrium Diagram of the System Al-Cu-Si

The paper presents a model for establishing the mathematical functions of the liquidus and solidus curves, from the binary diagrams Al-Si, Si-Cu, Cu-Al and their use in the prognosis of the phase equilibrium diagram from the ternary system Al-Cu-Si. We have studied the model of the non-ideal liquid solution of the regular type. The calculus and graphic plotting of the equations for the binary systems has been performed on the computer

1. Introduction

The CAD (Computer Aided Design) software include the part of creation, analysis and optimisation of those models, which results in the completion of the partially plotted equilibrium diagrams, the correction of the experimental equilibrium diagrams, the qualitative analysis and systematic classification of the possible types of equilibrium diagrams. The theoretical studies of the phase equilibrium diagrams in the multiple systems of chemical elements are based on the structure, physical and chemical properties and thermodynamic functions of substances, on the elements' interactions in the binary systems, using the appropriate CAD software. Thus we obtain the theoretical models of the phase equilibrium diagrams for unary, binary or polynary systems of chemical elements, which haven't been determined experimentally so far.

2. The computerised model for the ternary diagram Al-Cu-Si

Building a *mathematical-statistic model* for the phase equilibrium diagram in the ternary system Al-Cu-Si, is based on the *establishment of the structure and the elaboration of the statistic model*, using the data from the literature for the three binary phase diagram Si-Al (Aloman, 1999), Al-Cu (Chang, 2001), Cu-Si (Olesinski, 1986). The mathematical computerised modelling of the ternary phases' diagram of equilibrium Al-Cu-Si was realised by generating the liquidus and solidus

surfaces from the liquidus and solidus curves of the binary phase diagrams Al-Si, Si-Cu, Cu-Al. The spatial model of the ternary phase diagram starts from the Gibbs triangle, and the lateral faces are constituted by the binary phase equilibrium diagrams, represented in temperature-composition co-ordinates. Figure 1 presents the model of the spatial diagram.

The construction of the mathematical model of the ternary phases diagram Al-Cu-Si was performed on a computer with the software MathCAD 2000 Professional, Curve Expert 1.3 and *3D StudioMax Version 5.0*, *Statistica 6,* which analyses the concatenated functions of the liquidus and solidus curves form the binary diagrams Al-Si, Al-Cu, Cu-Si, as well as B-spline functions (Cziple, 2002). The continuity of the liquidus curves (optimised with the Curve Expert 1.3software) and solidus form the perimeter of the corresponding surfaces.

The phase equilibriums liquid-solid from the binary diagram Al-Si, Al-Cu, Cu-Si were treated analytically (Aloman, 2001), rigorously deducing he equations of the phase transformation curves delimiting the monophase liquid domain form the biphase liquid-solid domain based on the models of the ideal and the regular non-ideal solution.

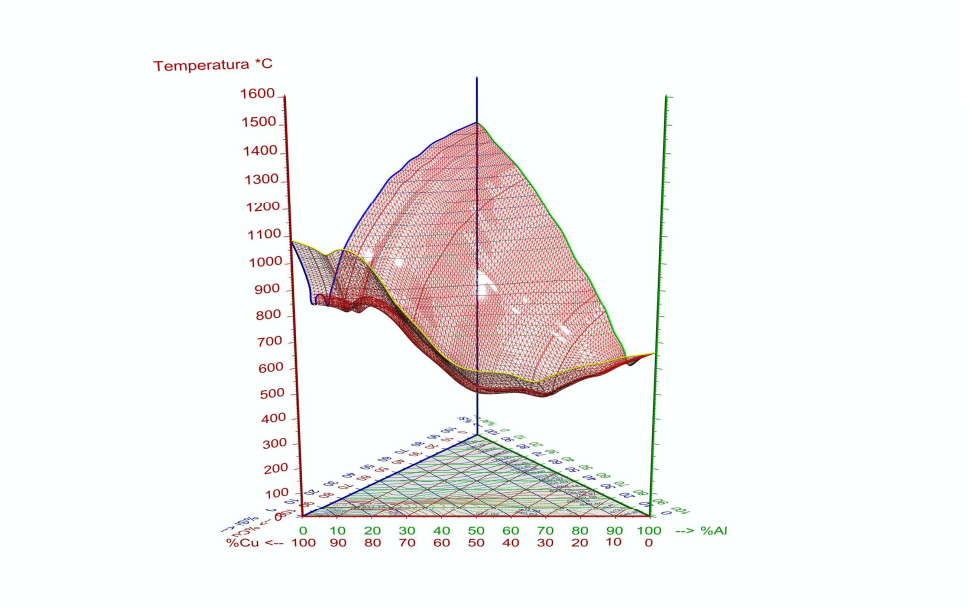

Figure 1 The three binary diagrams Si-Al, Al-Cu, Cu-Si, which are swung over in the plane of the Gibbs compositional triangle of the system Al-Cu-Si

The plotting (Fig.2) starts from the Gibbs triangle with the concentration (atomic %), and the axis perpendicular on the triangle plane represents the temperature (K). The acknowledged term for discretisation is „mesh".

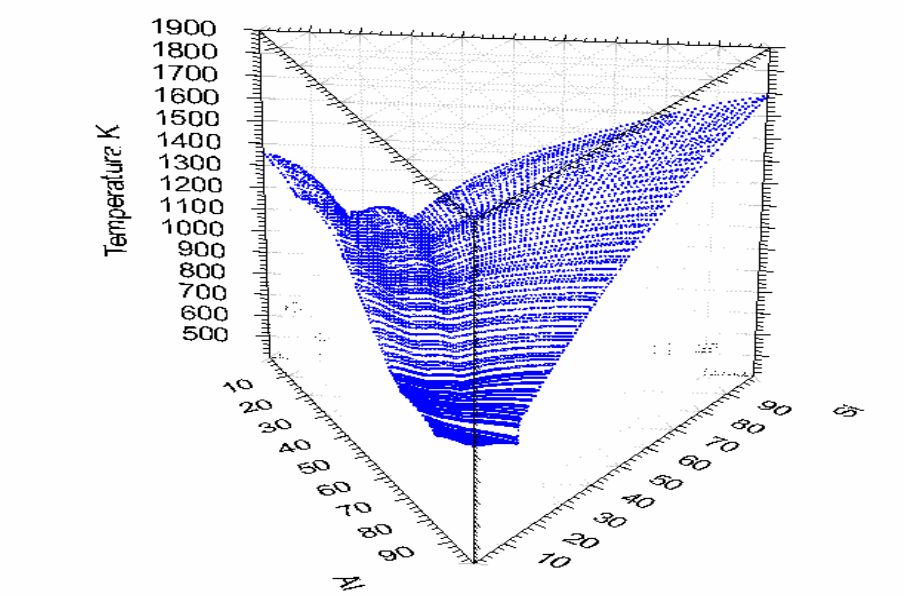

Figure 2 The liquidus surface mathematically modelled, in the ternary system Al-Cu-Si

Computed for the co-ordinates temperature (^{o}C) – concentration (%), the theoretical liquidus or solidus surfaces obtained, thus plotted are smooth, but in reality, at the solid-liquid interface, at the microscopic level, the surfaces contain a series of prominences due to the preferential concentration of different species of atoms, following the modification of the concentration of phases when the temperature drops.

The plotting is based on the Gibbs triangle of the concentrations expressed in atomic %, and the axis perpendicular on the triangle plane is graded in temperature units, (K) [4]. The projection on the Gibbs triangle of the points of co-ordinates: temperature (K) – atomic % (Al, Cu, Si) on the theoretic liquidus is presented in Figure 3.

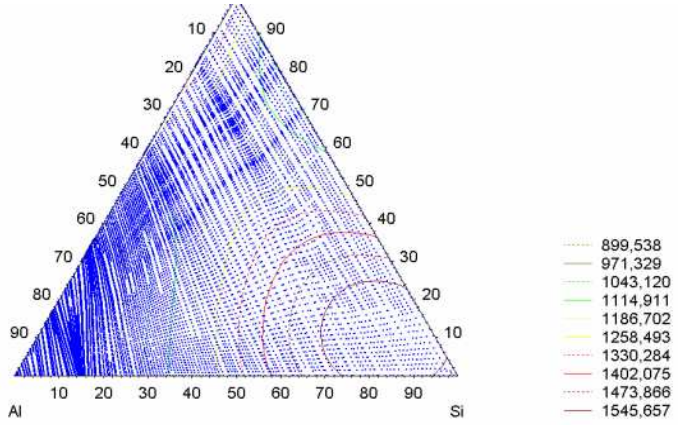

Figure 3. Projection on the Gibbs triangle of the points having generated the theoretic liquidus surface.

The studies performed on the prognosis of the diagram of phase equilibrium Al-Cu-Si (ternary phase diagram Al-Cu-Si) show the practical applicability of the equation of the statistic model (2), (3) and of the graphic plotting (Fig. 1-7) of the liquidus surface determined theoretically. It is thus possible to approximate the temperature of the beginning of solidification of any alloy of the Al-Cu-Si type, if we know its chemical composition. Furthermore, we can determine the composition of the alloy, knowing only the solidification beginning temperature of one of the components.

3. The statistic interpretation of the mathematical model

Using the database of the mathematical model of the liquidus surface, we have selected with the help of the computer 15466 points on the surface (Fig.2), having the co-ordinates : x_{Al}, x_{Si}, $x_{Cu,}$ concentrations (atomic %) and temperature (K). With these data, with the help of the Statistica 6 software, we have determined the equation of approximation of the liquidus surface (equation 2) through non-linear multiple regression, selecting the full-cubic approximation model (reliability coefficient 95%).

$$T = 918{,}959 \cdot x + 1491{,}086 \cdot y + 1355{,}557 \cdot z + 409{,}962 \cdot x \cdot y - 249.939 \cdot x \cdot z$$
$$- 811{,}233 \cdot y \cdot z - 1354{,}968 \cdot x \cdot y(x - y) - 1396{,}364 \cdot x \cdot z(x - z)$$
$$+ 2416{,}135 \cdot y \cdot z(y - z) + 2564{,}369 \cdot x \cdot y \cdot z \qquad (1)$$

where: T- temperature (K) ; x- atomic % Al ; y- atomic % Si : z- atomic % Cu.

The computerised 3D plotting (Statistica 6 software) of the equation (2) and the thermal characteristics of the surface are shown in Figure 3.

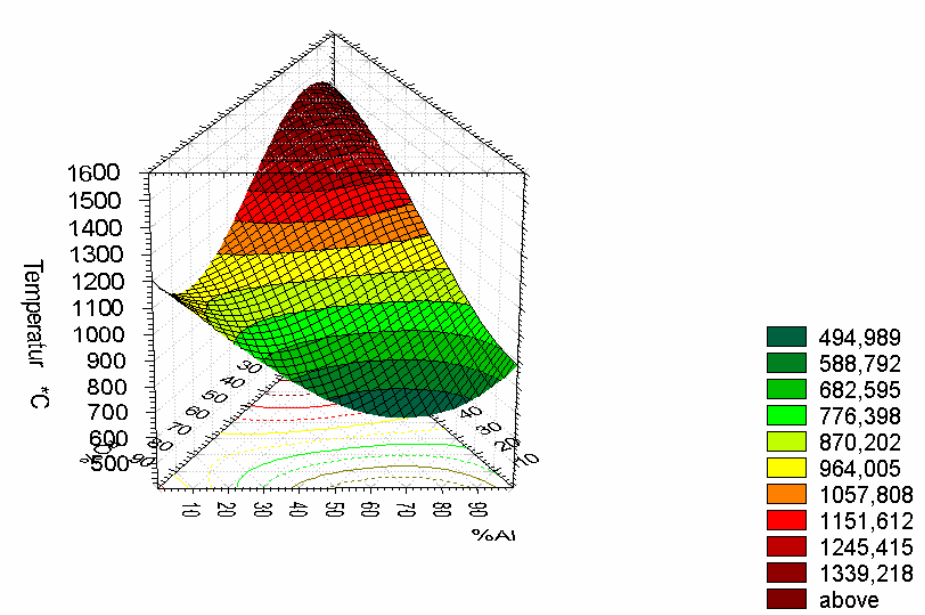

Figure 4. The equation surface (2) obtained with the Statistica 6 software.

4. Conclusions

The ternary diagram of phase equilibrium modelled thorough mathematical and thermodynamic calculus (Fig.7) delimits the domains of phase transformation (the liquid monophase domain, the bi-phase liquid-solid domain, the domain of solid phases), without indicating the number and nature of phases from the domains.

In the Al-Cu-Si system, through solidification depending on the system composition, ten condensed phases are separated: 1)Al2Cu3; 2)Al2Cu; 3)Al9Cu11; 4)Cu19Si6; 5)Cu33Si7; 6)Cu4Si; 7)Cu56Si11; 8)Cu85Si15; 9)Cu87Si13; 10)Si (GTT's Technical Termochemistry) The delimitation of these phases is not indicated by the computerised model presented.

The crystallisation process in alloys differs from that in pure metals and depends on the number and nature of phases separating from the melted material as a result of the way the atoms of the composing elements interact. Being a mixture of different atoms, alloys solidify within a temperature range to be found

in the thermal range between the liquidus and solidus surfaces. This range may be different in value, depending on the experiment conditions. Possible causes of differences may be: researchers' errors, different sensitivities of the experimental methods used for the diagram plotting, different purity of the initial materials (impurities can provoke the apparition of eutectic transformations), the various degrees of closeness to the equilibrium of alloys due to the different rates of cooling and the maintenance duration.

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[7] *** 3D StudioMax, 5.0 Portions Copyrighted © 1989–2002 mental images GmbH & Co. KG Berlin, Germany.

Address:

- S.L.Dr. Eng. Florentina Cziple, "Eftimie Murgu" University of Reşiţa, Piaţa Traian Vuia, nr. 1-4, 320085, Reşiţa, cziplechim@uem.ro