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## **The Computerised Calculus in the Prognosis of the Phase Equilibrium Diagram of the Ternary 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 with the software programmes MathCad 2000 Professional, Statistica 5, Curve Expert, and for the ternary system Al-Cu-Si, with the 3D StudioMax software.*

### **1. Introduction**

The present-day technical activities utilise a various range of materials, most of them being binary, ternary or polynary alloys. The general trend, intensely manifested these past decades, is the progressive mathematisation in the research of materials, the wider and wider use of mathematical methods and of computerised calculus in:

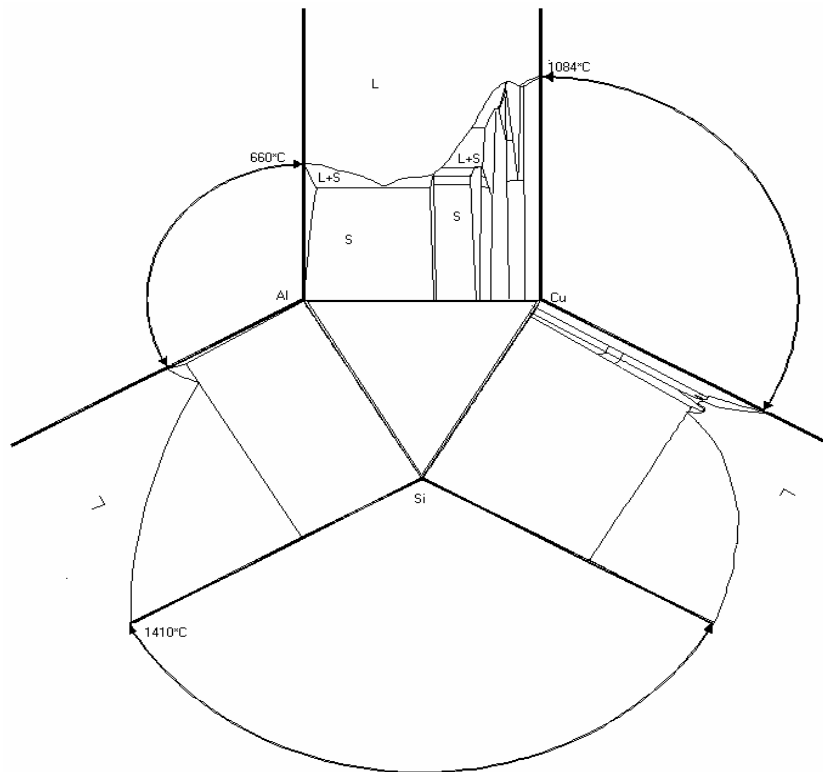
- Physical-chemical-mathematical modelling;
- Planning of the physical-chemical experiment;
- Processing experimental data;
- Optimisation of the physical-chemical properties;
- The prognosis of the equilibrium diagrams.

As nowadays there is no possibility to completely and accurately solve the issue of the prognosis of equilibrium diagrams, many researchers confer great attention to searching and elaborating qualitative and quantitative laws.

The main method of such works is the analysis of the known equilibrium diagrams as they enclose and contain all the laws and correlations we must find. The statistical method for the prognosis of a phase equilibrium diagram in a ternary system is a theoretical method for assessing the character of the components' interaction in the binary systems. The prognosis of the general aspect of binary equilibrium diagrams and of their fragments is performed with the help of

criteria and statistical processing of data from the known diagrams, plotting statistical graphs, obtained through the use of the main characteristics of the atomic-crystalline structure of the components. The reliability of such a prognosis may well go over 90% [1].

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 (Fig.1). The liquidus and solidus curves of the binary diagrams lead to the graphic plots of curves forming the perimeter of the liquidus and solidus surfaces of the ternary system Al-Cu-Si (Fig. 2a, 3a).



**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 construction of the mathematical model of the ternary phases diagram Al-Cu-Si was performed on a computer with the software *3D StudioMax Version 5.0* [7], which analyses the concatenated functions of the liquidus and solidus curves [6] from the binary diagrams Al-Si [1], Al-Cu [4], Cu-Si [5], as well as B-

spline functions. In the terminology of the mechanical drawing the term „spline” indicates an elastic band for drawing smooth curves along a set of control points (the NURBS <Non Uniform Rational B-Spline> concept). Mathematically, such curves may be described by portions as approximations of polynomial functions of the third grade, with all three orders of continuity (continuity of the zero, first and second order) in the control points [2].

## 2. The computerised plotting of the liquidus and solidus surfaces

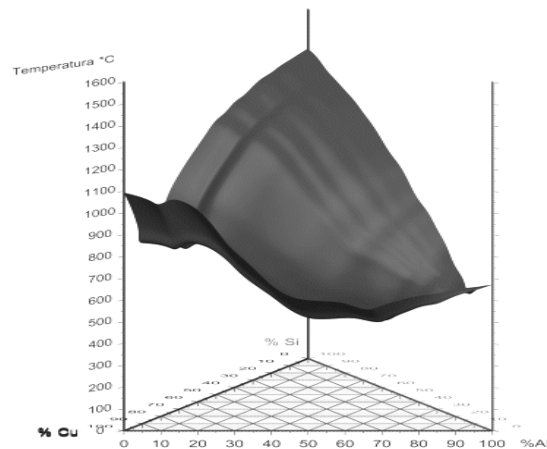
The definition of the spline surface obtained for the liquidus and solidus surfaces is made through the topological product of the mixture functions of the three B-spline functions representing the liquidus and solidus curves from the diagrams Al-Si, Si-Cu, Cu-Al, used for the computation of the vector of each point of the spline surface, expressed in the relations [2]:

$$P_{(u,v,z)} = \sum_{i=0}^l \sum_{j=0}^m \sum_{k=0}^n p_{i,j,k} \cdot N_{i,s}(u) \cdot N_{j,t}(v) \cdot N_{k,w}(z) \quad (1)$$

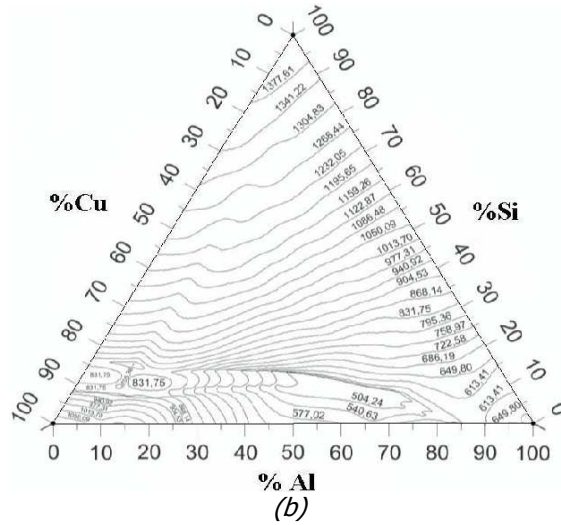
where:

$u, v, z$  – the parameters of variation of the mixture functions;  $p_{i,j,k}$  – the vector of one of the  $(l+1)(m+1)(n+1)$  control points on the surface;  $N_{i,s}(u)$ ,  $N_{j,t}(v)$ ,  $N_{k,w}(z)$  – mixture functions, mixture polynomials;  $l, m, n$  – number of control points of the respective polynomials;  $s, t, w$  – points of the  $(l+1)$ ,  $(m+1)$ ,  $(n+1)$  control points;

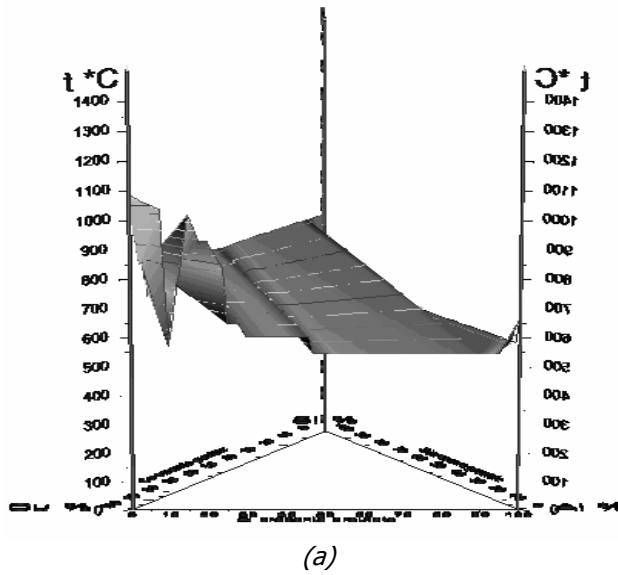
The projection of the liquidus and solidus surfaces on the plane of the Gibbs triangle (fig.3b-4b) allows the positioning of the isotherms in the plane, which offers information on the physical shape and thermal characteristics of the surface.

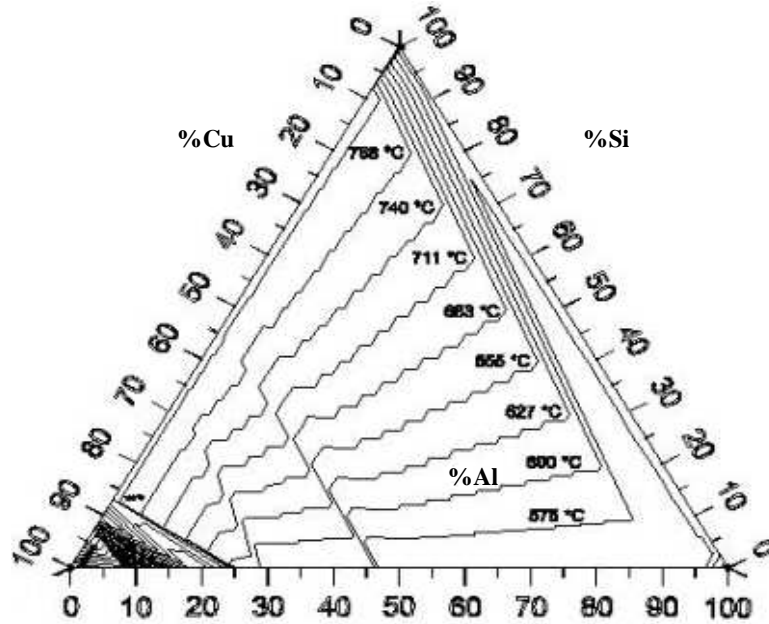


(a)



**Figure 2** The liquidus surface of the system Al-Cu-Si. (a) space plotting; (b) projection of the liquidus surface on the plane of the Gibbs triangle (at.%) Al,Cu,Si





(b)

**Figure 3** The solidus surfaces of the ternary phases diagram Al-Cu-Si.  
 (a) Perspective view. Vertical close-up view: the solidus curve (Cu-Al)  
 (b) projection of the liquidus surface on the plane of the Gibbs triangle (% Al, Cu, Si).

The surfaces 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.

### 3. Testing the mathematical model

The testing of the mathematical model of the liquidus and solidus surface was performed by determining the correlation coefficient  $r$  [8] of the mathematical model against the real model made of alloys from the system Al-Cu-Si [3]:

$$r \equiv \sqrt{\frac{S_t - S_r}{S_t}} \quad (2)$$

where -  $S_t$  is the *standard deviation*, quantifying the spreading of data around the medium experimental value  $\bar{y}$ , according to the relation [8]:

$$S_t = \sqrt{\sum_{i=1}^n (\bar{y} - y_i)^2} \quad (3)$$

where -  $S_r$  is defined as the *deviation of the model compared to the experiment* calculated (4),  $S_r = \sigma^2$  [8]:

$$\sigma^2 = \frac{\sum_{i=1}^n (y_{i,exp} - y_{i,calc})^2}{2n} \quad (4)$$

The data resulted from the experiment [3] are presented in Table 1.

**Table 1** The values of temperatures from the database of the mathematical model (calculated value) and the real model (experimental value)

Sample alloys	Beginning of solidification (°C)		End of solidification (°C)		Solidification range (°C)	
	Comp. value	Exp. value	Comp. value	Exp. value	Comp. value	Exp. value
AlSi6Cu4	628	$y_1$ : 615	576	$y_1$ : 540	52	$y_1$ : 75
		$y_2$ : 610		$y_2$ : 530		$y_2$ : 80
		$\bar{y}$ : 612,5		$\bar{y}$ : 535		$\bar{y}$ : 77,5
AlSi9Cu3	618	$y_1$ : 580	555	$y_1$ : 490	63	$y_1$ : 90
		$y_2$ : 578		$y_2$ : 479		$y_2$ : 99
		$\bar{y}$ : 579		$\bar{y}$ : 484,5		$\bar{y}$ : 94,5
AlSi12Cu	630	$y_1$ : 580	558	$y_1$ : 515	72	$y_1$ : 65
		$y_2$ : 570		$y_2$ : 529		$y_2$ : 41
		$\bar{y}$ : 575		$\bar{y}$ : 522		$\bar{y}$ : 53

After the statistical analysis performed by comparison with the real model [3], the mathematical model of the liquidus and solidus surfaces determined theoretically (Fig. 2a, 3a) exhibit a correlation coefficient of  $r=0,91$ .

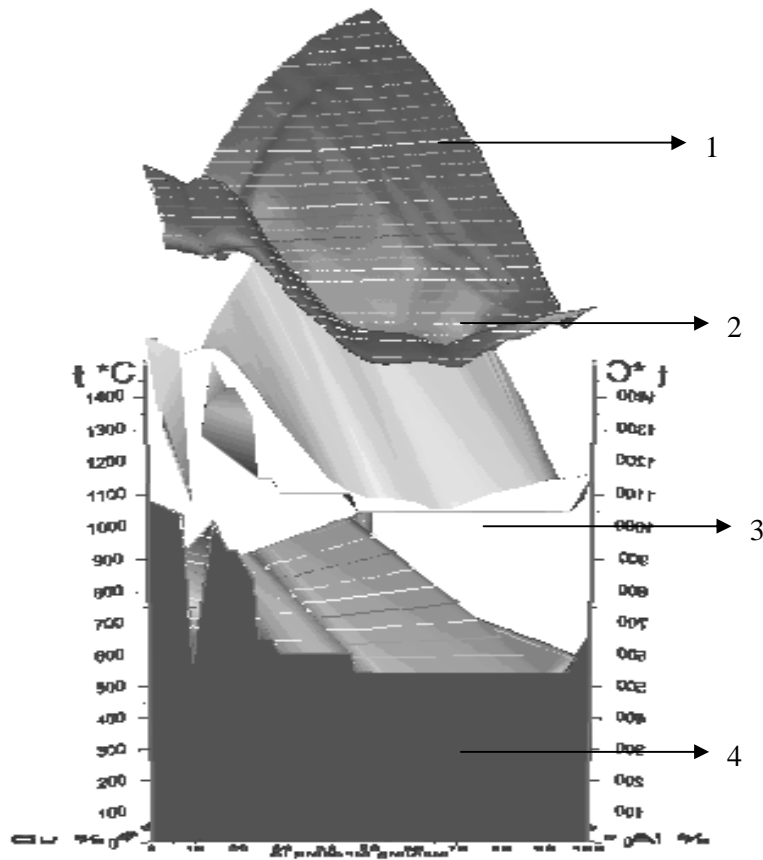
#### 4. Conclusions

- The ternary diagram of phase equilibrium modelled through mathematical and thermodynamic calculus (Fig.4), delimits the domains of phase transformation

(the liquid monophasic domain, the bi-phase liquid-solid domain, the domain of solid phases), without indicating the number and nature of phases from the domains.

- The correlation coefficient  $r=0,91$  of the liquidus and solidus surfaces leads to the conclusion that the mathematical model conceived has a rather satisfying reliability degree.

- The mathematical model of the liquidus surface plotted through the projection of isotherms on the plane of the basic Gibbs triangle allows the placement of the ternary eutectic area within the perimeter of the isotherm of  $504,24^{\circ}\text{C}$  (Fig. 2b).



**Figure 4** The theoretical ternary phase diagram Al-Cu-Si, the liquidus surface (1), the liquid-solid interval (2), the solidus surface (3), the solid phases space (4).

- The practical applicability of the model consists in the fact that with the help of the database one may approximate the melting temperature of any type of alloy from the system Al-Cu-Si.

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