

SPECIAL CUBE MODEL FOR MULTIPLE REGRESSION IN TRIANGULAR COORDINATES

This paper presents a multiple regression calculation Methodology in Triangular Coordinates. For the special cubic model is defined: the equations of theoretical regression model, the determination of regression coefficients using the least square method, checking the adequacy of mathematical models, and graphical representation of a mathematical model with the triangular contour and surface diagram.

INTRODUCTION

Three-component systems can be displayed graphically in two-dimensional space using triangular plots. The basic condition for applying triangular plots is:

$$0 \leq X_i \leq 1; \quad \sum_{i=1}^3 X_i = 1 \quad (1)$$

X_i - relative weight of the component in the mixture.

From the above stated condition it is evident that the weight of each component in the mixture depends on the share of the remaining two components.

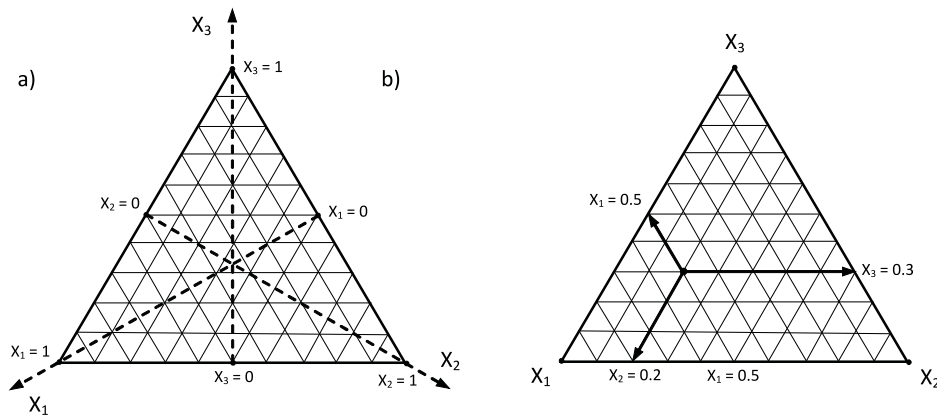


Fig. 1. Triangular diagram: a) display of vertical sections and the direction of the increase of the share of individual components, b) determining the composition of the alloy in the ternary system

Each point inside the triangle represents the corresponding composition of the three-component system. The vertices of the triangle represent pure substances while the points on the sides of the triangle represent two-component systems. For a point inside the triangle, the content of each of the components is determined by drawing lines through the point that are parallel to the sides of the triangle, to the remaining two sides of the triangle.

For a three-component system, regression models can generally be set in the form of lower-degree polynomials (usually the first, second and third) which are usually defined by the following canonical forms [1] [2]:

1. Linear regression model

$$y = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 \quad (2)$$

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2. Square regression model

$$y = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 \quad (3)$$

3. Incomplete cube regression model

$$y = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 + \beta_{123} X_1 X_2 X_3 \quad (4)$$

4. Complete cube regression model

$$y = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 + \delta_{12} X_1 X_2 (X_1 - X_2) + \dots \\ + \delta_{13} X_1 X_3 (X_1 - X_3) + \delta_{23} X_2 X_3 (X_2 - X_3) + \beta_{123} X_1 X_2 X_3 \quad (5)$$

INCOMPLETE CUBE MODEL FOR MULTIPLE REGRESSION

General canonical form of the *theoretical regression model* of the three-component system assumed by equations of the incomplete cube multiple regression can be shown by the analytic expression:

$$\hat{Y} = b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3 \quad (6)$$

Unknown values of multiple regression coefficients $b_1, b_2, b_3, b_{12}, b_{13}, b_{23}$ and b_{123} are determined based on the lowest square method [3],[4],[7], i.e. from the condition that the sum of squared deviation

$$S = S(b_1, b_2, b_3, b_{12}, b_{13}, b_{23}) = \sum_{i=1}^N \varepsilon_i^2 = \sum_{i=1}^N (Y_i - \hat{Y}_i)^2 \\ S = \sum_{i=1}^N \varepsilon_i^2 = \sum_{i=1}^N [Y_i - (b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3)_i]^2 \quad (7)$$

be minimal.

Function $S = S(b_1, b_2, b_3, b_{12}, b_{13}, b_{23}, b_{123})$ will have a minimum only for those variable values $b_1, b_2, b_3, b_{12}, b_{13}, b_{23}$ and b_{123} whose partial derivatives are equal to zero:

$$\frac{\partial S}{\partial b_1} = 0, \frac{\partial S}{\partial b_2} = 0, \frac{\partial S}{\partial b_3} = 0, \frac{\partial S}{\partial b_{12}} = 0, \frac{\partial S}{\partial b_{13}} = 0, \frac{\partial S}{\partial b_{23}} = 0, \frac{\partial S}{\partial b_{123}} = 0 \quad (8)$$

which leads to a system of 7 equations with 7 unknown parameters that need to be calculated:

$$2 \sum_{i=1}^N [Y_i - (b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3)_i] (-X_1)_i = 0 \\ 2 \sum_{i=1}^N [Y_i - (b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3)_i] (-X_2)_i = 0 \\ 2 \sum_{i=1}^N [Y_i - (b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3)_i] (-X_3)_i = 0 \\ 2 \sum_{i=1}^N [Y_i - (b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3)_i] (-X_1 X_2)_i = 0 \\ 2 \sum_{i=1}^N [Y_i - (b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3)_i] (-X_1 X_3)_i = 0 \\ 2 \sum_{i=1}^N [Y_i - (b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3)_i] (-X_2 X_3)_i = 0 \\ 2 \sum_{i=1}^N [Y_i - (b_1 X_1 + b_2 X_2 + b_3 X_3 + b_{12} X_1 X_2 + b_{13} X_1 X_3 + b_{23} X_2 X_3 + b_{123} X_1 X_2 X_3)_i] (-X_1 X_2 X_3)_i = 0 \quad (9)$$

This system of equations (9) can be reduced to a system of seven homogeneous linear equations with seven unknowns:

$$\begin{aligned}
& b_1 \sum_{i=1}^N X_1^2 + b_2 \sum_{i=1}^N X_1 X_2 + b_3 \sum_{i=1}^N X_1 X_3 + b_{12} \sum_{i=1}^N X_1^2 X_2 + b_{13} \sum_{i=1}^N X_1^2 X_3 + b_{23} \sum_{i=1}^N X_1 X_2 X_3 + b_{123} \sum_{i=1}^N X_1^2 X_2 X_3 = \sum_{i=1}^N X_1 Y \\
& b_1 \sum_{i=1}^N X_1 X_2 + b_2 \sum_{i=1}^N X_2^2 + b_3 \sum_{i=1}^N X_2 X_3 + b_{12} \sum_{i=1}^N X_1 X_2^2 + b_{13} \sum_{i=1}^N X_1 X_2 X_3 + b_{23} \sum_{i=1}^N X_2^2 X_3 + b_{123} \sum_{i=1}^N X_1 X_2^2 X_3 = \sum_{i=1}^N X_2 Y \\
& b_1 \sum_{i=1}^N X_1 X_3 + b_2 \sum_{i=1}^N X_2 X_3 + b_3 \sum_{i=1}^N X_3^2 + b_{12} \sum_{i=1}^N X_1 X_2 X_3 + b_{13} \sum_{i=1}^N X_1 X_3^2 + b_{23} \sum_{i=1}^N X_2 X_3^2 + b_{123} \sum_{i=1}^N X_1 X_2 X_3^2 = \sum_{i=1}^N X_3 Y \\
& b_1 \sum_{i=1}^N X_1^2 X_2 + b_2 \sum_{i=1}^N X_1 X_2^2 + b_3 \sum_{i=1}^N X_1 X_2 X_3 + b_{12} \sum_{i=1}^N X_1^2 X_2^2 + b_{13} \sum_{i=1}^N X_1^2 X_2 X_3 + b_{23} \sum_{i=1}^N X_1 X_2^2 X_3 + b_{123} \sum_{i=1}^N X_1^2 X_2^2 X_3 = \sum_{i=1}^N X_1 X_2 Y \\
& b_1 \sum_{i=1}^N X_1^2 X_3 + b_2 \sum_{i=1}^N X_1 X_2 X_3 + b_3 \sum_{i=1}^N X_1 X_3^2 + b_{12} \sum_{i=1}^N X_1^2 X_2 X_3 + b_{13} \sum_{i=1}^N X_1^2 X_3^2 + b_{23} \sum_{i=1}^N X_1 X_2 X_3^2 + b_{123} \sum_{i=1}^N X_1^2 X_2 X_3^2 = \sum_{i=1}^N X_1 X_3 Y \\
& b_1 \sum_{i=1}^N X_1 X_2 X_3 + b_2 \sum_{i=1}^N X_2^2 X_3 + b_3 \sum_{i=1}^N X_2 X_3^2 + b_{12} \sum_{i=1}^N X_1 X_2^2 X_3 + b_{13} \sum_{i=1}^N X_1 X_2 X_3^2 + b_{23} \sum_{i=1}^N X_2^2 X_3^2 + b_{123} \sum_{i=1}^N X_1 X_2^2 X_3^2 = \sum_{i=1}^N X_2 X_3 Y \\
& b_1 \sum_{i=1}^N X_1 X_2 X_3 + b_2 \sum_{i=1}^N X_2^2 X_3 + b_3 \sum_{i=1}^N X_2 X_3^2 + b_{12} \sum_{i=1}^N X_1 X_2^2 X_3 + b_{13} \sum_{i=1}^N X_1 X_2 X_3^2 + b_{23} \sum_{i=1}^N X_2^2 X_3^2 + b_{123} \sum_{i=1}^N X_1^2 X_2^2 X_3^2 = \sum_{i=1}^N X_1 X_2 X_3 Y
\end{aligned} \tag{10}$$

In regression analysis, these equations are called normal equations. The calculation of the system of equations (10) is best done using the matrix calculus. In the matrix form this system has the form:

$$\begin{bmatrix}
\sum_{i=1}^N X_1^2 & \sum_{i=1}^N X_1 X_2 & \sum_{i=1}^N X_1 X_3 & \sum_{i=1}^N X_1^2 X_2 & \sum_{i=1}^N X_1^2 X_3 & \sum_{i=1}^N X_1 X_2 X_3 & \sum_{i=1}^N X_1^2 X_2 X_3 \\
\sum_{i=1}^N X_1 X_2 & \sum_{i=1}^N X_2^2 & \sum_{i=1}^N X_2 X_3 & \sum_{i=1}^N X_1 X_2^2 & \sum_{i=1}^N X_1 X_2 X_3 & \sum_{i=1}^N X_2^2 X_3 & \sum_{i=1}^N X_1 X_2^2 X_3 \\
\sum_{i=1}^N X_1 X_3 & \sum_{i=1}^N X_2 X_3 & \sum_{i=1}^N X_3^2 & \sum_{i=1}^N X_1 X_2 X_3 & \sum_{i=1}^N X_1 X_3^2 & \sum_{i=1}^N X_2 X_3^2 & \sum_{i=1}^N X_1 X_2 X_3^2 \\
\sum_{i=1}^N X_1^2 X_2 & \sum_{i=1}^N X_1 X_2^2 & \sum_{i=1}^N X_1 X_2 X_3 & \sum_{i=1}^N X_1^2 X_2^2 & \sum_{i=1}^N X_1^2 X_2 X_3 & \sum_{i=1}^N X_1 X_2^2 X_3 & \sum_{i=1}^N X_1^2 X_2^2 X_3 \\
\sum_{i=1}^N X_1^2 X_3 & \sum_{i=1}^N X_1 X_2 X_3 & \sum_{i=1}^N X_1 X_3^2 & \sum_{i=1}^N X_1^2 X_2 X_3 & \sum_{i=1}^N X_1^2 X_3^2 & \sum_{i=1}^N X_1 X_2 X_3^2 & \sum_{i=1}^N X_1^2 X_2 X_3^2 \\
\sum_{i=1}^N X_1 X_2 X_3 & \sum_{i=1}^N X_2^2 X_3 & \sum_{i=1}^N X_2 X_3^2 & \sum_{i=1}^N X_1 X_2^2 X_3 & \sum_{i=1}^N X_1 X_2 X_3^2 & \sum_{i=1}^N X_2^2 X_3^2 & \sum_{i=1}^N X_1 X_2^2 X_3^2 \\
\sum_{i=1}^N X_1^2 X_2 X_3 & \sum_{i=1}^N X_1 X_2^2 X_3 & \sum_{i=1}^N X_1 X_2 X_3^2 & \sum_{i=1}^N X_1^2 X_2^2 X_3 & \sum_{i=1}^N X_1^2 X_2 X_3^2 & \sum_{i=1}^N X_1 X_2^2 X_3^2 & \sum_{i=1}^N X_1^2 X_2^2 X_3^2
\end{bmatrix} \cdot \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_{12} \\ b_{13} \\ b_{23} \\ b_{123} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^N X_1 Y \\ \sum_{i=1}^N X_2 Y \\ \sum_{i=1}^N X_3 Y \\ \sum_{i=1}^N X_1 X_2 Y \\ \sum_{i=1}^N X_1 X_3 Y \\ \sum_{i=1}^N X_2 X_3 Y \\ \sum_{i=1}^N X_1 X_2 X_3 Y \end{bmatrix} \tag{11}$$

Or the short form:

$$\mathbf{X} \cdot \mathbf{B} = \mathbf{Y} \tag{12}$$

Values of regression coefficients are calculated from the relation:

$$\mathbf{B} = \mathbf{X}^{-1} \mathbf{Y} \tag{13}$$

EXAMPLE OF USING THE INCOMPLETE CUBE MODEL

For this example, the values of hardness of the ternary alloy, i.e. three-component Sb-Bi-Zn system, are used. For each alloy, with its mole fractions shown in Table 1, three measurements were conducted, and then the mean hardness value was calculated.

Table 1. Mole fraction of components Sb, Bi and Zn and mean hardness value HB

<i>i</i>	<i>Sb</i>	<i>Bi</i>	<i>Zn</i>	<i>HB</i>
	<i>X1</i>	<i>X2</i>	<i>X3</i>	<i>Y</i>
1	0,00	0,50	0,50	132,0
2	0,10	0,45	0,45	46,0
3	0,20	0,40	0,40	52,0
4	0,30	0,35	0,35	87,0
5	0,40	0,30	0,30	45,9
6	0,50	0,25	0,25	45,0
7	0,60	0,20	0,20	51,5
8	0,70	0,15	0,15	56,1
9	0,80	0,10	0,10	49,7
10	0,90	0,05	0,05	52,0
11	1,00	0,00	0,00	412,0

<i>i</i>	<i>Sb</i>	<i>Bi</i>	<i>Zn</i>	<i>HB</i>
	<i>X1</i>	<i>X2</i>	<i>X3</i>	<i>Y</i>
12	0,50	0,00	0,50	32,0
13	0,45	0,10	0,45	25,3
14	0,40	0,20	0,40	42,0
15	0,35	0,30	0,35	46,0
16	0,30	0,40	0,30	79,6
17	0,25	0,50	0,25	83,0
18	0,20	0,60	0,20	77,3
19	0,15	0,70	0,15	87,0
20	0,10	0,80	0,10	85,7
21	0,05	0,90	0,05	48,6
22	0,00	1,00	0,00	294,0

<i>i</i>	<i>Sb</i>	<i>Bi</i>	<i>Zn</i>	<i>HB</i>
	<i>X1</i>	<i>X2</i>	<i>X3</i>	<i>Y</i>
23	0,50	0,50	0,00	82,0
24	0,45	0,45	0,10	56,4
25	0,40	0,40	0,20	32,1
26	0,35	0,35	0,30	30,6
27	0,30	0,30	0,40	49,7
28	0,25	0,25	0,50	53,2
29	0,20	0,20	0,60	67,2
30	0,15	0,15	0,70	74,8
31	0,10	0,10	0,80	89,7
32	0,05	0,05	0,90	88,2
33	0,00	0,00	1,00	94,2

The hardness measurement was conducted according to Brinell HB (SRBS C.A4.032). Values of the mole fractions of the components are marked with X1, X2 i X3 and mean hardness with Y. Experimental points are distributed along the three quasi-binary sections, Sb-BiZn, Bi-SbZn and Zn-SbBi (Fig. 2).

The diagram on the Fig. 3. shows the dependence of the hardness on the antimony (Sb) mole fraction and it can be seen that the hardness value for the antimony mole fraction from 0 to 0.4 varies between 40-130HB, then it stabilizes around 50HB, and with values larger than 0.9 there is a rapid growth from 50 to 412HB.

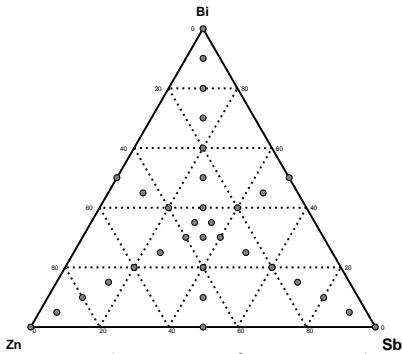


Fig. 2. The position of experimental points in the experimental plan

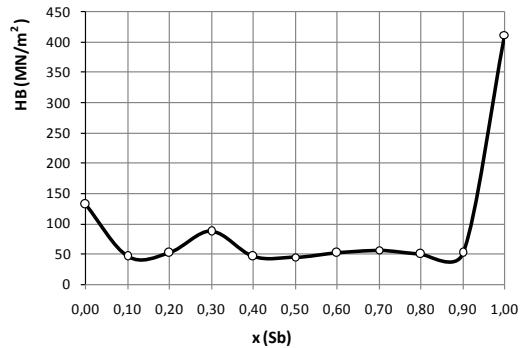


Fig. 3. Mean hardness value in the quasi-binary section Sb-BiZn

The influence of the mole fraction of bismuth (Bi) can be seen along the quasi-binary section from the Fig. 4. The hardness value slightly grows with bismuth mole fractions from 0 to 0.9 after which there is a rapid growth like with antimony. Unlike these two elements, the influence of the zinc (Zn) mole fraction is such that it causes a drop in hardness from 80 to 30HB in interval 0-0.3. However, mole fractions higher than 0.3 causes constant increase of hardness up to a value of 94.2 HB which can be seen on the quasi-binary section show in Fig. 5.

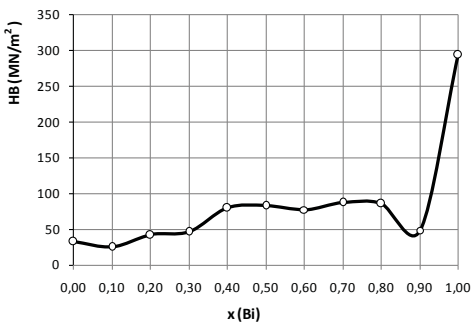


Fig. 4. Mean hardness value in the quasi-binary section Bi-SbZn

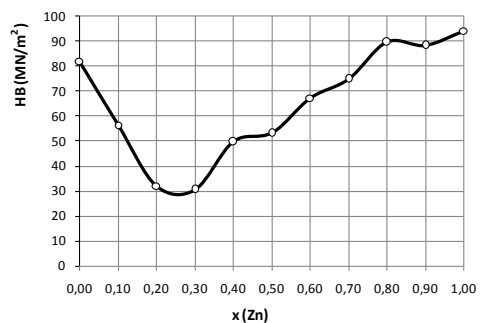


Fig. 5. Mean hardness value in the quasi-binary section Zn-BiSb

To establish a relation between the dependant variable, i.e. the object of the research (hardness in HB) and the selected influential parameters (mole fraction of Sb, Bi and Zn) the dependence is assumed in form of an equation (6).

Values of the matrices X and Y were obtained based on experimental data.

$$X = \begin{bmatrix} 5,77500 & 2,61250 & 2,61250 & 0,99688 & 0,99688 & 0,61875 & 0,20625 \\ 2,61250 & 5,77500 & 2,61250 & 0,99688 & 0,61875 & 0,99688 & 0,20625 \\ 2,61250 & 2,61250 & 5,77500 & 0,61875 & 0,99688 & 0,99688 & 0,20625 \\ 0,99688 & 0,99688 & 0,61875 & 0,32498 & 0,20625 & 0,20625 & 0,06198 \\ 0,99688 & 0,61875 & 0,99688 & 0,20625 & 0,32498 & 0,20625 & 0,06198 \\ 0,61875 & 0,99688 & 0,99688 & 0,20625 & 0,20625 & 0,32498 & 0,06198 \\ 0,20625 & 0,20625 & 0,20625 & 0,06198 & 0,06198 & 0,06198 & 0,01785 \end{bmatrix}, Y = \begin{bmatrix} 951,2950000 \\ 957,0850000 \\ 739,4200000 \\ 155,6860000 \\ 136,7382500 \\ 176,8907500 \\ 34,9646500 \end{bmatrix}$$

The calculated values of regression coefficients are shown in Table 2.

Table 2. Values of regression coefficients

b_1	268,55843
b_2	206,21587
b_3	125,87913
b_{12}	-872,99402
b_{13}	-776,72974
b_{23}	-240,00684
b_{123}	1579,85191

The mathematical model assumed by the equation (6) can now written in the form:

$$\hat{Y} = 268,55843X_1 + 206,21587X_2 + 125,87913X_3 - 872,99402X_1X_2 - 776,72974X_1X_3 - 240,00684X_2X_3 + 1579,85191X_1X_2X_3 \quad (14)$$

Checking the adequacy of the mathematical model

For the incomplete cube model for multiple regression shown by the equation (14), the squared deviation of the empirical points from the regression equation were calculated, and the received value of the sum of squared deviation is SK=78515,932 (Table 3). Median standard deviation is:

$$\sigma = \sqrt{\frac{\sum_{i=1}^N (Y_i - \hat{Y}_i)^2}{N}} = 48,7778$$

Since the absolute value of the biggest deviation $\varepsilon_{\max}=143,44157$ is less than $3\sigma=146,333$ it can be considered, based on the *three-sigma* rule, that the assumed functional dependence is good .

Table 3. Calculated sum of squared deviation for the regression line

i	Y_i	\hat{Y}_i	ε_i	ε_i^2
1	132,0	106,05	25,95	673,62
2	46,0	85,45	-39,45	1556,43
3	52,0	66,73	-14,73	216,85
4	87,0	52,24	34,76	1208,36
5	45,9	44,36	1,54	2,37
6	45,0	45,46	-0,46	0,21
7	51,5	57,90	-6,40	41,00
8	56,1	84,07	-27,97	782,13
9	49,7	126,32	-76,62	5870,18
10	52,0	187,02	-135,02	18231,59
11	412,0	268,56	143,44	20575,48
12	32,0	3,04	28,96	838,89
13	25,3	22,74	2,56	6,57
14	42,0	36,26	5,74	32,99
15	46,0	45,96	0,04	0,00
16	79,6	54,23	25,37	643,81
17	83,0	63,42	19,58	383,49
18	77,3	75,90	1,40	1,95
19	87,0	94,06	-7,06	49,81
20	85,7	120,25	-34,55	1193,56
21	48,6	156,84	-108,24	11716,76
22	294,0	206,22	87,78	7706,05
23	82,0	19,14	62,86	3951,55
24	56,4	35,69	20,71	428,74
25	32,1	44,62	-12,52	156,82
26	30,6	48,30	-17,70	313,12
27	49,7	49,08	0,62	0,38
28	53,2	49,35	3,85	14,83
29	67,2	51,47	15,73	247,41
30	74,8	57,81	16,99	288,51
31	89,7	70,75	18,95	359,08
32	88,2	92,65	-4,45	19,79
33	94,2	125,88	-31,68	1003,57
Sum of squared deviation				78515,932

Graphic interpretation of the mathematical model

There is a number of software for drawing graphs in a triangular system. However, for our own research needs stemming from the cooperation of the Faculty of Mechanical Engineering Kraljevo and the Technical Faculty in Kosovska Mitrovica, the regression analysis for the three-component system and the procedure for obtaining a triangular 3D graph and a contour 2D diagram in a triangular system was done in the software package MATLAB 2008b.

The obtained mathematical model of the dependence of the surface hardness (in HB) on the mole fraction Sb-Bi-Zn, i.e. the selected parameters X_1 , X_2 and X_3 defined by the equation (14) is graphically represented with a surface triangular graph and its corresponding contour 2D plot in Figures 6 and 7. The possibility of obtaining such a mathematical model and graphic representations eliminates the need for drawing plots for quasi-binary sections and clearly shows the dependence of the observed characteristic on the dependant variables.

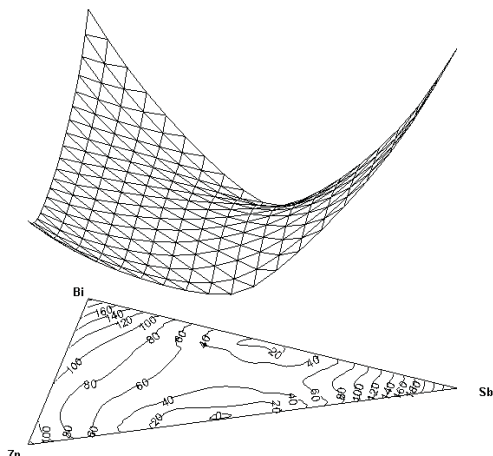


Fig. 6. Triangular 3D diagram of the surface hardness dependence on the mole fraction of Sb-Bi-Zn

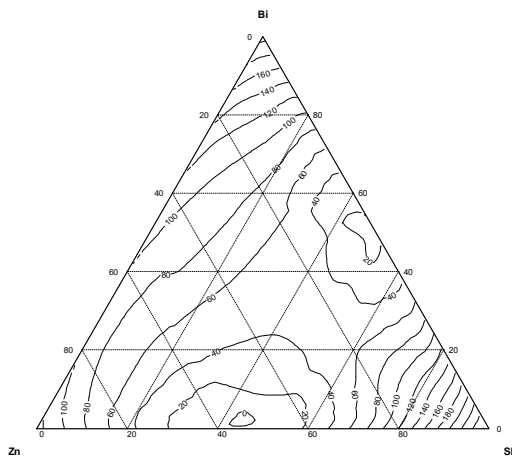


Fig. 7. Contour 2D diagram of the surface hardness dependence on the mole fraction Sb-Bi-Zn

CONCLUSION

In the process of exploring electrical and mechanical properties of alloys, three-component systems have a significant role. The theoretical dependence of these values on the mole fraction of certain components in the mixture is obtained based on experimental results. It often occurs that the linear (1) and the square model (2) cannot describe this phenomenon in a satisfactory way so it is necessary to use canonical models in the form of higher-degree polynomials.

When it comes to multidimensional problems, in regression analysis it is extremely important to show this correlation, apart from obtained analytical dependencies, with visually adequate graphic representations (diagrams). The advantage of the Ternary graph is that with the space curved surface it is possible to represent and analyze four-dimensional and with categorized Ternary graph even five-dimensional problems.

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