

# A methodology for forming the regression model of ternary system

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**SUMMARY.** This paper presents a methodology of multiple regression analysis of three-component systems. There are several stages: 1) calculation of the parameters of regression models, 2) checking the adequacy of mathematical models, 3) selection of regression model, 4) assessment of the significance of model parameters, 5) calculation of confidence limits of regression coefficients and 6) graphical representation of a mathematical model with the triangular surface plots or contour plots.

**Keywords:** Multiple regression, Triangular Coordinates, Contour plot, Surface plot

## 1. INTRODUCTION

Three-component systems can be graphically displayed in two-dimensional space using triangular plots. The basic conditions for application of the triangular plots are:

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

$X_i$  – the relative weight of the components in the mixture.

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

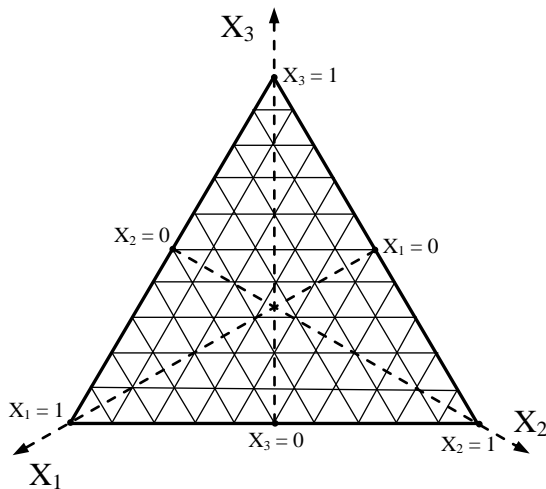


Fig. 1. Display of vertical sections and direction increase of share of individual component in a triangular diagram

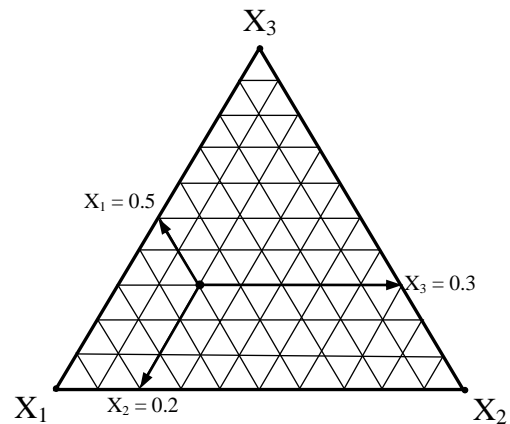


Fig. 2. Determining the composition of alloys in the ternary system

Each point within the triangle represents an appropriate composition of a three-component system. The vertices of the triangle represent a pure substance, while points on the sides of the triangle represent two-component systems. For a point inside the triangle, the content of each component is determined by drawing lines parallel to the sides of the triangle, and reading the value that corresponds to intersections between the lines and the sides of the triangle.

## 2. REGRESSION ANALYSIS

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

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- Linear regression model

$$y = b_1X_1 + b_2X_2 + b_3X_3 \quad (2)$$

- Square regression model

$$y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 \quad (3)$$

- Incomplete cube regression model

$$y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{123}X_1X_2X_3 \quad (4)$$

- Complete cube regression model

$$y = b_1X_1 + b_2X_2 + b_3X_3 + b_{12}X_1X_2 + b_{13}X_1X_3 + b_{23}X_2X_3 + b_{123}X_1X_2X_3 + \delta_{12}X_1X_2(X_1 - X_2) + \delta_{13}X_1X_3(X_1 - X_3) + \delta_{23}X_2X_3(X_2 - X_3) \quad (5)$$

Selection of the regression model for ternary system depends primarily on available number of experimental points (Table 1). However, when a sufficient number of experimental points exist, it still does not mean that the model of the highest level will be the best.

Table 1. The required number of experimental points for the formation of the regression model at ternary system

Regression model	Response subscripts	Number of regression coefficients	$\Sigma$
Linear	<i>i</i>	3	3
Second degree	<i>ij</i>	3	6
Incomplete third degree	<i>i</i>	3	7
	<i>ij</i>	3	
Complete third degree	<i>ijk</i>	1	10
	<i>i</i>	3	
	<i>ijj</i>	6	
	<i>ijk</i>	1	

In order to undergo the procedure of regression analysis of the ternary system and to select an appropriate regression model is necessary to implement the following steps:

- Selection of possible canonical forms of regression models
- Calculation of regression coefficients
- Checking the adequacy of the mathematical model
- Selection of regression model
- Assessment of significance of regression coefficients of the selected model

- Calculation the confidence limits of regression coefficients at the selected model
- Graphical interpretation of the mathematical model.

Procedure for implementation of regression analysis is shown in the example of measuring the electrical conductivity of ternary alloys *Ga-Sb-Zn* (Table 2). Mole fractions of component values are indicated by *X1*, *X2* and *X3* and the mean value of electrical conductivity (*MS /m*) with *Y*.

Table 2. Experimental values of electrical conductivity of ternary alloys *Ga-Sb-Zn*

	<i>Ga</i>	<i>Sb</i>	<i>Zn</i>	<i>EP [MS/m]</i>
	<i>X1</i>	<i>X2</i>	<i>X3</i>	<i>Y</i>
1	0	0,5	0,5	0,198
2	0,4	0,3	0,3	0,352
3	1	0	0	6,780
4	0,5	0	0,5	2,324
5	0,3	0,4	0,3	0,743
6	0	1	0	2,880
7	0,5	0,5	0	0,224
8	0,3	0,3	0,4	0,604
9	0	0	1	16,600

### 3. CALCULATION OF MODEL PARAMETERS

Modern software tools enable selection of all possible regression models depending on the number of available experimental points. Based on data from Table 1 it is possible to perform regression analysis for linear, quadratic and incomplete cubic regression model. Equations (2) - (4) can be written in matrix form:

$$Y = X b \quad (6)$$

where:

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_k \end{bmatrix}, X = \begin{bmatrix} x_{11} & x_{12} & \cdot & \cdot & \cdot & x_{1k} \\ x_{21} & x_{22} & \cdot & \cdot & \cdot & x_{2k} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x_{n1} & x_{n2} & \cdot & \cdot & \cdot & x_{nk} \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_k \end{bmatrix}$$

Unknown coefficients of multiple regression  $b_i$ ,  $b_{ij}$  and  $b_{ijk}$  are determined by the method of least squares [3], [4], [7] i.e. from the condition that the sum of squared deviations:

$$S = \sum_{i=1}^N \varepsilon_i^2 = \sum_{i=1}^N (Y_i - \hat{Y}_i)^2 \quad (7)$$

becomes minimal.

The function  $S = S(b_i, b_{ij}, b_{ijk})$  will have a minimum only for those values of the variables  $b_i, b_{ij}, b_{ijk}$  which are its partial derivatives equal to zero:

$$\frac{\partial S}{\partial b_i} = 0, \quad \frac{\partial S}{\partial b_{ij}} = 0, \quad \frac{\partial S}{\partial b_{ijk}} = 0, \quad (8)$$

which leads to systems of 3, 6 and 7 equations with 3, 6 and 7 unknown parameters. This system of equations can be reduced to a system of seven normal homogeneous linear equations with seven unknowns. Regression coefficients are calculated from the equation:

$$B = (X'X)^{-1}XY \quad (9)$$

From data in table 2 matrix X and vector Y are:

$$X = \begin{bmatrix} 0.0 & 0.5 & 0.5 & 0.00 & 0.00 & 0.25 & 0.000 \\ 0.4 & 0.3 & 0.3 & 0.12 & 0.12 & 0.09 & 0.036 \\ 1.0 & 0.0 & 0.0 & 0.00 & 0.00 & 0.00 & 0.000 \\ 0.5 & 0.0 & 0.5 & 0.00 & 0.25 & 0.00 & 0.000 \\ 0.3 & 0.4 & 0.3 & 0.12 & 0.09 & 0.12 & 0.036 \\ 0.0 & 1.0 & 0.0 & 0.00 & 0.00 & 0.00 & 0.000 \\ 0.5 & 0.5 & 0.0 & 0.25 & 0.00 & 0.00 & 0.000 \\ 0.3 & 0.3 & 0.4 & 0.09 & 0.12 & 0.12 & 0.036 \\ 0.0 & 0.0 & 1.0 & 0.00 & 0.00 & 0.00 & 0.000 \end{bmatrix}, Y = \begin{bmatrix} 0.198 \\ 0.352 \\ 6.780 \\ 2.324 \\ 0.743 \\ 2.880 \\ 0.224 \\ 0.604 \\ 16.600 \end{bmatrix}$$

Matrix  $X'X$  is:

$$X'X = \begin{bmatrix} 1.840 & 0.580 & 0.580 & 0.236 & 0.236 & 0.108 & 0.036 \\ 0.580 & 1.840 & 0.580 & 0.236 & 0.108 & 0.236 & 0.036 \\ 0.580 & 0.580 & 1.840 & 0.108 & 0.236 & 0.236 & 0.036 \\ 0.236 & 0.236 & 0.108 & 0.099 & 0.036 & 0.036 & 0.0119 \\ 0.236 & 0.108 & 0.236 & 0.036 & 0.099 & 0.036 & 0.0119 \\ 0.108 & 0.236 & 0.236 & 0.036 & 0.036 & 0.099 & 0.0119 \\ 0.036 & 0.036 & 0.036 & 0.012 & 0.0119 & 0.0119 & 0.0039 \end{bmatrix}$$

Vektor  $X'Y$  is:

$$X'Y = \begin{bmatrix} 0.00 & 0.40 & . & . & . & 0.0 \\ 0.50 & 0.30 & . & . & . & 0.0 \\ 0.50 & 0.30 & . & . & . & 1.0 \\ 0.00 & 0.12 & . & . & . & 0.0 \\ 0.00 & 0.12 & . & . & . & 0.0 \\ 0.25 & 0.09 & . & . & . & 0.0 \\ 0.00 & 0.036 & . & . & . & 0.0 \end{bmatrix} \begin{bmatrix} 0.198 \\ 0.352 \\ 6.780 \\ 2.324 \\ 0.743 \\ 2.880 \\ 0.224 \\ 0.604 \\ 16.600 \end{bmatrix} = \begin{bmatrix} 8.599 \\ 3.675 \\ 18.431 \\ 0.241 \\ 0.763 \\ 0.243 \\ 0.061 \end{bmatrix}$$

Values of inverse matrix  $(X'X)^{-1}$  are:

$$(X'X)^{-1} = \begin{bmatrix} 0.640 & -0.153 & -0.153 \\ -0.153 & 0.640 & -0.153 \\ -0.153 & -0.153 & 0.640 \end{bmatrix}$$

$$(XX)^{-1} = \begin{bmatrix} 0.987 & -0.0115 & -0.0115 & -1.7593 & -1.7593 & 0.2565 \\ -0.0115 & 0.987 & -0.0115 & -1.7593 & 0.2565 & -1.7593 \\ -0.0115 & -0.0115 & 0.987 & 0.2565 & -1.7593 & -1.7593 \\ -1.7593 & -1.7593 & 0.2565 & 18.853 & -0.989 & -0.989 \\ -1.7593 & 0.2565 & -1.7593 & -0.989 & 18.853 & -0.989 \\ 0.2565 & -1.7593 & -1.7593 & -0.989 & -0.989 & 18.853 \end{bmatrix}$$

$$(X'X)^{-1} = \begin{bmatrix} 0.9989 & 0.0005 & 0.0005 & -2.0053 & -2.0053 & 0.0105 & 2.963 \\ 0.0005 & 0.9989 & 0.0005 & -2.0053 & 0.0105 & -2.0053 & 2.963 \\ 0.0005 & 0.0005 & 0.9989 & 0.0105 & -2.0053 & -2.0053 & 2.963 \\ -2.005 & -2.005 & 0.0105 & 23.895 & 4.0525 & 4.0525 & -60.741 \\ -2.005 & 0.0105 & -2.005 & 4.0525 & 23.895 & 4.0525 & -60.741 \\ 0.0105 & -2.005 & -2.005 & 4.0525 & 4.0525 & 23.895 & -60.741 \\ 2.963 & 2.963 & 2.963 & -60.741 & -60.741 & -60.741 & 731.687 \end{bmatrix}$$

Based on the method of least squares from equation (9) values of regression coefficients are:

a) for a linear model

$$B_{lin} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} 2.1131 \\ -1.7946 \\ 9.9165 \end{bmatrix}$$

b) for a quadratic model

$$B_{kv} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_{12} \\ b_{13} \\ b_{23} \end{bmatrix} = \begin{bmatrix} 6.5284 \\ 2.6600 \\ 16.3430 \\ -13.3042 \\ -32.7144 \\ -33.1010 \end{bmatrix}$$

c) for incomplete cubic model

$$B_{sk} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_{12} \\ b_{13} \\ b_{23} \\ b_{123} \end{bmatrix} = \begin{bmatrix} 6.7713 \\ 2.9029 \\ 16.5859 \\ -18.2825 \\ -37.6928 \\ -38.0794 \\ 59.9695 \end{bmatrix}$$

#### 4. CHECKING ADEQUACY OF MODEL

After determining the numerical values of model parameters (regression coefficients), it is needed in the next phase to check the adequacy of selected models. Checks are conducted using **F**-test. The test relies on the following hypotheses:

$$H_0 \dots b_1 = b_2 = \dots = b_k = 0; \quad H_1 \dots \exists b_i \neq 0, i = 1, 2, \dots, k.$$

The claim contains a null hypothesis that neither variable in the regression model was not significant, i.e. that all the parameters of the regression variables are equal to zero. An alternative hypothesis *H1* states that out of the *k* regression variables, there is at least one that is

significant in explaining the variability of the dependent variable, i.e. that there is at least one parameter different of zero. For testing is used F-ratio:

$$F = \frac{\frac{SS_R}{v_1}}{\frac{SS_E}{v_2}} = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2 / k}{\sum_{i=1}^n (y_i - \hat{y}_i)^2 / n - k} \quad (10)$$

where:  $n$  – total number of experimental points  
 $k$  – number of regression coefficients  
 $SS_R$  – regression sum of squares  
 $SS_E$  – error sum of squares  
 $v_1, v_2$  – degrees of freedom

Sums of squares can be calculated using the matrix:

$$SS_R = (\hat{Y} - \bar{Y})' (\hat{Y} - \bar{Y}) \quad (11)$$

$$SS_E = (Y - \hat{Y})' (Y - \hat{Y})$$

The decision on the adequacy of the model is made based on comparison of empirical values of the size of  $F$  and theoretical values of  $F$ -distribution. Area of accepting the null hypothesis is  $F < F_{\alpha, v_1, v_2}$ . Area of rejection of the null hypothesis is  $F > F_{\alpha, v_1, v_2}$ .

Table 3. *Checking the adequacy of the model*

	Model		
	Linear	Quadratic	Inc.cubic
$SS_R$	149,452	286,036	290,951
$v_1=k$	3	6	7
$SS_E$	142,0065	5,4230	0,5078
$v_1=n-k$	6	3	2
$F$	2,105	26,373	163,696
$F_{\alpha, v_1, v_2}$	4,757	8,941	19,353
Adequacy	Model is not adequate	The model is adequate	The model is adequate
$\hat{\sigma}^2$	23,6678	1,8077	0,2539

By accepting the null hypothesis, it is also accepted the assumption that the regression variables in the model are not significant. Otherwise, it is considered that there is at least one of the  $k$  regression variables that significantly contributes to explaining of the variability of the dependent variable  $Y$ . After calculations with the data from the example for a significance level of

$\alpha = 0.05$ , we can conclude that only the linear model is not significant (Table 3).

### 5. SELECTION OF REGRESSION MODEL

For quality evaluation of the model and a comparison of regression models are available the following statistical and analytical indicators [7]:

- coefficient of determination  $R^2$
- corrected coefficient of determination  $\bar{R}^2$
- variance of regression  $\hat{\sigma}^2$
- Mallows indicator  $C_p$
- Prediction Sum of Squares Statistic - *PRESS*
- Akaike's Information Criterion - *AIC*
- Schwartz's Bayesian Criterion - *SBC*
- Bayes' Information Criterion - *BIC*
- Amemiya's Prediction Criterion - *PC*

For the purpose of this study, it was selected criterion is the minimum value of variance regression model, which is calculated as the ratio of residual sum of squares (sum of squared errors  $SS_E$ ) and the associated number of degrees of freedom  $v_1=n-k$ , i.e.

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n - k} \quad (12)$$

Statistical representativeness of the model increases with decrease of value of variance regression model and it is logical that between the available models, whose adequacy has been confirmed, the one with the lowest estimate of the variance regression is selected. In the example (Table 3), are adequate quadratic and incomplete cubic model. Incomplete cubic model is better, because it has a smaller value of variance.

Finally, we can write the expression for the selected regression model:

$$\hat{y} = 6.7713X_1 + 2.9029X_2 + 16.5859X_3 - 18.2825X_1X_2 - 37.6928X_1X_3 - 38.0794X_2X_3 + 59.9695X_1X_2X_3 \quad (13)$$

### 6. EVALUATION OF THE SIGNIFICANCE OF MODEL PARAMETERS

Assessment of the significance of the parameter model is reduced to testing of the hypotheses about the significance of the parameter  $b_j$  (regression variable  $X_j$ ). The claim contains a null hypothesis that the parameter  $b_j$  is zero, i.e. that

the variable  $X_j$  in the model is redundant. An alternative hypothesis claims the opposite. For evaluation of significance are available **t**-test or **F**-test because there is a their correlation at the shape  $F(1;\nu) = t^2(\nu)$ . Hypothesis and decision-making by **t**-test is given in Table 4. Test indicator is an empirical t-ratio

$$t = \frac{\hat{b}_j}{\sigma_{\hat{b}_j}} \quad (14)$$

which is distributed by the Student distribution with  $\nu = nk$  degrees of freedom.

Table 4. Evaluation of significance of parameters by t-test

Null hypothesis	$H_0...b_j=0$
Alternative hypothesis	$H_1...b_j \neq 0$
Acceptance area $H_0$	$ t  < t_{\alpha/2}$
Rejection area $H_0$	$ t  > t_{\alpha/2}$

It can also be applied to **F**-test with a test indicator empirical F-ratio

$$F = \left[ \frac{\hat{b}_j}{\sigma_{\hat{b}_j}} \right]^2$$

which has F distribution with  $\nu_1=1$  and  $\nu_2=n-k$  degrees of freedom. The decision is made by comparing the empirical values with the theoretical value of F distribution in the familiar way.

Table 5. Evaluation of the significance of parameters

$\hat{\sigma}$	$C_{jj}$	$\sigma_{\hat{b}_j}$	$t$	$t_{\alpha}$
0,5039	0,999	0,50363	13,4448	4,303
	0,999	0,50363	5,7638	
	0,999	0,50363	32,9324	
	23,895	2,46317	-7,4223	
	23,895	2,46317	-15,3025	
	23,895	2,46317	-15,4594	
	731,687	13,63026	4,3997	

Standard error of regression coefficient is:

$$\sigma_{\hat{b}_j} = \hat{\sigma} \sqrt{C_{jj}} \quad (15)$$

where:  $\hat{\sigma}$  - estimates the standard deviation

$C_{jj}$  - diagonal element of matrix  $(X'X)^{-1}$

The group parameters of the model which are insignificant can be excluded from the model without correcting of the values of other

parameters that remain significant in the model. Evaluation of the significance of parameters in the selected regression model is shown in Table 5. The value of  $t_{\alpha}=4,303$  is taken for  $\alpha=0.05$  and  $\nu=n-k=9-7=2$ . It may be noted that all parameters are eligible ( $|t| > t_{\alpha/2}$ ).

### 7. CONFIDENCE INTERVAL OF PARAMETERS OF MODEL

For information about the precision of parameters of model it is not enough just to make estimation of parameters, but is necessary to determine and limits of confidence interval. These are the limits defined by the general expression:

$$P(\hat{b}_j - t_{\alpha,n-k} \sigma_{\hat{b}_j} < b_j < \hat{b}_j + t_{\alpha,n-k} \sigma_{\hat{b}_j}) = (1-\alpha) \quad (16)$$

where the following notation is adopted:

$\hat{b}_j$  - estimate the parameters  $b_j$  with number

$t_{\alpha,n-k}$  - value  $t$ -distribution for the probability of  $\alpha$  and  $n-k$  degrees of freedom

$(1-\alpha)$  - reliability of evaluation

$\sigma_{\hat{b}_j}$  - standard error of regression coefficient

The values of the interval of evaluation of regression coefficients in the regression model is adopted for the significance level of  $\alpha=0,05$  are shown in Table 6.

Table 6. Confidence interval of the regression coefficients

	$\hat{b}_j - t_{\alpha,n-k} \sigma_{\hat{b}_j}$	$\hat{b}_j$	$\hat{b}_j + t_{\alpha,n-k} \sigma_{\hat{b}_j}$
$b_1=$	4,6043	6,7713	8,9382
$b_2=$	0,7359	2,9029	5,0698
$b_3=$	14,4189	16,5859	18,7528
$b_{12}=$	-28,8807	-18,2825	-7,6843
$b_{13}=$	-48,2910	-37,6928	-27,0946
$b_{23}=$	-48,6776	-38,0794	-27,4812
$b_{123}=$	1,3232	59,9695	118,6158

### 8. GRAPHIC INTERPRETATION OF MATHEMATICAL MODEL

There is a lot of software for drawing diagrams in a ternary system. However, for our own research needs arising from the cooperation of Mechanical Engineering in Kraljevo and the Technical Faculty in Kosovska Mitrovica, the regression analysis for the three-component system and procedure for obtaining triangular surface plot and respective 2D contour plot of triangular

system were developed using MATLAB 2008b software package.

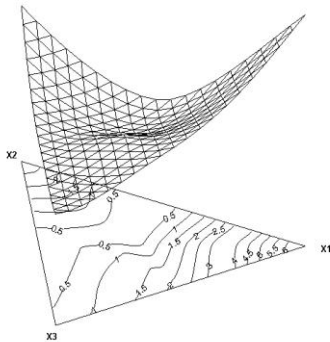


Fig. 3. 3D triangular graph of dependence of the electrical conductivity of the mole fraction of Ga-Sb-Zn

The mathematical model of the dependence electrical conductivity (in MS/m) of the mole fraction of Ga-Sb-Zn, i.e. from selected parameters X1, X2 and X3 defined by equation (13) is graphically represented with surface triangular graph and its corresponding 2D contour graph in Fig. 3 and Fig. 4.

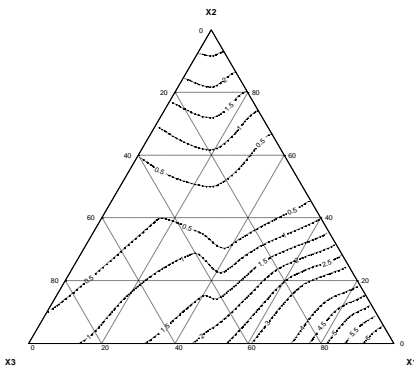


Fig. 4. 2D contour graph of dependence of the electrical conductivity of the mole fraction of Ga-Sb-Zn

The possibility of obtaining such a graphic display allows easy interpretation of the observed features of the dependence of the dependent variables in the ternary system.

## 9. CONCLUSION

In the process of exploring of electrical and mechanical properties of alloys, three-component systems play an important role. Regression analysis provides an opportunity to obtain

theoretical dependence of the size of the mole fraction of individual components of the mixture. To obtain an adequate regression model, it is necessary to implement the presented methodology.

Application of computers provides the ability to analyze several possible regression models and select one that is the best for description of a given phenomenon. Being that this is a multi-dimensional problem, it is of great importance to visually display the results with graphic diagrams. The advantage of a triangular diagram (Ternary graph) is that it can be visualize five dimension problems with the categorized Ternary graph.

## 10. ACKNOWLEDGEMENTS

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