Bulgarian Chemical Communications, Volume 50, Special Issue G (pp. 187 - 196) 2018

Mathematical modelling concerning the influence of chemical composition upon hardness of cadmium telluride crystal
- Part 2-

T. L. Severin*, A. Potorac, C. Dulucheanu, L. Irimescu

University Stefan cel Mare, Suceava, Faculty of Mechanical Engineering, Mechatronics and Management, Department of Mechanics and Technologies, 13 University St., 720229 Suceava, Romania

Cadmium telluride is an alloy with semiconductor properties and is currently the basic material for manufacturing photovoltaic cells. This material has been studied in the literature only in terms of properties defining characteristics of semiconductors, without presenting any data concerning the influence of micro-alloying elements upon hardness values. The mathematical model developed in this paper is aimed to determine hardness of cadmium telluride crystals depending on the chemical composition and expresses the hardness values of cadmium telluride crystal, depending on the micro-alloying elements. In order to establish a link between the micro alloying elements and cadmium telluride crystal hardness, experimental researches were carried out using ablation laser equipment UP213 New Wave Research, coupled to ICP-MS 750 Agilent, respectively Martens method for hardness measuring with hardness testing device Shimadzu DUH-211S. By applying the mathematical model developed, the calculated hardness values correspond within the predetermined limits with the hardness values determined experimentally by the Martens method. From the theoretical and experimental researches, it appears that the hardness of crystals of cadmium tellurium, an important mechanical characteristic in the subsequent mechanical processing of their shape and dimensions, can be predicted with a probability of 95%, using the mathematical model presented in this paper, starting from the concentrations of micro alloying elements.

Keywords: hardness, laser ablation, alloy, hardness tester, cadmium telluride

INTRODUCTION

"Cadmium telluride is an alloy with semiconductor properties, obtained through melting in special furnaces tellurium and cadmium semimetals and is currently the base material for manufacturing photovoltaic cells. Furthermore, through micro-alloying (crystal doping) with mercury, the base material for high performance infrared detectors used in spectrometry and remote sensing is manufactured, whereas through micro-alloying with zinc is obtained the base material for manufacturing Röntgen and Gamma detectors [2,3].

Cadmium telluride is characterized through a crystal, hence fragile structure. In the process of manufacturing large areas solar panels, the cadmium telluride, as base material, should provide corresponding mechanical characteristics depending on operating conditions. That is why a thorough study and an advanced characterization of the mechanical behavior of cadmium telluride crystal could be extremely useful.

The paper proposes a mathematical model which provides the hardness values of cadmium telluride crystal depending on the micro alloying elements. This material has been studied in the literature only in terms of defining the properties of semiconductor properties [4, 5, 6, 7, 8], without presenting any data concerning the influence of micro-alloying elements upon hardness values. That is why, providing a model and, consequently, having the possibility to predict the mechanical behavior and especially the hardness of cadmium telluride is of the last importance for practical issues depending on operating particularities [1].

EQUIPMENT USED FOR THE ACQUISITION OF EXPERIMENTAL DATA

"LA-ICP-MS technique is particularly useful for in situ samples analyzes, that is, for applications that require understanding of elementary spatial variation for the sample. Laser ablation (*LA*) coupled to an ICP-MS equipment (mass spectrometry with inductively coupled plasma) may perform direct analysis on almost all materials.

This technology was used in determining the composition of cadmium telluride crystal, by the instrumentality of a LA model UP213 of New Wave Research Company, coupled with a model Agilent 7500 ICP-MS, Agilent Technologies, from the laboratory of Instrumental Analysis of the Faculty of Food Engineering, University of Suceava Romania (Fig.1). The UP 213 (213 nm laser ablation) releases atomic vapors of the material absorbed in the ICP MS to quantitatively determine its elements.

* To whom all correspondence should be sent:
severin.traian@fim.usv.ro

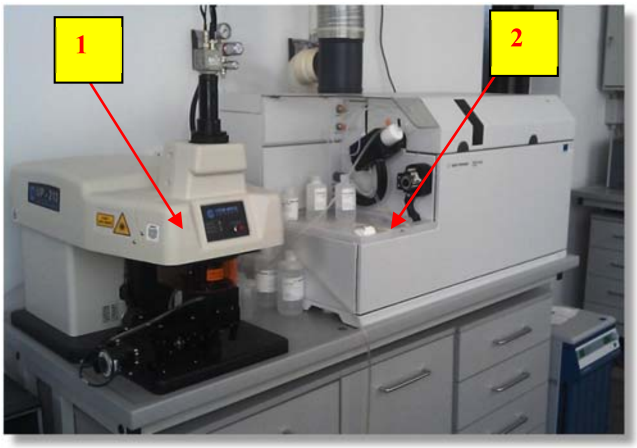

Fig.1. Laser ablation system UP-213 New Wave (1) – ICP-MS Agilent 7500 (2)

The UP series of laser ablation equipment manufactured by New Wave Research Company is specially designed to work with *ICP-MS* and *ICP-OE* systems. The *YAG* laser of *UP213* ablation equipment is operating in *213 nm UV* region, Fig.2" [1]. The Ablation zone on surface *CdTe* crystal after a qualitative and quantitative analysis performed with NewWave UP213 spectrometer coupled to an Agilent 7500 ICP-MS; laser continuously 10Hz rate, scan speed 10 µm/s, working energy 0.721 mJ, channel length 1 mm.

Using ICP MS type spectroscopy to study hardness allows highlighting the influence of micro alloying elements traces upon the hardness.

Micro hardness of cadmium telluride crystal was investigated and evaluated using the Shimadzu DUH-211S micro hardness tester, and three micro-indentation were made in each area on the crystal (Fig.2) [1].

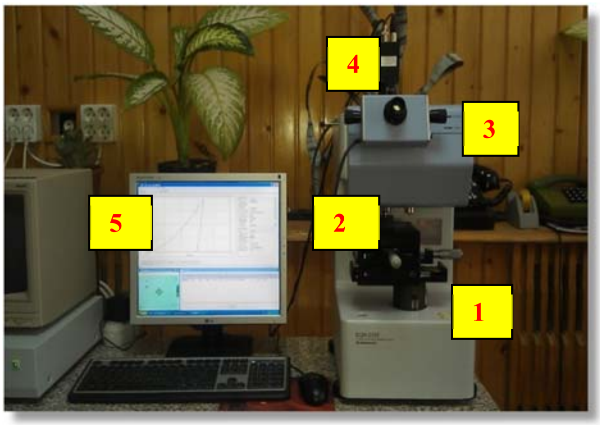

Fig.2. Shimadzu DUH-211S micro hardness tester (1), sample manual positioning system (2), footprint optical viewing system (3) image pickup video system CCD (4), hardness measurement and footprint inspection software (5) [1]

RESULTS

In this experimental research, cadmium telluride single crystal has the composition, concentrations of components and mechanical characteristics consistent with those presented in Tab.1 and determined by ICP-MS-LA technique. Moreover, the research was focused also on the distribution of the segregation of chemical elements of micro alloying with respect to the geometrical position of a point down the axis of the crystal, distribution enabling further correlation of the composition and concentration with the semiconductor, mechanical and thermal properties of cadmium telluride. To this end cadmium telluride crystal was mechanically cut lengthwise and on the symmetry axis have been marked distances of 5 mm on 5 mm (17 areas) [1].

The analysis of the distribution of micro alloying elements of cadmium telluride crystal was extended to all ten chemical elements, whose average concentration (mean concentrations of all the seventeen measurement areas) is shown in Tab. 1. Determination of the crystal hardness (HMV) depending on the micro alloying elements for the 17 analyzed areas was instrumented through the Martens method for determining hardness, using an automatic hardness testing device Shimadzu DUH-211S (Tab.1) [1].

Checking the homogeneity of hardness values variances for cadmium telluride crystal was performed using Bartlett Test and finally verifying χ^2_B which should obey to the law χ^2 with *k-1* degrees of freedom [1]. The decision according to the results shown in Article part 1 Tab. 3 with respect to checking the homogeneity of variance for hardness values recorded for the *CdTe* crystal, should be accepted as: $\chi^2_{B-calculated}$ = **(17,68)** < $\chi^2_{B-table}$ **(27,58)**. Consequently, it was clear that using Bartlett test, the results concerning the influence of micro alloying elements upon the hardness obtained for cadmium telluride crystal is confirmed by 95% confidence level.

Micro alloying elements identified and considered for mathematical model are expressed in parts per billion (*ppb*): vanadium (*ppb*) (x_1), chromium (*ppb*) (x_2), cobalt (*ppb*) (x_3), nickel (*ppb*) (x_4), copper (*ppb*) (x_5), zinc (*ppb*) (x_6), tin (*ppb*) (x_7), tungsten (*ppb*) (x_8), thallium (*ppb*) (x_9), lead (*ppb*) (x_{10}), (Tab. 2), for the target function the values of the hardness of the crystal *HMV=Z* are considered (Tab. 2). In order to elaborate the empirical model of the investigated process we used the programming of the experiment in the factorial space, moving from the real values of the influence factors to the coded equivalent values.

In Tab. 2, after encoding the concentrations of the influence factors used in order to develop the mathematical model, the minimum values of the components are represented with -1 (the lower level of the range), maximum values with +1 (the upper level of the interval), whereas the arithmetic mean of the minimum and maximum values is the 0 level of the interval.

The choice of the mathematical model

In order to obtain the mathematical model of prediction of hardness according to the microalloying elements, it was started from an order 1 polynomial (rel. 1), explaining the behavior of the studied system, [12].

$$Z = b_0 + \sum_{i=1}^{k} b_i \, x_i \qquad (1)$$

where Z represents the value of the hardness response for each experiment, b_0 represents the intersection term and b_i represents the terms of the linear coefficient.

Table 1. Influencing factors for developing the mathematical model used for *CdTe* crystal

No.	Elements / Exp. no.	x_1 (ppb)	x_2 (ppb)	x_3 (ppb)	x_4 (ppb)	x_5 (ppb)	x_6 (ppb)	x_7 (ppb)	x_8 (ppb)	x_9 (ppb)	x_{10} (ppb)	HMV (N/mm^2)
1.	Area 0	120	334	29	37	31	5100	3,4	46	0,21	0,57	**697**
2.	Area 1	120	250	28	36	30	3800	3,8	33	0,21	0,51	**681**
3.	Area 2	130	220	27	33	33	2500	3,9	25	0,18	0,35	**679**
4.	Area 3	150	210	25	25	35	1800	5	19	0,19	0,41	**674**
5.	Area 4	154	180	24	25	36	1660	9,5	17	0,21	0,37	**667**
6.	Area 5	154	168	24	24	37	1610	9,4	18	0,22	0,44	**663**
7.	Area 6	159	165	25	24	38	1590	8,6	20	0,2	0,45	**662**
8.	Area 7	161	163	24	24	40	1580	9,2	18	0,25	0,43	**661**
9.	Area 8	161	155	24	23	42	1570	9,6	17	0,17	0,54	**660**
10.	Area 9	168	148	25	22	44	1550	9,6	20	0,16	0,42	**657**
11.	Area 10	170	134	26	21	48	1420	9,5	17	0,2	0,41	**649**
12.	Area 11	171	132	25	20	49	1419	9,5	15	0,15	0,46	**649**
13.	Area 12	173	129	25	19	50	1411	9,4	13	0,19	0,71	**644**
14.	Area 13	180	127	24	19	53	1405	9,4	12	0,16	0,57	**640**
15.	Area 14	220	125	24	19	58	1400	9,3	11	0,18	0,44	**639**
16.	Area 15	221	125	23	18	60	1398	9,2	11	0,18	0,33	**638**
17.	Area 16	229	124	22	18	61	1398	9,4	11	0,14	0,47	**635**

Table 2. Coding the influence factors used to develop the mathematical model for *CdTe* crystal

Nr crt	Elements / Exp. no.	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	HMV (N/mm^2)
1.	Area 0	-1	1	1	1	-0,935	1	-1	1	0,272	0,263	**697**
2.	Area 1	-1	0,2	0,714	0,894	-1	0,297	-0,871	0,257	0,272	-0,052	**681**
3.	Area 2	-0,816	-0,085	0,428	0,578	-0,806	-0,404	-0,838	-0,2	-0,272	-0,894	**679**
4.	Area 3	-0,449	-0,181	-0,142	-0,263	-0,677	-0,782	-0,483	-0,542	-0,090	-0,578	**674**
5.	Area 4	-0,376	-0,466	-0,428	-0,263	-0,612	-0,858	0,967	-0,657	0,272	-0,789	**667**
6.	Area 5	-0,376	-0,581	-0,428	-0,368	-0,548	-0,885	0,935	-0,6	0,454	-0,421	**663**
7.	Area 6	-0,284	-0,609	-0,142	-0,368	-0,483	-0,896	0,677	-0,485	0,090	-0,368	**662**
8.	Area 7	-0,247	-0,628	-0,428	-0,368	-0,354	-0,901	0,871	-0,6	1	-0,473	**661**
9.	Area 8	-0,247	-0,704	-0,428	-0,473	-0,225	-0,907	1	-0,657	-0,454	0,105	**660**
10.	Area 9	-0,119	-0,771	-0,142	-0,578	-0,096	-0,917	1	-0,485	-0,636	-0,526	**657**
11.	Area 10	-0,082	-0,904	0,142	-0,684	0,161	-0,988	0,967	-0,657	0,090	-0,578	**649**
12.	Area 11	-0,064	-0,923	-0,142	-0,789	0,225	-0,988	0,967	-0,771	-0,818	-0,315	**649**
13	Area 12	-0,027	-0,952	-0,142	-0,8947	0,290	-0,993	0,935	-0,885	-0,090	1	**644**
14	Area 13	0,101	-0,971	-0,428	-0,8947	0,483	-0,996	0,935	-0,942	-0,636	0,263	**640**
15	Area 14	0,834	-0,990	-0,428	-0,8947	0,806	-0,998	0,903	-1	-0,272	-0,421	**639**
16	Area 15	0,853	-0,990	-0,714	-1	0,935	-1	0,871	-1	-0,272	-1	**638**
17	Area 16	1	-1	-1	-1	1	-1	0,935	-1	-1	-0,263	**635**

The experimental domains and levels of independent variables (x_1, x_2,…,x_{11}), used to obtain the prediction model of cadmium tellurium crystals, depending on the micro alloying elements are shown in Tab. 3.

The regression coefficients of the empirical model are calculated using Eq.(2) [12, 13, 14].

$$B = (X^T \cdot X)^{-1} \cdot X^T \cdot Y \qquad (2)$$

where B represents matrix regression coefficients, X is the matrix of the encoded variables, X^T is transposed to the matrix X, Y is the matrix of the response values.

Table 3. Experimental domain and levels of independent variables

Independent variable	Code	The level of the variables			Domain
		-1	0	+1	Δ = 2
V, (ppb)	x_1	120	174,5	229	109
Cr, (ppb)	x_2	124	229	334	210
Co, (ppb)	x_3	22	25,5	29	7
Ni, (ppb)	x_4	18	27,5	37	19
Cu, (ppb)	x_5	30	45,5	61	31
Zn, (ppb)	x_6	1398	3249	5100	3702
Sn, (ppb)	x_7	3,4	6,5	9,6	6,2
W, (ppb)	x_8	11	28,5	46	35
Tl, (ppb)	x_9	0,14	0,195	0,25	0,11
Pb, (ppb)	x_{10}	0,33	0,52	0,71	0,38

For the calculation of the coefficient b_0, the following equations, that is Eq.(3), (4), (5) are used and where b, b_0 represent intercept term [12, 13]

$$b_0 = b_0' - \sum_{i=1}^{k} b_{ii} \left(\frac{\sum_{u=1}^{N} x_{i\,u}^2}{N}\right)$$
$$b'_0 = \frac{\sum_{u=1}^{N} x_{0_u} y_u}{\sum_{u=1}^{N} x^2{}_{0_u}} \qquad (3)$$

Calculation of coefficients for simple effects (b_i)

$$b_i = \frac{\sum_{u=1}^{N} x_{i_u} y_u}{\sum_{u=1}^{N} x^2{}_{i_u}} \qquad (4)$$

Calculating coefficients for interaction effects (b_{ij})

$$b_{ij} = \frac{\sum_{u=1}^{N} x_{i_u} x_{j_u} y_u}{\sum_{u=1}^{N} (x_{i_u} x_{j_u})} \qquad (5)$$

where the total number of experiments is $N = 17$. Thus, the values of polynomial coefficients calculated with the above equations are presented in Tab. 4.

Table 4. Polynomial coefficient values

b_0	b_1	b_2	b_3	b_4	b_5
665,6381	-9,1569	3,9332	-9,7158	-0,0005	-8,1460
b_6	b_7	b_8	b_9	b_{10}	
-6,0448	-4,5125	21,0411	-0,1321	-2,1940	

Therefore, the mathematical model has the expression according to the Eq.(1), where the response function Z has the form:

$$Z = 665{,}6380 - 9{,}1568x_1 + 3{,}9331x_2 - 9{,}7158x_3 + 0{,}0005x_4 - 8{,}14603x_5 - 6{,}0448x_6 - 4{,}5124x_7 + 21{,}0410x_8 - 0{,}1321x_9 - 2{,}1939x_{10} \qquad (6)$$

Testing the significance of the mathematical model

The significance of coefficients of the regression model is tested by comparing the absolute value of the coefficients b_i with the confidence interval calculated with the Eq.7 (Student test).

Coefficients have significant effects if the condition presented in equation 8 is met:

$$\Delta b_i = t_{\alpha;N} \cdot S_{bi} \qquad (7)$$

$$|b_i| \geq |\Delta b_i| \qquad (8)$$

The calculation of the Student test for the mathematical model presented in Eq.7 used the following parameters:

$N = 17$ (number of degrees of freedom - experiences) (9)

$\alpha = 0{,}05$ (threshold of significance) (10)

$t_{0,05;17} = 2{,}110$ (Student test value) [13] (11)

$S^2 = 7{,}5294$ (data reproducibility dispersion) (12)

S_{bi}- average square deviation for the coefficient b_{ij}

The confidence intervals of the coefficients are shown in Tab. 5.

Table 5. Confidence intervals for the mathematical model

Δb_0	Δb_1	Δb_2	Δb_3	Δb_4	Δb_5
0,312	0,312	0,312	0,312	0,312	0,312
Δb_6	Δb_7	Δb_8	Δb_9	Δb_{10}	
0,312	0,312	0,312	0,312	0,312	

Table 6. Significant coefficients of the mathematical model

b_0	b_1	b_2	b_3	b_4	b_5
665,638	-9,156	3,933	-9,715	**0**	-8,146
b_6	b_7	b_8	b_9	b_{10}	
-6,044	-4,512	21,041	**0**	-2,193	

Since the terms x_4 and x_9 do not meet the condition, they were eliminated (Tab. 6), and the predictive mathematical model of prediction of crystal hardness of the analyzed cadmium telluride becomes according to Eq.(13).

$$\mathbf{Z} = 665{,}6380 - 9{,}1568x_1 + 3{,}9331x_2 - 9{,}7158x_3 - 8{,}14603x_5 - 6{,}0448x_6 - 4{,}5124x_7 + 21{,}0410\, x_8 - 2{,}1939x_{10} \quad (13)$$

Testing the adequacy of the mathematical model

The Fisher test is used to test the adequacy of the model [12,14].

The Fisher test was performed for a confidence level of $\alpha=0{,}05$ and for the degrees of freedom $v_1 = 8$ and $v_2 = 10$. The value of the Fisher test calculated ($F_c=0{,}8068$) was compared to the Fischer tabulated score ($F_{T(v1,\, v2)}= 2{,}42$).

Because $F_c<F_T$, the mathematical model obtained is appropriate and can be used in optimization processes.

The following chart shows a comparison of analysed crystal hardness values obtained experimentally (blue columns) with those calculated using the regression model (red columns) Eq.(13.).

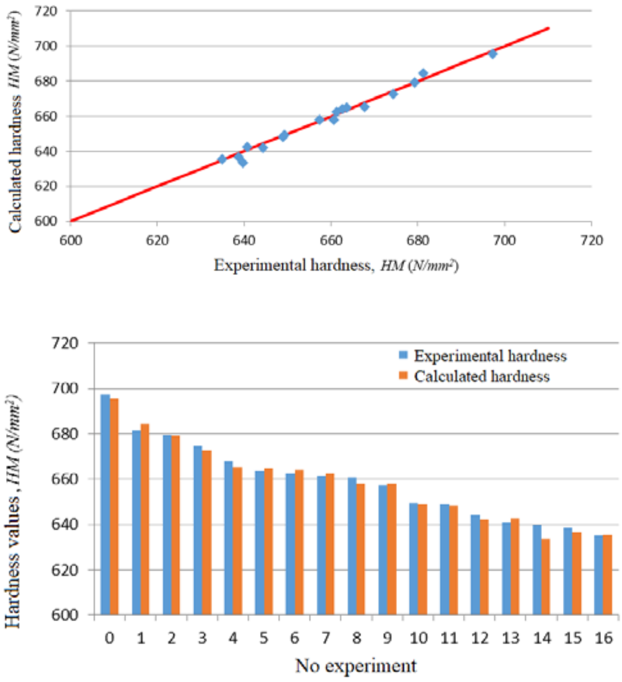

Fig.3. Comparison of the hardness values of the crystal of cadmium telluride obtained experimentally with those calculated using the regression model

Analysing the graphs from Fig.3, one can see a deviation below *5%* of the hardness values obtained with the experimental mathematical model against the values obtained by experimental measurements with the *DUH-211S* Shimadzu.

These small differences demonstrate that the mathematical model can be used to predict the hardness of crystals of cadmium tellurium with the concentrations of the micro-alloying elements contained in the fields presented in Tab. 3.

Micro-alloying elements influence on cadmium telluride crystal hardness using a mathematical model proposed

In this subchapter are presented some of the graphs that represent the influence of the alloying elements on the crystal hardness of the cadmium tellurium.

Fig.4 shows the influences of vanadium and chromium concentrations on the hardness of cadmium telluride crystal. The value *+1* of hardness on graph is the maximum encoded value of hardness *678,73 HM* for the cadmium tellurium crystal, whose *V* composition has been modified between *120 ppb* and *229 ppb* and *Cr* in the range *124-334 ppb*.

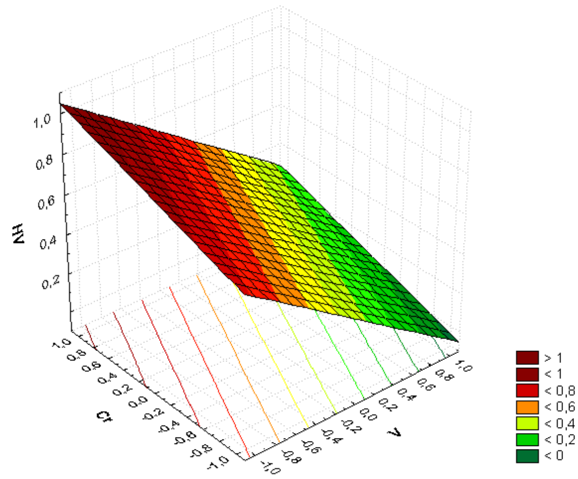

Fig.4. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *V* and *Cr*

The value *0* of hardness is the minimum encoded value of hardness *652,55 HM* for the cadmium tellurium crystal, whose *V* composition has been modified between *120 ppb* and *229 ppb* and the *Cr* in the range *124-334 ppb*.

The graph of variation of crystal hardness was represented by coding with *-1 V* content of *120 ppb* (minimum interval value), and with *+1* V content of *229 ppb* (maximum interval value), for the *Cr* content the value of *-1* is corresponding to *124 ppb* (minimum interval value) and *+1* to 334 *ppb* (maximum interval value).

According to the graph in Fig.4 the crystal hardness increases linearly with the increase of the content of *Cr* and decreases when increasing concentration of *V*. Maximum hardness values are obtained for the maximum content of *Cr* (*334 ppb*) and to minimum content of *V* (*120 ppb*).

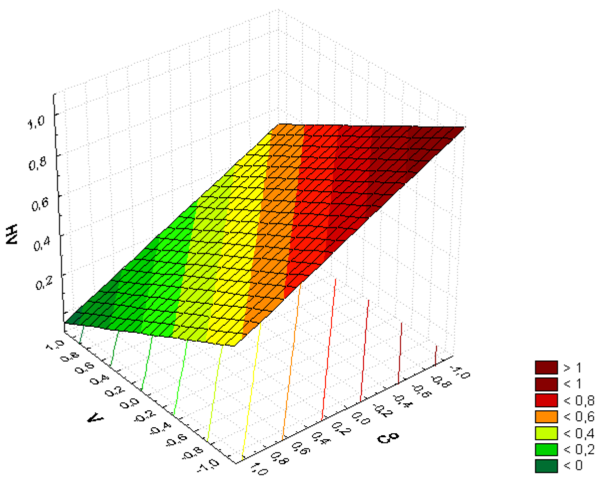

Fig.5. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *V* and *Co*

By graphical representation of the regression model (Fig.5), the hardness of the crystal decreases with the increase of the content of *V* and *Co*. Maximum values of crystal hardness are obtained for the minimum content of *V* (*120 ppb*) and *Co* (*22 ppb*).

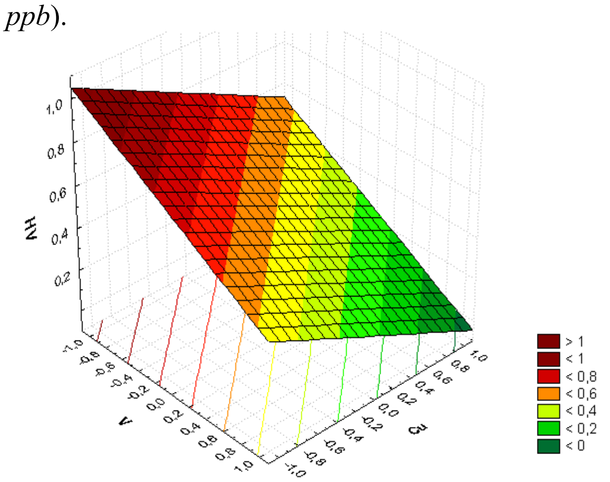

Fig.6. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *V* and *Cu*

In the representation of Fig.6, the hardness of the crystal is negatively influenced by the increase of the *V* content, respectively, of *Cu*. The maximum values of the crystal hardness are obtained for the minimum values of the *V* content *(120 ppb)* and *Cu* (*30 ppb*).

According to the graph in Fig.7, the hardness of the crystal decreases when increasing *Zn* and *V* concentration. The maximum values of the crystal hardness are obtained for the minimum *Zn* content (*1398 ppb*) and *V* (*120 ppb*).

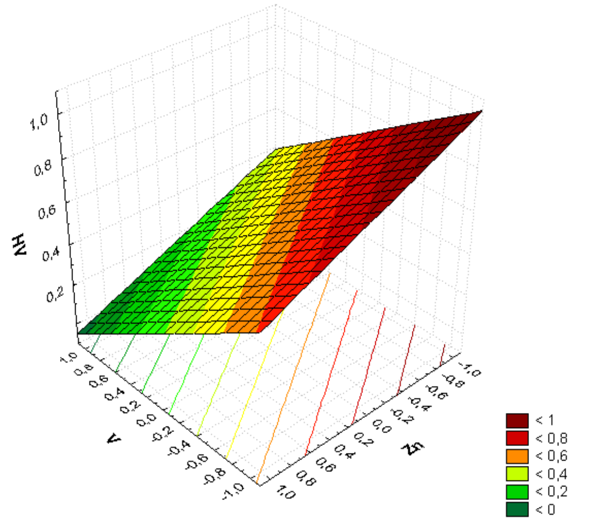

Fig.7. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *V* and *Zn*

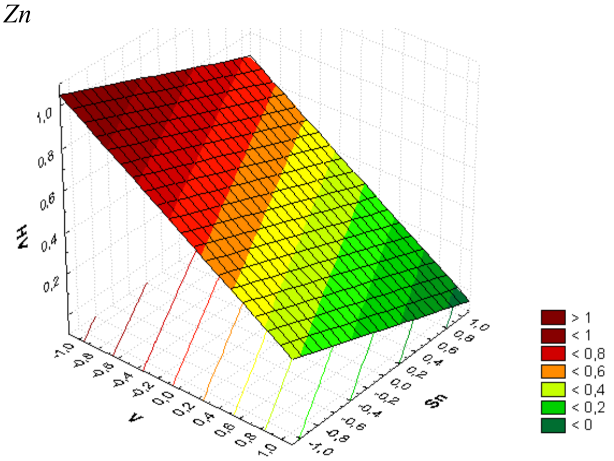

Fig.8. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *V* and *Sn*

In the situation presented in Fig.8, the hardness of the crystal increases less significantly when decreasing the concentration of *Sn* and more pronounced when increasing concentration of *V*. The maximum values of the crystal hardness are obtained for the minimum values of the *Sn* content (*3,4 ppb*) respectively of the *V* content (*120 ppb*).

In Fig.9 the value of crystal hardness increases sharply as the percentage of tungsten increases and decreases when increasing concentration of *V*. Maximum crystalline hardness values are obtained for the minimum content of *V* (*120 ppb*) and maximum *W* values (46 *ppb*).

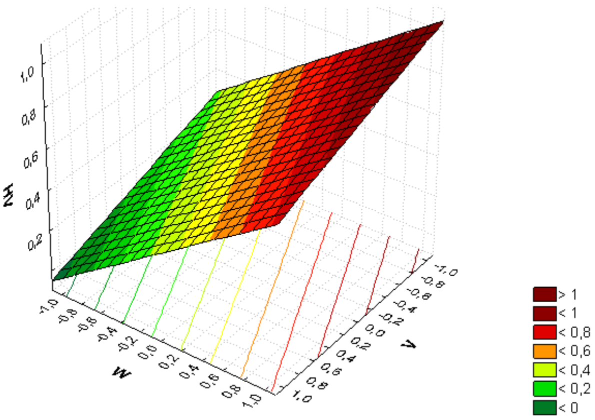

Fig.9. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *V* and *W*

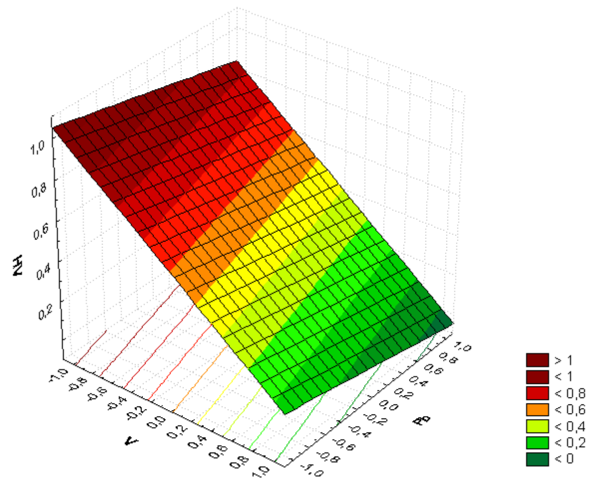

Fig.10. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *V* and *Pb*

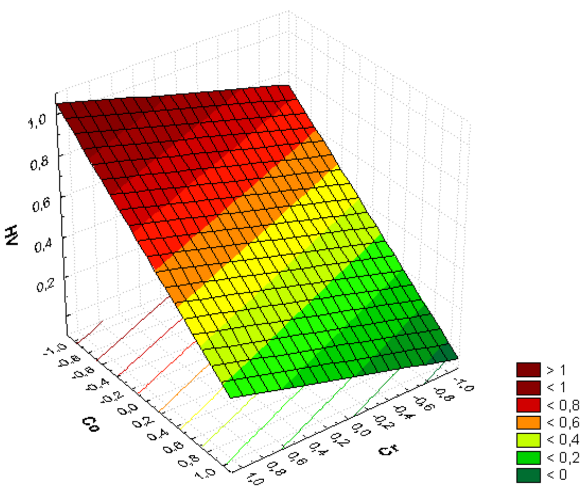

Fig.11. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Cr* and *Co*.

Not the same situation is presented in Fig.10 where maximum crystal hardness values are obtained at the minimum contents of *V* (120 ppb) respectively of *Pb* (0,33 ppb).

By graphical representation of the regression model Fig.11, the hardness of the crystal increases with the increase in the content of *Cr* and decreases more pronouncedly when increasing concentration of *Co*. The maximum values of the crystal hardness are obtained for the maximum values of the *Cr* content (*334 ppb*) and minimum *Co* values (*22 ppb*).

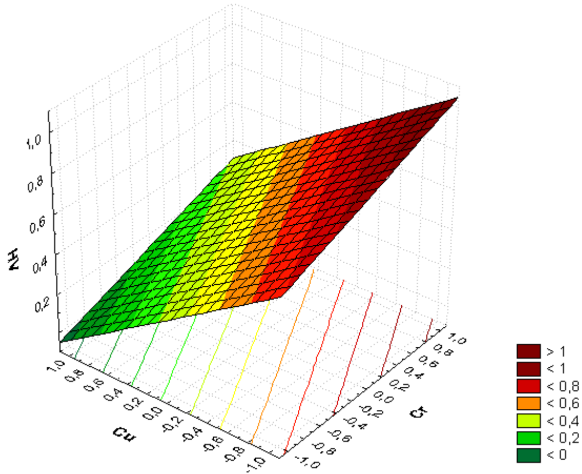

Fig.12. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Cr* and *Cu*.

In Fig.12 the hardness of the crystal increases with the increase of *Cr* content and decreases sharply with the increase of *Cu* concentration. Maximum crystalline hardness values are obtained for the maximum *Cr* content (*334 ppb*) and at minimum *Cu* values (*30 ppb*).

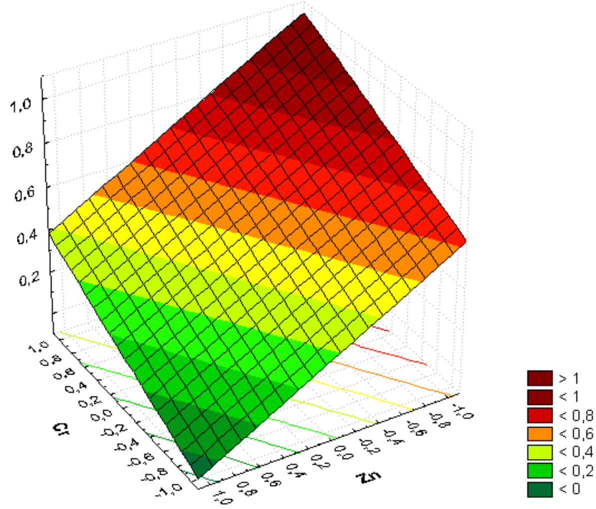

Fig.13. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Cr* and *Zn*.

According to the graphical representation in Fig.13, the hardness of the crystal increases with the increase of the *Cr* concentration and decreases with the increase of the *Zn* content. Maximum crystalline hardness values are obtained at the maximum *Cr* content (*334 ppb*) and at low Zn concentrations (*1398 ppb*).

In Fig.14, the hardness of the crystal increases with the increase of *Cr* concentration and increases sharply with the increase of the percentage of *W*.

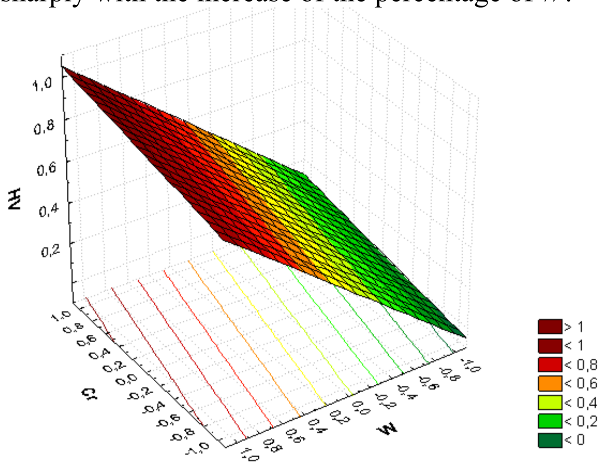

Fig.14. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Cr* and *W*

Maximum crystalline hardness values are obtained at the maximum *Cr* content (*334 ppb*) and *W* (*46 ppb*).

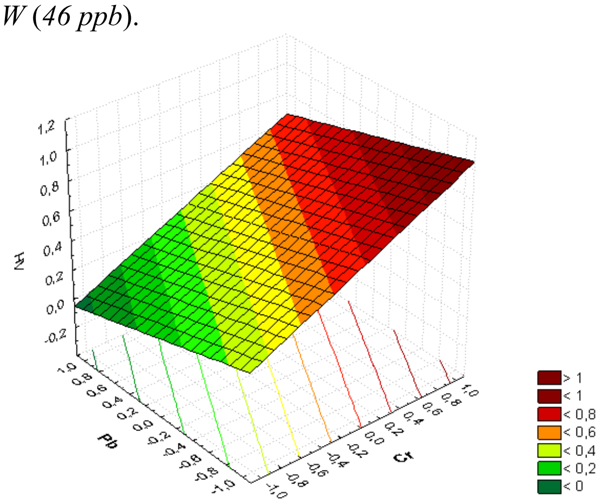

Fig.15. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Cr* and *Pb*

The hardness of the crystal of cadmium tellurium increases with the increase in *Cr* content and decreases with the growth of *Pb*. Maximum hardness values are obtained at the maximum *Cr* content (334 ppb) and at minimum *Pb* values (0,33 ppb) (Fig.15).

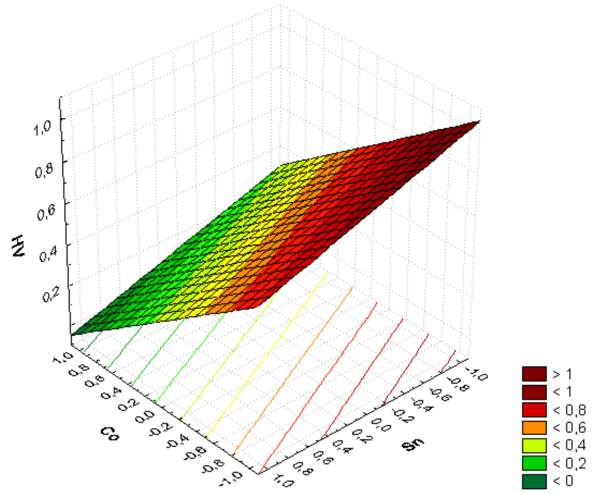

Fig.16. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Co* and *Sn*

Fig.16 shows the decrease of the crystal hardness value with the increase of the content of *Co* and *Sn*. Maximum crystalline hardness values are obtained at the minimum *Co* content (*22 ppb*) and *Sn* (*3,4 ppb*).

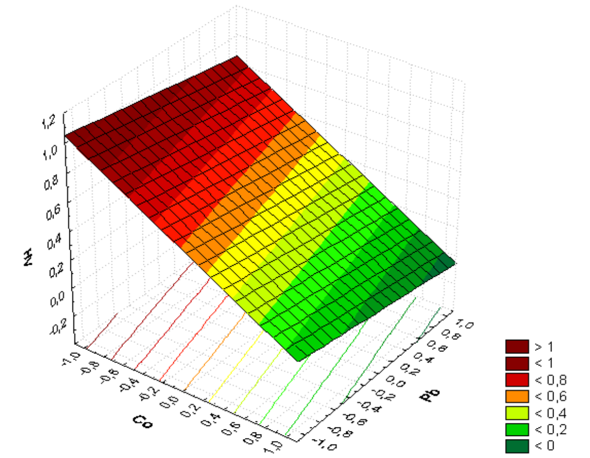

Fig.17. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Co* and *Pb*

The hardness of the crystal of cadmium is decreasing with the increase in *Pb* content and even more pronouncedly with the increase of the percentage of *Co*. Maximum crystalline hardness values are obtained at the minimum *Co* content (22 ppb) and *Pb* (0,33 ppb) (Fig.17).

According to the representation in Fig.18, the hardness of the crystal decreases with the increase of *Cu* and *Zn* concentration. Maximum crystalline hardness values are obtained at the minimum content of *Cu* (*30 ppb*) respectively of *Zn* (*1398 ppb*).

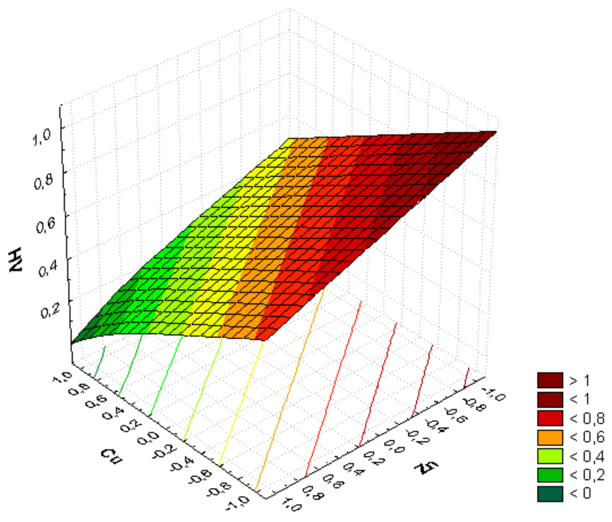

Fig.18. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Cu* and *Zn.*

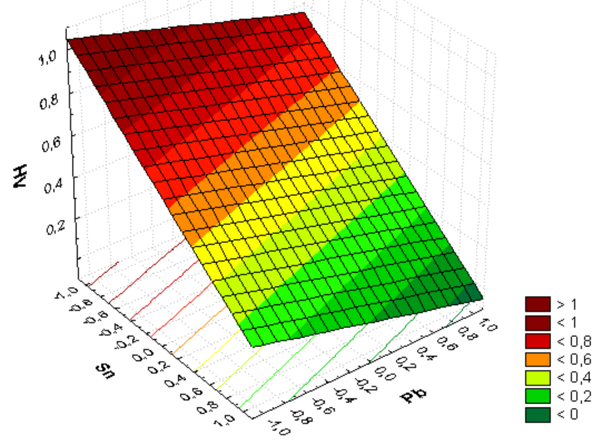

Fig.19. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *Sn* and *Pb.*

From the analysis of the obtained graph Fig.19, it turns out that the crystal hardness decreases when increasing the *Sn* content and decreases less sensitively with the *Pb*. The maximum values of the crystal hardness are obtained at the minimum values of the *Sn* content (*3,4 ppb*) respectively *Pb* (*0,33 ppb*).

The Fig. 20 highlights the sharp increase in crystal hardness with increased tungsten concentration and a less sensitive decrease in hardness when increasing lead percentage. Thus, the maximum hardness of the crystal is recorded at the maximum value of the tungsten concentration (*46 ppb)* and minimal of the lead (*0,33 ppb*).

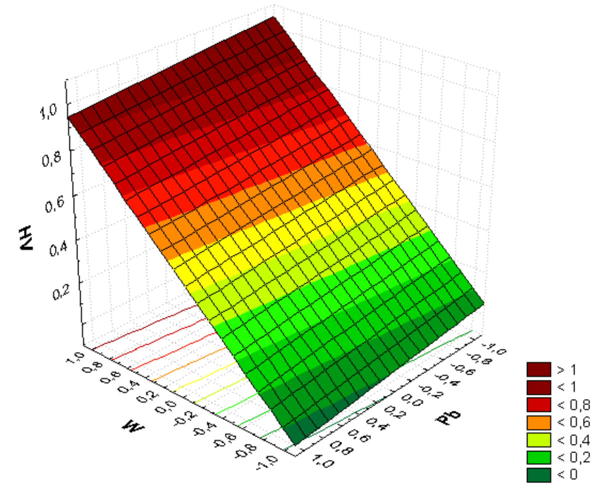

Fig.20. Variation of *Cd-Te* crystal hardness obtained using regression model based on the interaction of *W* and *Pb.*

CONCLUSIONS

In order to establish a link between the micro alloying elements and cadmium telluride crystal hardness experimental researches were carried out using ablation laser equipment UP213 New Wave Research, coupled to ICP-MS 750 Agilent, respectively Martens method for hardness measuring with hardness testing device Shimadzu DUH-211S. The significance of mathematical model coefficients was determined using the Student test, whereas mathematical model adequacy testing was performed using the Fisher test.

The mathematical model for the expression of hardness by micro alloying elements is a linear linkage.

By applying the mathematical model obtained, the calculated hardness values correspond within the predetermined limits with the hardness values determined experimentally by the Martens method.

The micro alloying elements that influence the hardness of the cadmium tellurium crystal are *V, Cr, Co, Cu, Zn, Sn, W, Pb*, whereas *Ni, T1* does not significantly affect hardness.

The results obtained from the theoretical research on cadmium tellurium crystal hardness using the developed mathematical model were plotted according to the concentration of micro alloying elements. The analysis of these surfaces highlights the sharp increase in crystal hardness with the increase in *Cr* and *W* content and drops with *V, Co, Cu, Zn, Sn, Pb.*

From the theoretical and experimental researches, it appears that the hardness of crystals of cadmium tellurium, an important mechanical characteristic in the subsequent mechanical processing of their shape and dimensions, can be predicted with a probability of 95% using the mathematical model presented in this paper, starting from the concentrations of micro alloying elements.

ACKNOWLEDGEMENTS

Financial support from the POSCCE project "Centru integrat de cercetare, dezvoltare si inovare pentru materiale Avansate, Nanotehnologii si Sisteme distribuite de fabricatie si control (MANSiD)", Contract No. 671/09.04.2015 is acknowledged.

REFERENCES

[1] **Severin, T.L., Potorac A.** Mathematical modelling concerning the influence of chemical composition upon hardness of cadmium telluride crystal - Part 1. *Bulgarian Chemical Communications*, **48 E**, 378-383 (2016).

[2] **Capper, P.** Properties of narrow gap cadmium-based compounds, IET. p. 39-40, ISBN 978-0-85296-880-2, (2012).

[3] **Brewer, P.D., Zinck, J.J., Olson, G.L.**, Surface composition changes and ablation dynamics in excimer laser irradiated CdTe Laser ablation for materials synthesis, *Book Series, Materials Research Society Symposium Proceedings*, 68-70, (1990).

[4] **Fochuk, P.; Nykonyuk, Ye, Verzhak, Ye, Dopant** content and thermal treatment of CdZnTe in effects on point-defect structures, *IEEE Nuclear Science Symposium and Medical Imaging Conference (2008 NSS/MIC),* **1-9**, 4880-4882, (2009).

[5] **Fochuk, P., Grill, R. Kopach, O**., Elimination of Te inclusions in Cd1-xZnxTe crystals by short-term thermal annealing, *IEEE Transactions on Nuclear Science*, **59** (2), 258-260 (2012).

[6] **Rzeszutek, J., Oszmaldowski, M., Savchuk, V,** Ablation of CdTe with 100 pulses from Nd:YAG laser: Velocity distribution of emitted particles, Nuclear Instruments & Methods in Physics Research Section B-beam Interactions with Materials and Atoms, **266**, Issue 21, 4766-4774, (2008).

[7] **Savchuk, Victor K.; Kotlyarchuk, Bohdan K.; Zaginey, Apollinary O.** Ablation species generated by high power laser pulses from Cd-Te target, 70091M, *Proceedings of the Society of Photo-Optical Instrumentation Engineers (SPIE)* **7009**, M91-M91 (2008).

[8] **Semaltianos, N. G., Logothetidis, S., Perrie, W.,** CdTe nanoparticles synthesized by laser ablation, *Applied Physics Letters*, **95** (3), no. 033302 (2009).

[9] **Gutt, S., Gutt, G., Severin, T. L., Vasilache, V., Poroch, M.,** Contribution to design and carry out an universal dynamic hardness tester for metalic materials testing, Annals of DAAAM for 2010 & *Proc. of 21st International Symposium*, ISBN 978-3-901509-73-5, ISSN 1726-9679, 0506, Vienna, Austria, (2010).

[10] **Iacob, D.,** Statistica, Ed. Universitatii Stefan cel Mare Suceava, ISBN 973-9408-57-5, p.114-132, (2000).

[11] **Bulgaru, M., Bolboaca, L.,** Ingineria calitatii. Mangementul calitatii, statistica si control, masurari în *3D*, Ed. Alma Mater, ISBN 973-85153-0-0, Cluj-Napoca, p.188-209, (2001).

[12] **Macoveanu, M., Nicu V., Curievici I.,** Bazele tehnologiei chimice, metodologia elaborarii modelelor matematice din industria chimica, Ed. IPI, Iasi, România, (1991).

[13] **Cuceriu, I.,** Optimizari in industria chimica, Ed. Didactica si Pedagogica, Bucuresti, p. 67-82, (1990).

[14] **Severin T. L.,** Cercetari si contributii la realizarea si promovarea de noi metode si aparate pentru încercarea de duritate, teza de doctorat, Research and contributions to the development and promotion of new methods and devices for hardness testing, (2012).