ACADEMIA ROMÂNĂ
Revue Roumaine de Chimie
http://web.icf.ro/rrch/

Rev. Roum. Chim.,
2012, *57*(4-5), 369-381

Dedicated to Professor Ionel Haiduc on the occasion of his 75th anniversary

NEW INSIGHTS IN PHYSICAL PROPERTIES PREDICTION OF INDIUM BASED SOLID SOLUTION BY EXPERIMENTAL AND ARTIFICIAL INTELLIGENCE TECHNIQUES

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Received January 31, 2012

In order to discover new n-type or p-type transparent conductors numerous investigations have been carried out recently on transparent conducting oxides materials. Our work presents a new $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$ solid solutions prepared by solid-state reactions. Many expensive experiments for optical diffuse reflectance and electrical resistivity were realised to characterise this solid solution. To reduce the time and costs of future researches in order to improve or to obtain new transparent conducting oxides, predictions of new properties based on experimental measurements are important factors. To achieve this goal the paper implements ideas of artificial intelligence based on support vector machine in a minimax approach. The implemented procedure, named minimax decision procedure involving a link between artificial intelligence and material science, is able to predict particular variables, properties or trends. In a comparative manner, the paper presents the performance of the procedure with some established regression techniques.

INTRODUCTION

Due to significant advances in the field of electronic and optical properties of materials, and recently in the discovery of novel functionalities in display technologies, transparent conducting oxides (TCOs) have become an important topic in view of future applications. Although scientific investigations have produced basic knowledge of the underlying phenomena many problems still remain unsolved, where quantitative deterministic characterization or theoretical approaches are dismally lacking or are cumbersome. In the last years transparent conducting oxides have become an important topic in the field of optoelectronics and numerous investigations have been carried out recently on these materials, in order to discover new n-type or p-type transparent conductors. Besides the famous ITO indium-rich oxide, which crystallizes with the bixbyite structure, another oxide was identified for the composition $In_4Sn_3O_{12}$ with M_7O_{12} type structure. Introduction of antimony in the M_7O_{12} structure and the existence of a positive effect on the electrical conductivity have been previously demonstrated. Sb^{5+} can be introduced without difficulty into M_7O_{12} structure of $In_4Sn_3O_{12}$ until the formation of the antimonate $In_{5.5}Sb_{1.5}O_{12}$.[1] We know that the stability of M_7O_{12} structure of $In_{4+x}Sn_{3-2x}Sb_xO_{12}$ solid solution is strongly affected as the antimony content increases, leading in fact to its transformation into a bixbyite type structure. The electrical conductivity appears to benefit from the introduction of Sb^{5+}. Taking into account the existence of tungstate In_6WO_{12} previously reported [2-4] which shows the significant stabilizing effect due to the introduction of W^{6+} in a M_7O_{12} structure, we are interested in the problem of formation a solid solution

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between $In_{5.5}Sb_{1.5}O_{12}$ and In_6WO_{12}, implementing the fully compensated cationic substitution: $3Sb^{5+} \rightarrow In^{3+} + 2W^{6+}$. Mathematical or empirical models of fundamental phenomena are crosscutting area that promises major contribution to improve the quality of products or to develop new insights. Although scientific achievements on materials have supplied basic knowledge of the underlying phenomena, there remain many problems where theoretical treatments are cumbersome or dismally lacking. At the same time laboratory experiments and measurements to verify or to establish properties of solid solution are cumbersome, expansive and time consuming. Recent developments in the field of artificial intelligence can improve the investigations in this domain. Artificial intelligence procedures are capable of replicating a lot of variety of non-linear relationships of considerable complexity between the studied variables and have the ability to investigate new phenomenon cases where the information cannot be easily accessed theoretically or explicitly relational physics. Also these procedures can be used to examine the effect of any individual input on the output parameter, whereas this may be cumbersome and difficult or expensive to do experimentally. In the last years artificial intelligence techniques have been used to solve various problems from material science domain.[5-8] In order to reduce the number of laboratory experiments or to avoid cumbersome theoretically developments the present work implements a novel procedure based on artificial intelligence. The main advantage of the procedure is that if once an efficient predictive model is built then it can be successfully used to predict on any novel compounds of the same type. The procedure is able to predict new optical and electrical properties of a new indium based solid solution using a reasonable numbers of known experimental data. Therefore the procedure can reduce the time and costs of research and improve the study for new transparent conducting oxides. The procedure named minimax decision procedure is based on support vector machine in a minimax approach. Support vector machine (*SVM*) that is primarily a two-class classifier based on statistical learning theory was introduced by Vapnik, 1995,[9] and studied by many others.[9-13] Some important advantages of the support vector machine over other artificial intelligence techniques as artificial neural network are: (a) it makes no prior assumptions concerning the data distribution and does not assume normality of the data, as it is a non-parametric classifier, (b) provides better accuracy even with a small number of training samples, fast and simple in implementation, (c) avoids the specific problems such as over-fitting and local minima. A major drawback of the support vector machine consists in simple assessment of the same covariance for each class and thus the margin should be defined in a local way. Support vector machine in a minimax approach (*MSVM*) is a relative novelty research topic developed after 2002.[14-16] Some proved advantages of the support vector machine in minimax approach over basic support vector machine: (a) avoids the drawback of *SVM* consisting in the simple assessment of the same covariance for each class and defining the margin in a local way, (b) unlike *SVM*, for which the closest points to the decision boundary are most important, the minimax approach looks at the margin between the means of classes, (c) provides an explicit direct upper bound on the probability of misclassification of new data, without making any specific distribution assumptions and (d) obtains explicit decision boundaries based on available data. However, as with *SVM*, *MSVM* is computationally relatively expensive and requires extensive manually or cross validation experiments to choose functions and parameters that give good performance. *MSVM* presents many merits however little attention has been paid to apply *MSVM* in material science applications. Today we are unaware of others similar approaches related to this domain. Finally the paper presents a comparatively predictive study between a robust regression technique and our minimax decission procedure. For simplicity the study is reduced to predictions of new optical and electrical properties for indium based solid solution using existing experiments and experimental data. The results based on the developed procedure compared with new experimental measurements indicate a good agreement with experimental data. At the same time the results point out the ability of minimax decision procedure for predictive assessments in transparent conducting oxides systems and reveal the potential of minimax decision procedure in others engineering applications.

EXPERIMENTAL

1. Synthesis, homogeneity range and structure calculation

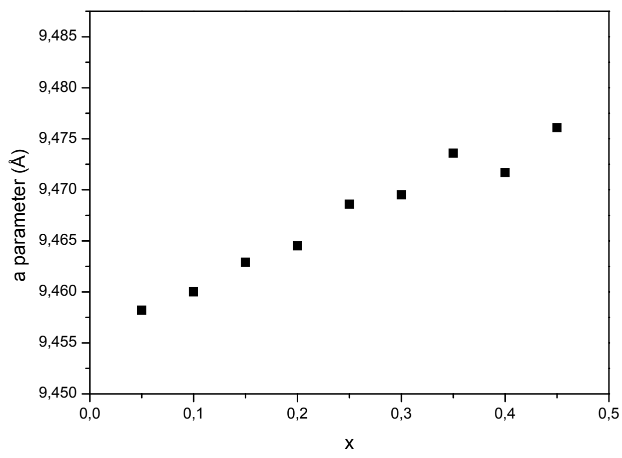
$In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$ solid solutions were prepared by solid-state reactions from mixtures of pure In_2O_3, SnO_2, WO_3 and Sb_2O_3 powdered oxides in alumina crucibles heated in air. After an initial heating at 600°C in order to ensure the full oxidation of Sb(III) into Sb(V), successive 12h annealing followed by air quenching were performed. In the case of $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$ solid solution the presence of Sb^{5+} greatly facilitates the formation of M_7O_{12} structure to the point that a final temperature of 1200 °C is sufficient to obtain a total reaction of precursors. Since this temperature is not enough to ensure a correct sintering of samples prepared for electrical resistivity measurements, we decided to systematically perform an additional annealing at 1300 °C. According to this experimental procedure, pure phases corresponding to the entire range of solid solution $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$ (composition: $0 \leq x \leq 0.45$) were isolated. The parameters (*a* and *c*) and volume (*V*) of the hexagonal cell were calculated and considered in their dependence on *x*. Fig. 1 presents the corresponding variation of the hexagonal cell constants versus *x*.

According to the experimental procedure described above, nine compositions of solid solution $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$ were obtained. The X-ray diffractograms were recorded on a Panalytical X'Pert diffractometer (Co Kα1 radiation) equipped with an X'Celerator detector, in the angular range 6-120º, 2θ. Their diffractogrammes are all very similar and also isotypic to $In_{5.5}Sb_{1.5}O_{12}$ confirming the existence of a complete homogeneity range of this solid solution (composition: $0 \leq x \leq 0.45$). In order to prove the stability and truthfully of solid solution described above structure calculations have been performed by Rietveld analysis of diffractogrammes in a series of nine compositions. As an example, Fig. 2 presents calculated and observed diffractograms for the composition x = 0.2, $In_{5.7}W_{0.4}Sb_{0.9}O_{12}$, prepared at 1300°C.

2. Physical properties measurements

Experiments for optical diffuse reflectance spectra (%R(a.u.)) for nine compositions (*x*) of $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$ solid solution registered with a double beam spectrophotometer (double beam Cary Varian 100 Scan spectrophotometer) show that the optical bandgap is shifted to higher energies with the introduction of W^{6+}. This increase becomes significant for values of $x \geq 0.4$ (80 cm^{-1}) and it is accompanied by strong increase of the maximum percentage reflectance (Fig. 3). Clearly the optical characteristics of TCOs are altered from the higher contents in W^{6+} (composition $x \geq 0.4$).

Electrical resistivity (ρ) measurements on pellets treated at 1300 °C in air were carried out by the four-probe method in the range of 5-320K, using a PPMS device. Fig. 4 includes the ρ = f (T) curves of the nine compositions of solid solution $In_{5,5+x}Sb_{1,5-3x}W_{2x}O_{12}$. An overall increase of electrical resistivity of the solid solution $In_{5,5+x}Sb_{1,5-3x}W_{2x}O_{12}$ as antimony content decreases, more specifically as Sb (V) is replaced by the pair 2/3 W (VI) + 1/3 In (III), was observed.



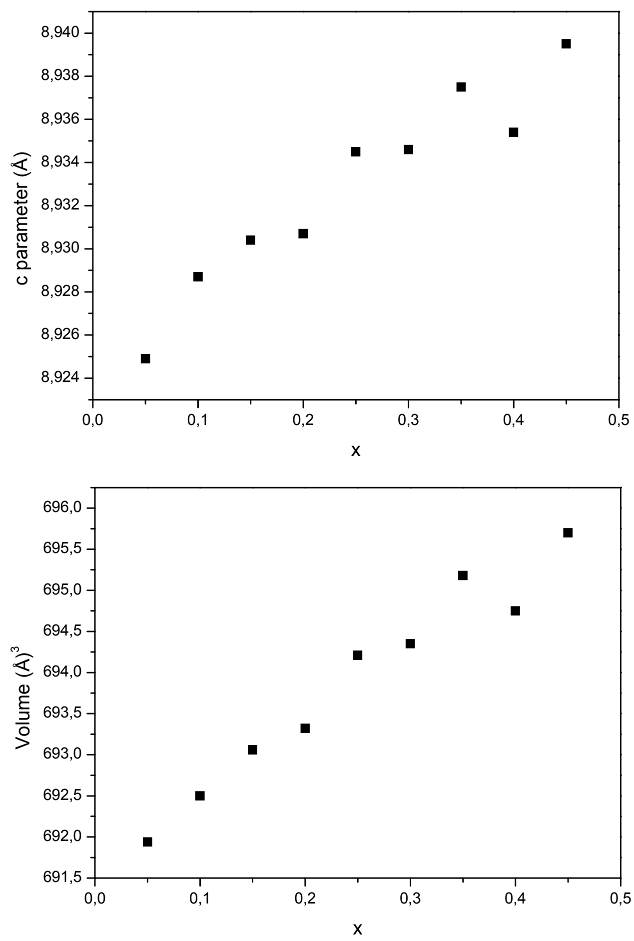


Fig. 1 – Variation of the hexagonal cell constants in the solid solution $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$ (after heating at 1300°C).

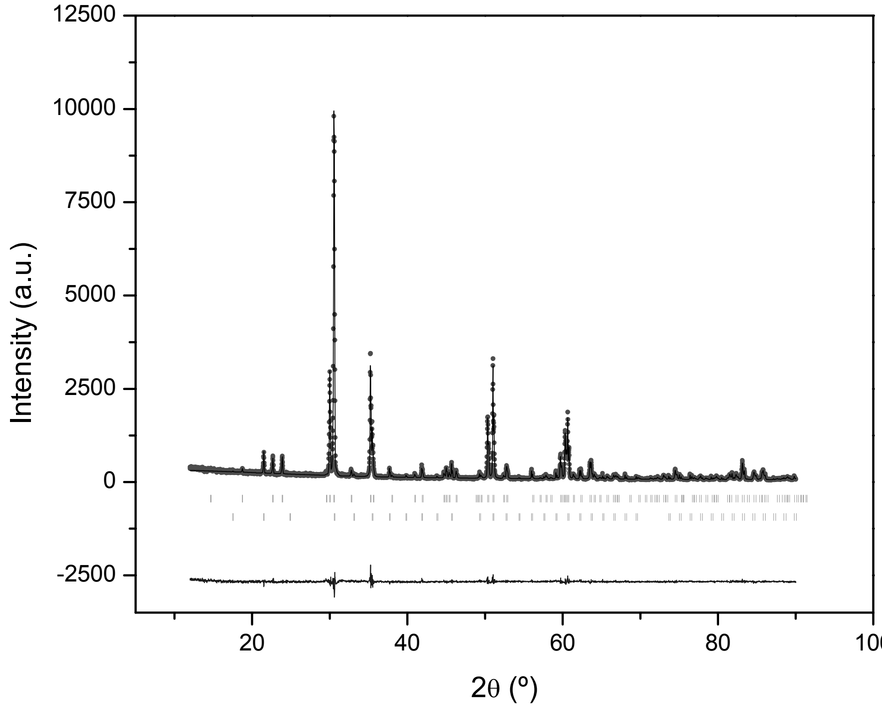


Fig. 2 – Observed (dots), calculated (lines) and difference XRPD pattern of $In_{5.7}Sb_{0.9}W_{0.4}O_{12}$ treated at 1300°C. Vertical bars indicate the positions of the reflections of the title phase (upper) and In_2O_3 (lower).

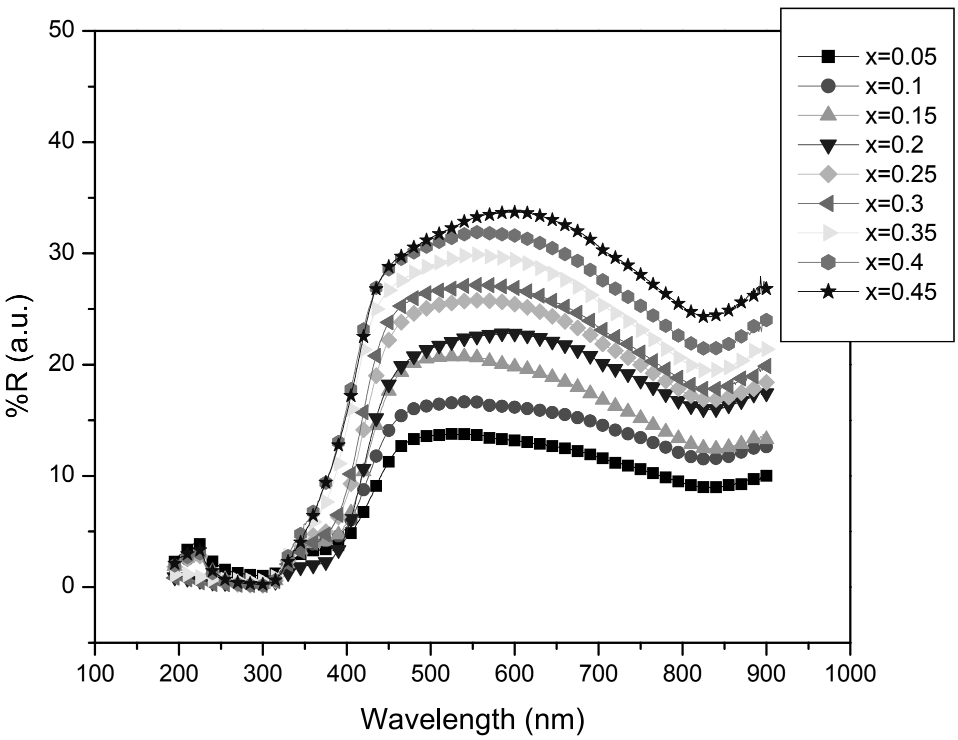


Fig. 3 – Measured optical reflectance in the compositions x =0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45 of the solid solution $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$ after 1300°C.

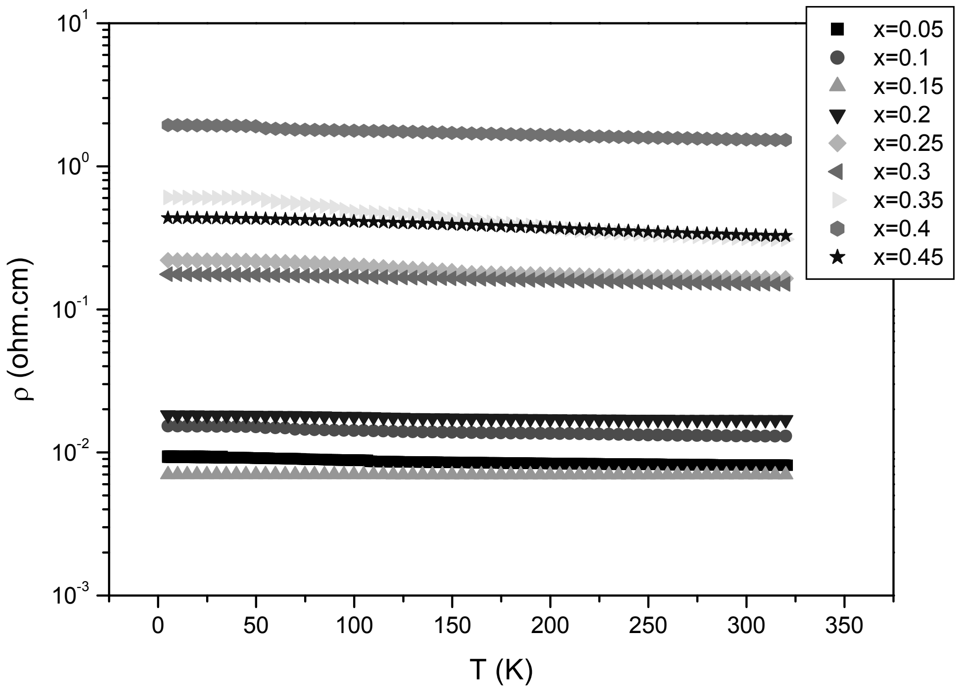


Fig. 4 – Electrical resistivity (Ω.cm) versus temperature (K) in solid solution $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$, after heating at 1300°C.

IMPLEMENTATION OF THE MINIMAX DECISION PROCEDURE

Unlike Support Vector Machines for which the closest points to the decision boundary are most important, the minimax approach named minimax probability machine[14-15] looks at the margin between the means of classes. Thus minimax classification is similar to maximum margin classification (minimising the maximum of distances between the classes) with respect to the mean of the classes, where a factor that depends on the covariance matrices of each of the classes pushes the threshold towards the class with lower covariance. Basically as was stated by Lanckriet[14] into a binary classification problem of **z** random vectors, with $\mathbf{z_1}$ and $\mathbf{z_2}$ denoting random vectors from each of two classes as $z_1 \in \text{Class 1}$ and $z_2 \in \text{Class 2}$, a hyper plane can separates these points, with maximal probability in respect to all distributions having mentioned means $\overline{z_1}, \overline{z_2}$ and covariance matrices $\sum z_1, z_2$ By kernel function $K(\mathbf{z}_i, \mathbf{z}) = \Phi(\mathbf{z}_i) \cdot \Phi(\mathbf{z})$ simply mapping data into a higher dimensional feature space through a non-linear mapping function ' Φ ', minimax probability machine can adapt them to become a non-linear classifier. In this context a kernel represents a legitimate inner product into a high dimensional space called feature space F ^{n} (that is basically a Hilbert space). It let to define a similarity measure from the dot product in F ^{n} and learning algorithm using linear algebra and analytic geometry. The basic idea is to map original d-dimensional input data points $\mathbf{Z}(z_1,..z_d) \in \mathbf{R^d}$ from real input space into a high-dimensional feature space F ^{n} through a non-linear mapping function '*Φ*' which is usually unknown. The choosing of the mapping function '*Φ*' will enable to design a large variety of learning algorithms. Into this feature space a linear classifier-surface between the two classes corresponds to a non-linear decision-hyperplane into original input space (Fig. 5). Based on the kernel formulation for minimax approach a regression model into feature space named minimax probability machine regression[15] was built as maximising the minimum probability of future predictions being within some bound of the true regression function (±ε).[15] Basically starting from some unknown regression function

$$f: R^d \rightarrow R \text{ with a general form as } \mathbf{y} = f(\mathbf{z}) + \rho \quad (1)$$

the main task is to construct an approximation for "*f*" such that

$$\text{for any } z \in R^d, \; \hat{\mathbf{y}} = \hat{f}(\mathbf{z}). \quad (2)$$

The minimax probability machine regression model will approximate this function only into feature space by nonlinear regression using the basis formulation:

$$\hat{\mathbf{y}} = \hat{f}(\mathbf{z}) = \sum_{i=1}^{N} \beta_i K(\mathbf{z}_i, \mathbf{z}) + b_k \qquad (3)$$

Here $K(\mathbf{z}_i,\mathbf{z}) = \Phi(\mathbf{z}_i)\cdot\Phi(\mathbf{z})$ in the feature space is so-called kernel function satisfying Mercer's conditions and N represents the number of learning examples (points). The others, β_i are weighting coefficients and 'b_k' offset of the minimax regression model, obtained as outputs of the minimax probability machine regression from the learning data. Generating two classes that are obtained by shifting the dependent variable ±ε the regression problem was reduce to a binary classification problem into features space (Fig. 6). The regression surface is interpreted as being the boundary that separates the two classes, successfully and wrongly predicted. The strength of this regression model comes from its ability to represent very high dimensional input space through kernel functions with great resistance to over-fitting. The resulting model is independent from the dimensionality of the input space. The nonlinear regression function eq. (3) is only a formal basis function formulation. Because $K(\mathbf{z}_i,\mathbf{z}) = \Phi(\mathbf{z}_i)\cdot\Phi(\mathbf{z})$ is done implicitly the issue is solved numerical. Thus, all computations related to '*Φ*', will be carried on by kernel function into a higher dimensional feature space. Instead of '*d*' features now '*n*' features represent inputs vectors and the kernel map evaluates at all of the other training inputs.[15] Based on these statements minimax decision procedure casts both regression (numerical values as outputs) and classification (class labels as outputs) into a global unified technique. Fundamentals principles also a basic flowchart of minimax decisions procedure and others details were previously presented.[17-19] The procedure was conducted in a crude manner, without outliers' detection and no features selection or reduction. The errors were estimated by testing rather than by calculation during the training steps (learning and testing) in order to build and estimate the model. To carry out the most basic testing method (simple testing) a random percentage of the database (10-30%) is set aside and used in testing step. To ensure a good distribution of the data in data sets and stability of the procedure the simulations was conducted based on data randomly divided into a number of distinct learning and testing subsets. The implementation was developed as a user-friendly computer application in MATLAB software environment and works in a multiple cyclic steps. This time for simplicity the performance of procedure was investigated based only on single metric criterion, the relative error between the predicted (outputs) and the corresponding test targets:

$$RE = \left(\frac{(Y_{predicted} - Y_{test})}{Y_{predicted}} \right) \times 100\ [\%]\ . \qquad (4)$$

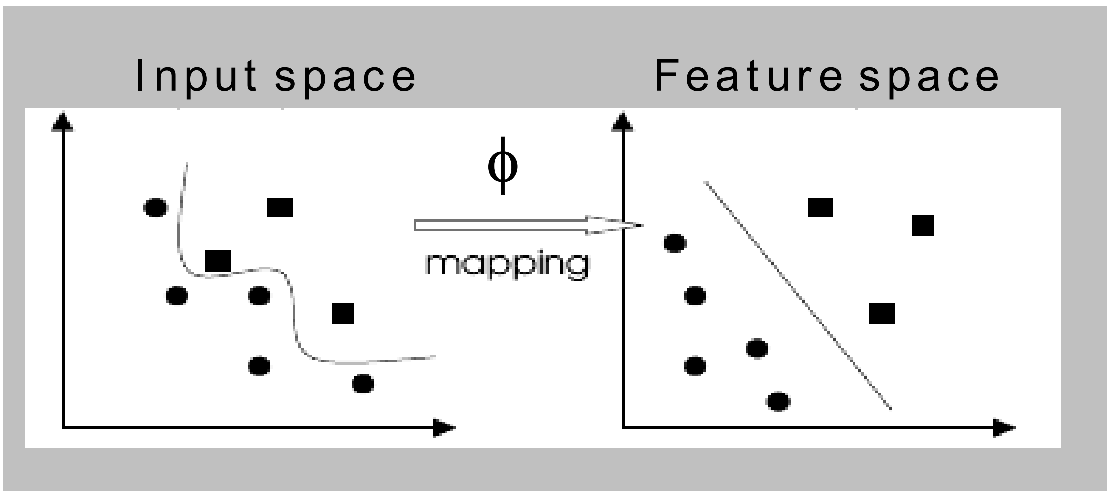


Fig. 5 – The principle of kernel map.

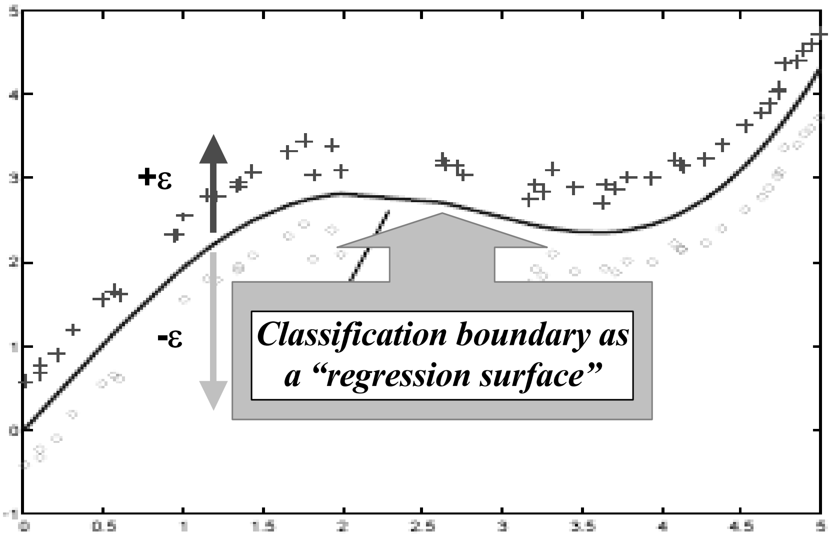


Fig. 6 – Formulating regression as a binary classification into feature space.

The performance criterions are evaluated with all values reconverted into the original real Euclidian R^d space. To obtain generalisation and robustness computer programs were coded in a convenient way to find the best models over a number of "*k*" cyclic experiments (simulations). Formally the best model means model that performs best. It involves best kernel function, kernel parameters and outputs. Basically as previously mentioned Lanckriet *et al.*[14] one typically has to choose manually or determine it by tenfold cross validation. This time we preferred a simple-empirical but heuristic principle for setting the type of the kernel function. Homogenous and inhomogeneous polynomial kernel also Gaussian radial basis function kernel were tested. The kernel type that yields to the best performance was put aside and considered for the best model. This time was a Gaussian radial basis function (Table 3-4) with standard width kernel (σ) tuned using 10-fold cross validation. The best model over these "*k*" cyclic simulations and the corresponding output values emerged from the minimax decision procedure was defined as the sample model. Long random trials ($k > 100$) do not get improved accuracy or more reliable predictions. Taking this aspect into account, it was considered appropriate to obey some statements[20,21] and to work with a reduced learning set limiting the trials to $k = \leq 100$. To avoid very different scales of variation between different inputs the data is scaled (brings the range of variation) between -0.5 ÷ +0.5. Also to ensure a good distribution of the data in every data set the data was randomised. The proper size and selection of the training set (randomly divided into learning and test subsets) is very important to produce optimal results and to increase the performance of the algorithm. So far, there are no uniquely agreed and generalised approaches to choose the suitable dimension and the selection of the training set. However, it is a commonly agreed statement that the training set must be sufficiently large compared with the number of features. In principle the procedure obey the statements.[12, 20] Subsequent to its establishment the sample model will be used for predictions on other new and unseen of the same type data set, accordingly any new targets.

RESULTS AND DISSCUSION

Data sets for numerical applications are obtained by measurements of optical diffuse reflectance related on wavelengths and electrical resistivity related on temperature. Details of database for the case studies are presented in Tables 1 and 2. Two comparative procedures, our minimax decision procedure and a robust regression technique (a Total Least Squares regression based on Principal Component Analysis) were conducted and reported to the same data sets. The applications are related to predictions of new diffuse reflectance and electrical resistivity values for mentioned compositions samples of indium-based solid solution. Experimental parameters of interests were wavelength, temperature and composition (x) of every experimental specimen. Because of relatively few variables of dependence related to measured properties we consider this robust regression technique suitable for the investigation of relationships between variables. For simplicity only the x = 0.2 sample compositions was considered for analyse and comparison with predictions. Also the performance of the application was investigated based only on the relative errors criterion Eq. (4).

Table 1

Values of experimental measured data for diffuse reflectance

Sample composition	**Optical reflectance %R [a.u.]**		
	Range	**Mean**	**Standard deviation**
Experimental parameter	Range of Wavelengths = 192÷900[nm]		
x1 = 0.05	13.7518 ÷0. 984	8.6374e	4.455
x2 = 0.1	16.6453 ÷0. 227	10.4741	5.8845
x3 = 0.15	20.7124 ÷0.288	12.2853	7.2658
x4 = 0.2	**22.8461 ÷0. 315**	**13.7726**	**8.7582**
x5 = 0.25	25.7969 ÷0. 157	15.7364	9.3717
x6 = 0.3	27.1506 ÷0. 179	16.4691	10.191
x7 = 0.35	29.9434 ÷0. 551	18.5490	10.8368
X8 = 0.4	31.9331 ÷0. 153	20.1809	11.5252
X9 = 0.45	33.7252 ÷0. 237	21.5595	12.3494

• *x* – content compositions of W^{6+} – defining sample specimen

Table 2

Values of experimental measured data for electrical resistivity

Sample composition	**Electrical resistivity [ohm.cm]**		
	Range	**Mean**	**Standard deviation**
Experimental parameter	Range of Temperature = 9.9667 ÷320[^{o}K]		
x1 = 0.05	$(8.14÷9.24)\times10^{-3}$	8.5731×10^{-3}	3.7155×10^{-4}
x2 = 0.1	$(1.3÷1.529)\times10^{-3}$	1.3911×10^{-3}	7.3821×10^{-4}
x3 = 0.15	$(6.98÷7.01)\times10^{-3}$	6.99×10^{-3}	1.0473×10^{-5}
x4 = 0.2	$\mathbf{(1.694÷1.827)\times10^{-2}}$	$\mathbf{1.7461\times10^{-2}}$	$\mathbf{4.7638\times10^{-4}}$
x5 = 0.25	$(1.646÷ 2.2018)\times10^{-1}$	1.8732×10^{-1}	2.0268×10^{-2}
x6 = 0.3	$(1.5059÷1.7603)\times10^{-1}$	1.6335×10^{-1}	8.3343×10^{-3}
x7 = 0.35	$(3.0882÷6.0503)\times10^{-1}$	4.3348×10^{-1}	1.0414×10^{-1}
X8 = 0.4	1.5285÷1.9373	1.7069	1.2855×10^{-1}
X9 = 0.45	$(3.2689÷4.3505)\times10^{-1}$	3.2689×10^{-1}	3.6662×10^{-2}

• *x* – content compositions of W^{6+} – defining sample specimen

1. Establish of sample model based on training steps

Main conditions of simulation and partial results are done in Tables 3 and 4. This time only for simplicity the performance of procedures is reported in terms of percentage relative error between the model predicted outputs and the corresponding test experimental measured. This shows the model performance in training steps. Based on these a kernel type having the form of an exponential radial basis function (Tables 3, 4) was proved to work well. Therefore the sample model was established based on this kernel type. For simplicity and for its "key point" we present model establishment and predictions related only to a single specimen of composition x = 0.2. Results are comparatively presented (Fig. 7). Differences regarding correspondences between predicted and test values (diffuse reflectance and electrical resistivity) are observed for both procedures. At first glance for diffuse reflectance, comparatively with minimax decision procedure the results of regression technique are unstable and lead to distorted predictions (Fig. 7a). It was found the percentage relative errors between -805 ÷ 55 [%]. These suggested that the robust regression technique model has poor generalisation capability.

Table 3

The main conditions and partial results of simulations for diffuse reflectance

	Minimax decission procedure	**Regression procedure**
Range of relative errors on test subset	-7.543÷ 0.464 [%] based on Fig. 7a	-805 ÷ 55 [%] based on Fig. 7a
Range of relative errors between new predictions and new experimental measurements	-0.21 ÷ 8.23 [%] based on Fig. 8	Not utilised
Wavelengths for new predictions and experimental measurements [nm]: 820, 827, 835, 842, 849, 856, 863, 871, 878, 885, 892, 899.		
Kernel functions for *minimax decision procedure*	$K(\mathbf{x}_i,\mathbf{x}_j)=exp\left(-\left\|\mathbf{x}_i-\mathbf{x}_j\right\|^2 \Big/ 2\sigma^2\right)$	

Note: predictions and analyse was related only to *x4 = 0.2* sample compositions.

Table 4

The main conditions and partial results of simulations for electrical resistivity

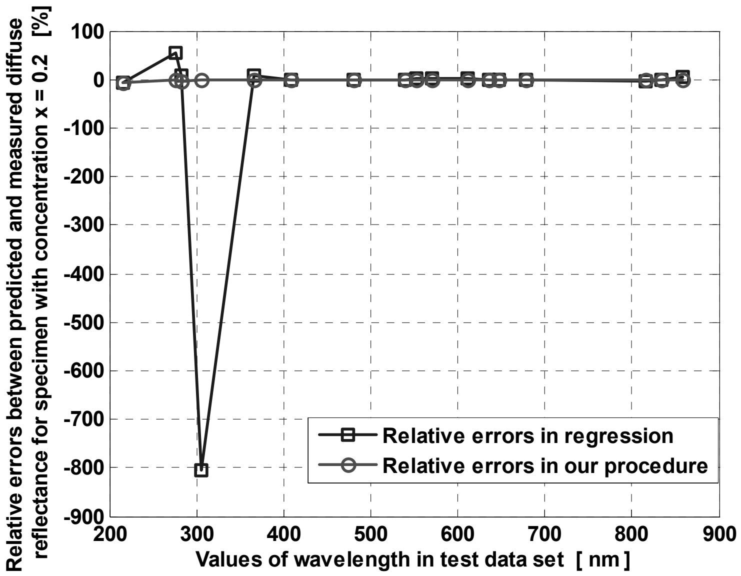
	Minimax decission procedure	**Regression procedure**
Range of relative errors on test subset	- 0.1056 ÷ 0.193 [%] based on Fig. 7b	-0.226÷ 0.317 [%] based on Fig. 7b
Range of relative errors between new predictions and new experimental measurements	-0.941÷ 5.083 [%] based on Fig.9.	-1.6÷ 6.077 [%] based on Fig. 9.
Temperature for new experimental measurements and predictions [^{o}K]: 114.8639, 134.9055, 154.9105, 174.8455, 194.9456, 214.8456, 234.8501, 254.8251, 274.8485, 294.8219, 314.7289.		
Kernel functions for *minimax decision procedure*	$K(\mathbf{x}_i,\mathbf{x}_j)=exp\left(-\left\|\mathbf{x}_i-\mathbf{x}_j\right\|^2 \Big/ 2\sigma^2\right)$	

Note: predictions and analyse was related only to *x4 = 0.2* sample compositions.

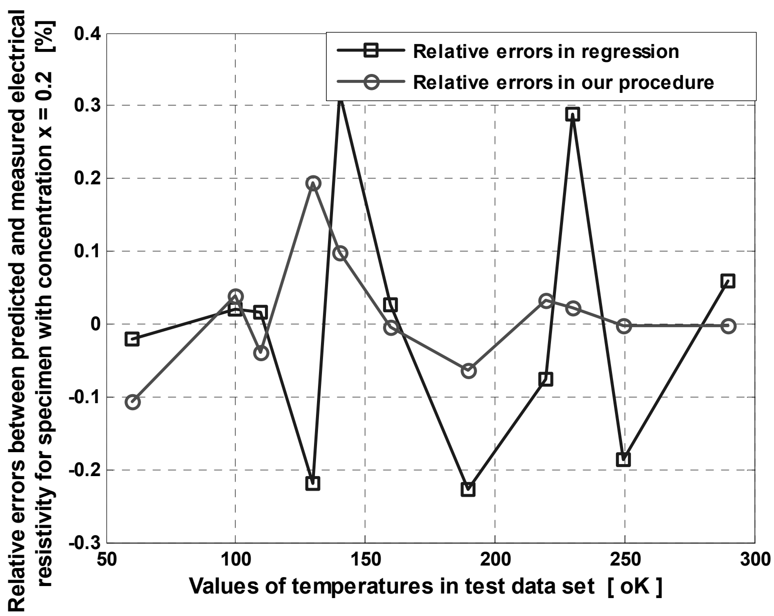
Because minimax decision procedure results' based on sample model have the percentage relative errors between -7.543 ÷ 0.464 [%] suggested that model has good generalisation capability. By this reason only minimax decision procedure was utilised into new predictions for diffuse on compounds of the same type. For electrical resistivity the results of minimax decision procedure are closed to regression technique (Fig. 7b). The percentage relative errors between -0.226 ÷ 0.317 [%] are in good agreement that suggested a good generalisation capability for both techniques. By of this reason into new predictions on compounds of the same type, for electrical resistivity both of the procedures were utilised.

2. New properties predictions of indium based solid solution

Because the procedure can be used to examine the effect of any individual input on the output parameter, based on established efficient predictive sample model new predictions of properties as optical and electrical properties of indium-based solid solution was realised. These new predictions were obtained based on two important experimental parameters: (a) wavelength for diffuse reflectance and (b) temperature for electrical properties of indium-based solid solution. These new predictions were obtained introducing in sample model a set of new unseen parameters (wavelength for diffuse reflectance and temperature for electrical properties). Comparatively new experimental measurements for optical and electrical properties at the same set of new unseen parameters were realised. The results are comparatively presented. Details of interests and some results for these new predictions are done in Tables 3 and 4. Fig. 8 presents predicted and new experimental measurements of diffuse reflectance values; also relative errors are reported. It was found that the percentage errors between new measured and predicted values are all within -0.21 ÷ 8.23 [%] which suggested that sample model has good generalisation capability. In the same manner Fig. 9 presents predicted and new experimental measured values of electrical resistivity. Range of relative errors between predictions and new experimental measurements are between -0.941 ÷ 6.077 [%]. Basically all predicted values are in good agreement with the new experimental values. At first glance, the minimax decision procedure results and the regression emerged results are in a reasonable good agreement, but the predictions obtained by the minimax decision procedure are superior to those obtained by the regression approach (Table 4 and Fig. 9). Therefore analyses based on minimax decision procedure can reduce the numbers experimental measurements and more, they can really to substitute experimental measurements with predicted values. Thus such analyses may decrease the number of experimental measurements and constitute a step in order to save time and costs in future research.

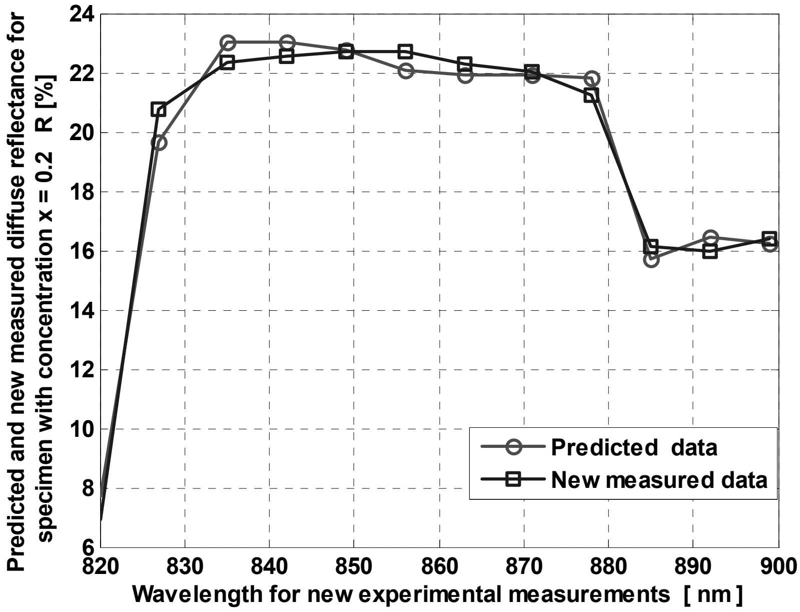


a.

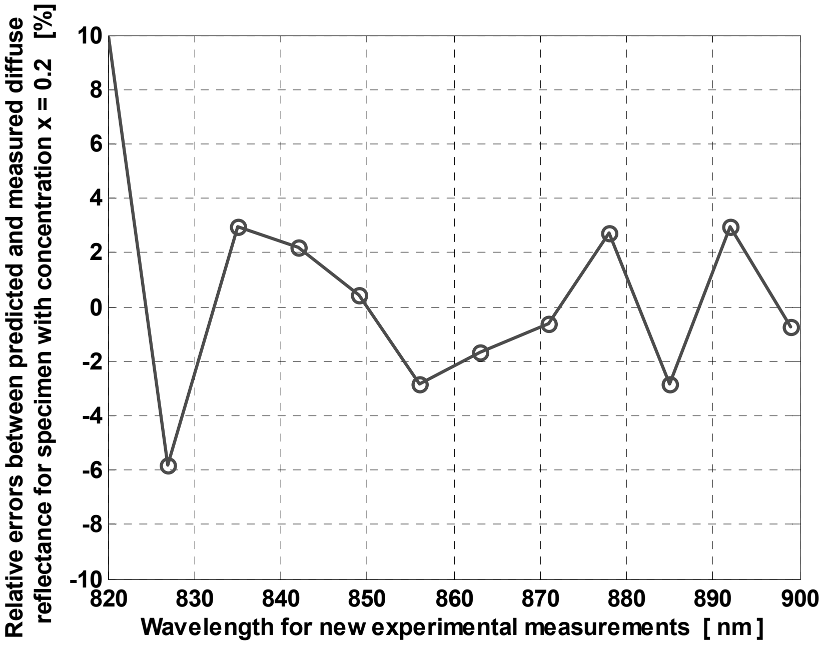


b.

Fig. 7 – Relative errors between predicted and measured diffuse reflectance values:
o Relative errors from our procedure; □ Relative errors from regression.
7a. Relative errors between predicted and measured diffuse reflectance values in test data set; **7b.** Relative errors between predicted and measured electrical resistivity values in test data set.

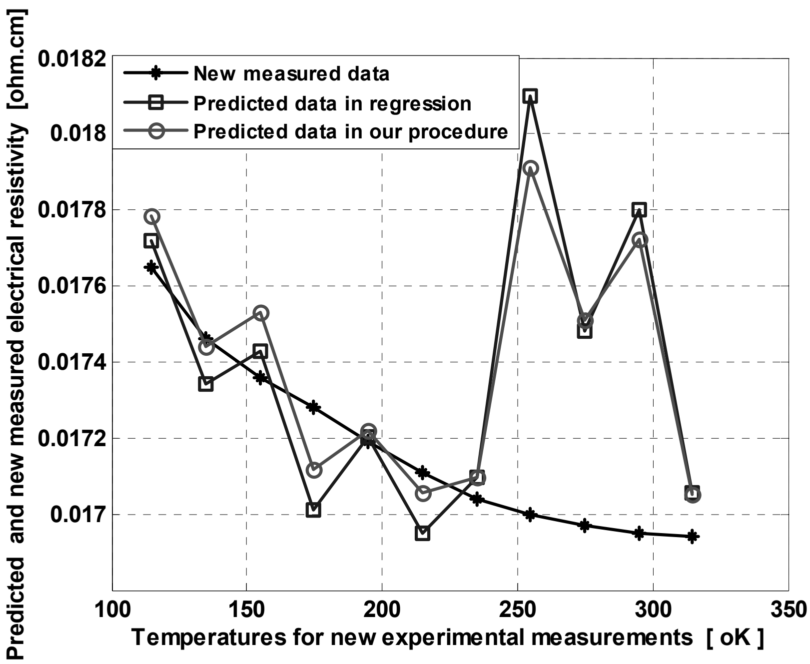


a.

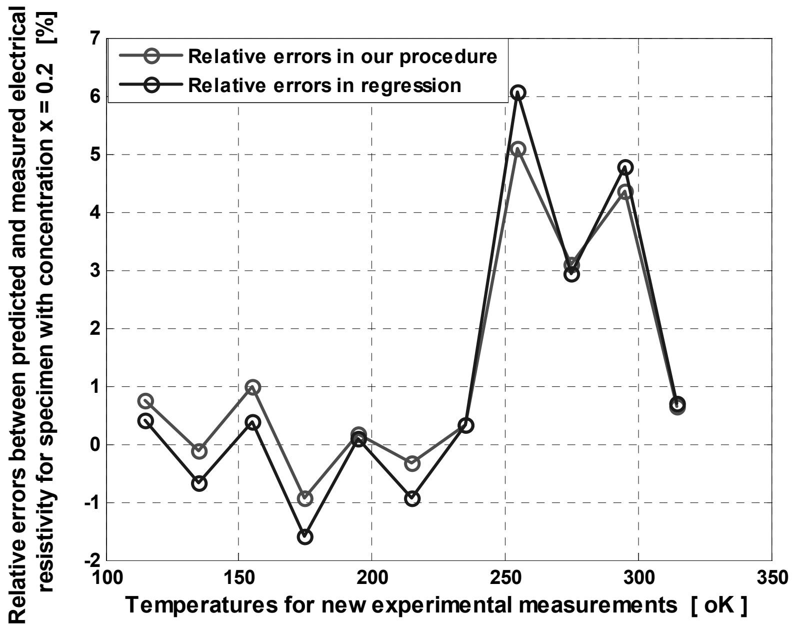


b.

Fig. 8 – Comparatively results for diffuse reflectance of specimen with concentration $x = 0.2$
o Predicted data from our procedure; □ New measured values.
8a. Predicted and new measured diffuse reflectance values; **8b.** Relative errors between predicted and new measured values.



a.



b.

Fig. 9 – Comparatively results for electrical resistivity of specimen with concentration *x = 0.2*
9a. Predicted and new measured values, ∗ New measured values; □ Predicted from regression; o Predicted from our procedure.
9b. Relative errors between predicted and new values, o Relative errors from our procedure; o Relative errors from regression.

CONCLUSIONS

Correlated predictions of properties based on experimental measurements are important factors to reduce the costs of researches in order to obtain new transparent conducting oxides. The paper implements minimax decision procedure based on support vector machine into a minimax approach developed in the MATLAB language. Numerical experiments demonstrate the capability of the proposed procedure. Instead of numerous and expensive experimental measurements the procedure is able to supply good prediction of particular variables of interest as diffuse reflectance values and electrical resistivity of solid solution $In_{5.5+x}Sb_{1.5-3x}W_{2x}O_{12}$. An important goal of the paper was to compare the performance of the procedure with a robust regression technique and to promote it as an effective technique in material science. This procedure proves to be an efficient instrument to build classification models instead of regression analysis or other cumbersome theoretical (sometimes inaccurate, simplified or incomplete) models. We may mention some advantages as: (1) the procedure works properly with a reduced training set, (2) the procedure needs relative few science-phenomena knowledge, (3) the procedure avoids cumbersome theoretical approaches. Furthermore, used with an appropriate experimental policy our framework is not limited to reduce the costs and the number of laboratory experiments. Future research will be focus on improving the properties of new transparent conducting oxides based on minimax decision procedure.

Acknoledgements: This work was possible with the financial support of the Sectoral Operational Programme for Human Resources Development 2007-2013, co-financed by the European Social Fund, under the project number POSDRU 89/1.5/S/60189 with the title "Postdoctoral Programs for Sustainable Development in a Knowledge Based Society".

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