



NEURAL NETWORKS USED FOR MODELING THE THERMAL STABILITY OF POLYDIMETHYLSILOXANE/SILICA COMPOSITES CONTAINING COMPLEXED LANTHANUM

Alexandra NISTOR,^{a,b} Gabriela LISA,^b Silvia CURTEANU,^b Angelica VLAD^a and Maria CAZACU^a

^a"Petru Poni" Institute of Macromolecular Chemistry Iasi, Roumania

^bTechnical University "Gh. Asachi", Faculty of Chemical Engineering and Environmental Protection, Iasi, Roumania

Received September 24, 2009

Polydimethylsiloxane/silica composites containing complexed lanthanum were prepared starting directly from tetraethylorthosilicate and 3-aminopropyltriethoxysilane as precursors for functionalized silica, 2,4-dihydroxybenzaldehyde as a modifier for silica, Lanthanum acetate as metal provider to be complexed, polydimethylsiloxane- α,ω -diol as polymer matrix, and dibutyltindilaurate as a condensation catalyst. The change in the feed molar ratios between the reaction components permitted to prepare a product series that were investigated by thermogravimetric analysis. The amounts of every reaction components assigned as inputs, and the main parameters of the thermogravimetric curves as outputs were used to develop artificial neural networks for the prediction of thermal stability of the approached materials. On the other hand, synthesis conditions, which lead to a pre-established thermal stability were predicted using inverse neural network method.

INTRODUCTION

The rare earth – based compounds are of interest in life sciences, mainly for the development of the chemical sensors or tools for medical diagnosis and therapy, mainly due to their high paramagnetism and fluorescence.¹ In order to use them in certain domains, such compounds are encapsulated in a matrix, usually an organic polymer. A possibility consists in the complexation of the rare earth ions by ligands that are covalently bound to the polymeric matrix.² Silica is commonly used as a rigid matrix for ligand immobilization. Silica xerogels doped with rare earth are of great interest for technological applications in the field of the optical devices.³ The immobilization of chelating groups on the silica gel surface can occur either by chemical modification of the silica or through simple physical adsorption processes.² The sol-gel process

based on hydrolysis/polycondensation reactions of the proper metal alkoxides is a convenient and versatile method for preparing transparent optical materials in mild conditions.^{4,5}

In recent years, the applications of artificial neural networks (ANN) have been extensively studied because they are promising instruments for process modeling. These types of intelligent instruments are information processing systems and have been used a lot in engineering application areas, in classification, pattern matching, structural systems identification, modeling of material behavior, pattern recognition, optimization and control-related problems.⁶

Pidaparti and Palakal were among the firsts which used artificial neural networks as constitutive models for composites.⁷ They demonstrated that neural models can predict uni-axial stress-strain behaviors with different off-axis angle and verified them with experiments.

* Corresponding author: silvia_curteanu@yahoo.com

However, these ANN models were limited because they cannot provide full multi-axial plane-stress constitutive models, required to performed structural analysis of laminated composites. Rami and Hoan-Kee presented a new approach to develop ANN constitutive models, which can generate nonlinear multi-axial stress-strain behaviors of fiber reinforced polymeric (FRP) composites for the entire plane-stress constitutive domain.⁸ The neural networks were also used to predict the behavior of reinforced concrete members (the shear resistance of rectangular reinforced concrete beams) using six parameters that influence this property. A back propagation neural network with sigmoid activation function proved to be a good model, due to the accuracy of prediction.⁶ Jiang applied the ANN technique for predicting the properties of the polymer-matrix composites. A well-trained artificial neural network was used to calculate some mechanical properties, such as compressive strength and modulus, the specific wear rate and frictional coefficient, having as starting point an experimental database for short fiber reinforced polyamide 4,6 composites.^{9,10}

In this paper we encapsulated lanthanum in functionalized silica by *in situ* complexation. Hydroxy-azomethine groups, known to form readily complexes with transition metal ions, are generated in this aim. Polydimethylsiloxane- α,ω -diol, PDMS, was added in different proportions in the sol-gel system, generating silica in order to obtain free standing flexible films. Taking into account the potential applications of such materials, besides the fluorescence that was investigated elsewhere¹¹, another property of practical interest is the thermal stability. Neural networks were developed and used to predict the thermostability property of the synthesized

composites. The influence of the reaction mixture composition on the thermostability was modeled, considering the amounts of every reaction components as inputs, and the main parameters of the thermogravimetric curves as outputs for the neural models. Neural networks have also been used in "inverse problem" in order to determine the reactants ratio, which lead to an imposed thermal stability of the compounds.

RESULTS AND DISCUSSION

Thermogravimetric analysis

The thermal degradation of the compounds was evaluated by dynamic thermogravimetric analysis in nitrogen atmosphere with a heating rate of 10°C/min. Figures 1 shows the obtained TG and DTG curves for the samples listed in Table 1. The shape of the resulted curves suggests a complex degradation mechanism consisting in three or four successive global processes. First and second steps are probably due to the volatile compounds (water and ethanol resulted by hydrolysis-polycondensation of the residual groups) emitting, followed by two thermo-oxidative processes. The position of the DTG maxima of the last degradation step is about the same (~579°C) in all cases, except the sample RL13, which does not contain PDMS. The peak value is higher as compared to that indicated for pure PDMS by Seema Ansari *et al.*¹² as being at 475°C, as well as to that obtained for a crosslinked polydimethylsiloxane/silica composite at about 470°C.¹³ Finally, a solid residue remains, SiO₂ and lanthanum oxide probably.

The summary of the important thermogravimetric characteristics obtained from the thermogram is given in Table 2.

Table 1

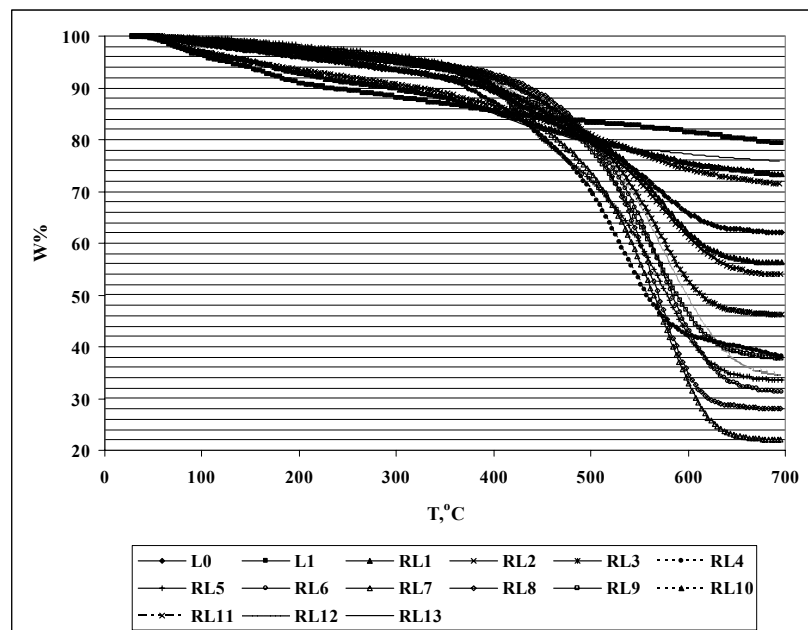
Experimental data for the sample preparation

Sample	Parameters				
	TEOS* (mmol)	APT* (mmol)	AR* (mmol)	LaAc ₃ * (mmol)	PDMS* (mmol)
L1	22	0.64	0.00	0.00	0.0000
L0	22	0.64	0.64	0.00	0.0000
RL1	22	0.64	0.64	0.25	0.0100
RL2	22	0.64	0.64	0.50	0.0125
RL3	22	0.64	0.64	0.75	0.0250
RL4	22	0.64	0.64	0.125	0.0500
RL5	22	0.64	0.64	0.25	0.0750

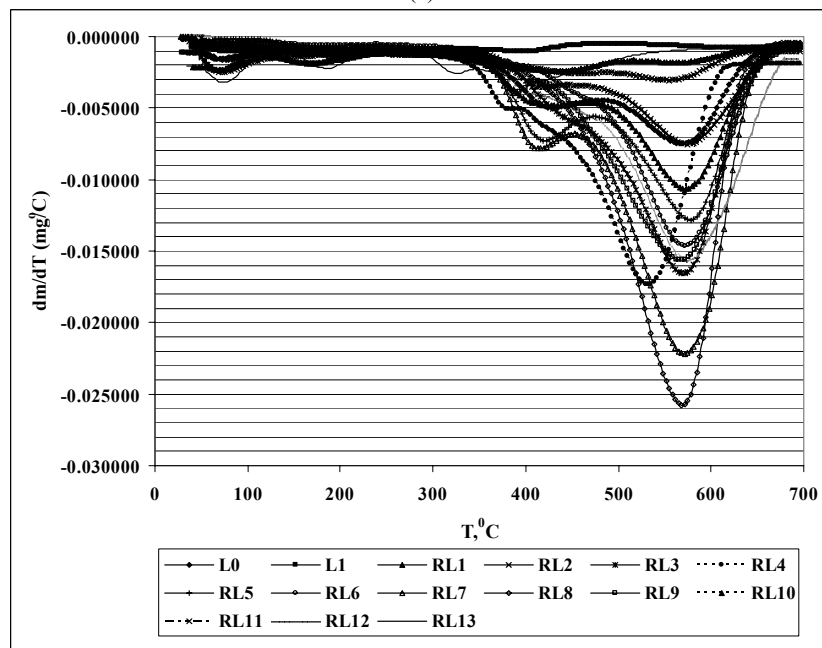
Table 1 (continued)

RL6	22	0.64	0.64	0.25	0.1000
RL10	22	1.28	1.28	0.50	0.0100
RL11	22	1.28	1.28	0.50	0.0250
RL12	22	1.28	1.28	0.50	0.0750
RL13	22	1.28	1.28	0.50	0.0000
RL7	11	0.64	0.64	0.25	0.1000
RL8	44	0.64	0.64	0.25	0.1000
RL9	66	0.64	0.64	0.25	0.1000

* TEOS is tetraethyl-orthosilicate, APT is 3-aminopropyltriethoxy-silane, AR is 2,4-dihydroxybenzaldehyde, LaAc₃ is lanthanum acetate and PDMS is polydimethylsiloxane α,ω -diol.



(a)



(b)

Fig. 1 – TG (a) and DTG (b) curves of the different samples used in experiments, at 10°C/min.

Table 2
Thermogravimetric characteristics

Sample	Stage of the thermal degradation	T _{onset} (°C) ^a	T _{peak} (°C) ^b	T _{endset} (°C) ^c	W% ^d	M _{Resid} (%) ^e
L0	I	60	72	150	2.60	61.81
	II	150	184	262	3.51	
	III	385	422	521	14.58	
	IV	521	571	625	17.50	
L1	I	45	68	99	4.62	79.13
	II	134	174	212	5.20	
	III	212	409	447	6.26	
	IV	549	589	700	4.79	
RL1	I	64	71	373	6.61	55.87
	II	373	413	523	13.61	
	III	523	576	623	23.91	
RL2	I	52	68	182	6.19	71.37
	II	182	431	478	12.39	
	III	478	559	611	10.05	
RL3	I	89	196	404	7.12	46.43
	II	404	572	618	46.45	
RL4	I	45	160	340	9.04	48.15
	II	340	533	586	51.85	
RL5	I	131	171	384	6.97	33.63
	II	385	418	516	23.45	
	III	516	577	630	35.95	
RL6	I	112	180	452	10.76	31.70
	II	452	572	630	57.54	
RL7	I	82	184	383	6.14	21.84
	II	383	410	497	19.67	
	III	497	571	623	52.35	
RL8	I	140	201	462	12.63	27.86
	II	462	570	611	59.51	
RL9	I	124	156	370	7.42	37.52
	II	370	389	460	8.51	
	III	460	569	616	46.55	
RL10	I	44	67	143	4.09	73.20
	II	143	164	348	7.77	
	III	348	439	465	7.33	
	IV	465	568	614	7.61	
RL11	I	63	289	380	9.10	53.56
	II	380	416	520	14.36	
	III	520	574	635	22.98	
RL12	I	104	209	376	6.91	34.30
	II	376	574	647	58.79	
RL13	I	44	74	99	4.52	72.50
	II	167	185	306	5.26	
	III	306	324	375	3.32	
	IV	375	409	514	14.40	

^a The onset temperatures of the polymer decomposition; ^b Thermal degradation peak temperatures of the samples decomposition; ^c Thermal degradation endset temperature in every stage; ^d Mass loss in every stage; ^e Weight loss of the samples after the end of a decomposition process.

The thermogravimetric characteristics listed in Table 2 indicated that thermal stability is slightly increased as the concentration of the PDMS in the complexed La-containing polydimethylsiloxane/silica composites increased (RL₅, RL₆, RL₇, RL₈, RL₉ and RL₁₂). The residue yields at 700°C (M_{Resid}) obtained from TG curves decreases as the concentration of the PDMS in the complexed La-containing polydimethylsiloxane/silica composites increased (Figure 2). Percentage of residue decreases as the concentration of the PDMS in the complexed La-containing polydimethylsiloxane/silica composites increased. One explanation would be the fact that in the analysing conditions, PDMS is degraded mainly by

the Si-O-Si bond breaking and formation of the volatile cyclic compounds.¹⁴

Neural network modeling

For modeling the thermal stability of polydimethylsiloxane/silica containing complexed La, two different types of modeling were used: direct neural network modeling, which means the determination of the dependence of thermostability (thermogravimetric properties) on the initial conditions and inverse neural network modeling, which determines the reaction conditions starting from the final imposed thermogravimetric properties.

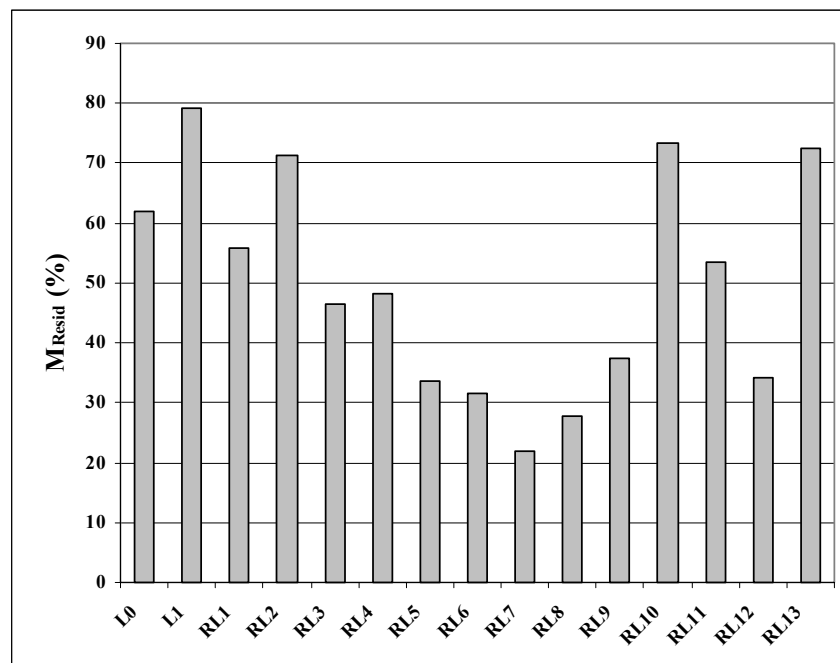


Fig. 2 – Weight loss of the samples at 700°C.

In direct modeling, different types of neural networks were built: MLP (multilayer perceptron), GFFN (generalized feed-forward networks) and MFN (modular feed-forward networks).

MLPs are layered feed-forward neural networks usually trained with static backpropagation algorithm. Their main advantage is that they are easy to use and can approximate any input/output map. The main disadvantages come from the slow train and the requirement of a lot of training data.

GFFNs are a generalization of the MLP such that connections can jump over one or more layers. GFFNs often solve the problem much more efficiently than MLPs because MLPs require hundreds of times more training epochs (iterations)

than the GFFNs with the same number of processing elements.¹⁵

MFNs are a special class of MLP. These networks process their input using several parallel MLPs, and then recombine the results. This tends to create some structure within the topology, which will foster specialization of function in each sub-module. MFNs do not have full interconnectivity between their layers. Therefore, a smaller number of weights are required for the same network size. This tends to speed up training times and reduce the number of required training exemplars.¹⁵

The neural network based modeling has the following stages: data acquisition, analysis and problem representation, architecture determination,

learning process, training of the networks and testing the trained network for generalization evaluation. After these stages, the ANN can supply good answers even when the data to be processed include errors or are incomplete and can process information rapidly when is applied to solve engineering problems.¹⁶

An important problem in the construction of neural networks is to determine the network architecture that is the number of hidden layers and the number of neurons in each hidden layer. In most cases, it is not necessary to increase the number of the hidden layers more than one or two because that does not improve the performance of the neural network, but increases the difficulties in training. The model has to be a simple one.^{16,17} Many hidden nodes cause the network to memorize the training set, leading to poor performance of generalization. Too few hidden nodes may not achieve the required error tolerance having difficulties in representing the nonlinear processes.¹⁸

Firstly, our experimental data is split into training and validation data sets (80 % and 20 %, approximately) because it is more important to evaluate the performance of the neural networks on “unseen” data that training data. In this way, we can appreciate the most important characteristic of a neural model - the generalization capability.¹⁹

Experimental data were used to train different types and topologies of neural networks which model the thermostability of polydimethylsiloxane/silica composites containing complexed La, as a function of components amounts which participate at the reaction. The thermostability was appreciated by the temperature when the first degradation process starts, T_{onset} , and the temperature corresponding to the maximal degradation rate, T_{peak} in this degradation step. Neural networks with three inputs: the amounts of TEOS, LaAc₃ and PDMS from Table 1 (considered as important factors which influence the thermostability) and two outputs parameters: T_{onset} and T_{peak} , (Table 3) were designed and trained.

Table 3

Experimental outputs for the direct neural network modeling.

	L1	L0	RL1	RL2	RL3	RL4	RL5	RL6	RL7	RL8	RL9	RL10	RL11	RL12	RL13
T_{onset}^a	45	59	64	52	89	45	131	112	82	140	124	44	63	104	44
T_{peak}^a	68	72	71	68	196	64	171	466	184	201	156	67	289	209	74

^aCorresponding to the first peak

Table 4 contains three types of neural networks (MLP, GFFN, MFN), with different topologies, and their performances: MSE (Mean Squared Error), r (correlation between experimental data and neural network outputs) and E_p (percent error).

The best network topology was determined by a trial and error method, based upon the mean of squared error. Consequently, two types of neural networks was found to have good performances, MLP(3:15:2) and MLP(3:12:4:2), that means networks with 3 input variables, one hidden layer with 15 neurons or two hidden layers with 12 and, respectively, 4 neurons, and 2 output variables. Compared with GFFN and MFN, neural networks of MLP type register better performance and benefit of simpler topologies, so they were chosen to model the thermal stability of polydimethylsiloxane/silica composites containing complexed lanthanum.

In the training phase, the neural network learns the behavior of the process. The training data set contains both input patterns and the corresponding output patterns. Neural network training leads to

finding values of connection weights that minimize differences between the network outputs and the target values.

Table 5 presents the predictions of the thermogravimetric characteristics obtained with the two neural networks, MLP(3:15:2) and MLP(3:12:4:2), compared to experimental data.

The relative errors were calculated using the formula:

$$E\% = \frac{P_{\text{exp}} - P_{\text{net}}}{P_{\text{exp}}} \cdot 100 \quad (1)$$

where P_{exp} is the experimental value and P_{net} is the value obtained with the neural network for both thermogravimetric properties (T_{onset} and T_{peak}).

The correlation between the experimental data and neural network prediction obtained with MLP (3:15:2) was 0.998513 for T_{onset} and 0.999974 for T_{peak} . For MLP (3:12:4:2) the two corresponding correlations were 0.999421 and 0.99996.

Table 4
Different topologies of neural networks in direct neural network modeling

	Neural network topology	MSE	r	E _p %
MLP				
1	3:4:2	0.003719	0.9951	4.6921
2	3:10:2	0.001339	0.9983	1.6324
3	3:15:2	0.001296	0.9983	1.5642
4	3:20:2	0.00126	0.9984	1.5475
5	3:9:3:2	0.002493	0.9968	1.8232
6	3:12:4:2	0.001171	0.9985	1.4502
7	3:24:8:2	0.001162	0.9985	1.2389
8	3:33:11:2	0.001168	0.9985	1.4606
9	3:42:14:2	0.001155	0.9985	1.2176
GFFN				
10	3:10:2	0.001681	0.9977	3.0002
11	3:12:4:2	0.001816	0.9973	3.1719
12	3:42:14:2	0.001315	0.9983	1.563
MFN				
13	$\begin{pmatrix} 12 & 12 \\ 3: & : \\ 4 & 4 \\ : & : \\ & & : & 2 \end{pmatrix}$	0.002061	0.9969	3.8036
14	$\begin{pmatrix} 42 & 42 \\ 3: & : \\ 14 & 14 \\ : & : \\ & & : & 2 \end{pmatrix}$	0.01916	0.9972	3.359

Table 5
Predictions of MLP(3:15:2) and MLP(3:12:4:2) compared to experimental training data.

Sample	T _{onset} exp	T _{peak} exp	MLP(3:15:2)				MLP(3:12:4:2)			
			T _{onset}	T _{peak}	E % T _{onset}	E % T _{peak}	T _{onset}	T _{peak}	E % T _{onset}	E % T _{peak}
L0	59	72	55	70	6.7797	2.7568	57	70	3.3898	2.7778
L1	45	68	48	70	6.6667	2.9634	48	70	6.6667	2.9412
RL1	64	71	64	71	0.0144	0.0604	64	71	0.0000	0.0000
RL3	89	196	89	196	0.0064	0.0112	89	196	0.0000	0.0000
RL4	45	64	45	64	0.0093	0.0303	45	64	0.0000	0.0000
RL5	131	171	131	171	0.0011	0.0032	131	171	0.0000	0.0000
RL6	112	466	112	466	0.0059	0.0064	112	466	0.0000	0.0000
RL9	124	156	124	156	0.0001	0.0163	124	156	0.0000	0.0000
RL10	44	67	47	67	6.4298	0.7440	45	65	2.2727	2.9851
RL11	63	289	63	289	0.1178	0.0067	63	289	0.0000	0.0000
RL13	44	74	43	74	2.2684	0.2499	44	75	0.0000	1.3514

Good agreement between experimental data and neural network results proved that the models learned well the behavior of the process. The aim of developing a neural model is to discover a network that finds out the essential relationships in the data. These formulae are then applied to new sets of inputs to produce corresponding outputs.²⁰ This is called generalization and represents

subsequent phase after training - validation phase. The learning algorithm should lead to a good fit to the training samples and to a network that has a good generalization capability. A network is said to “generalize well” when the input-output relationship, found by the network, is correct for the “unseen” data, which were never used in the training the network.²⁰ Figure 3 contains the

predictions for the two selected neural networks in the validation stage. The good results obtained in this phase mean that the chosen models have a

good robustness or generalization capability, because they perform well on unseen data. The relative errors were under 7 %.

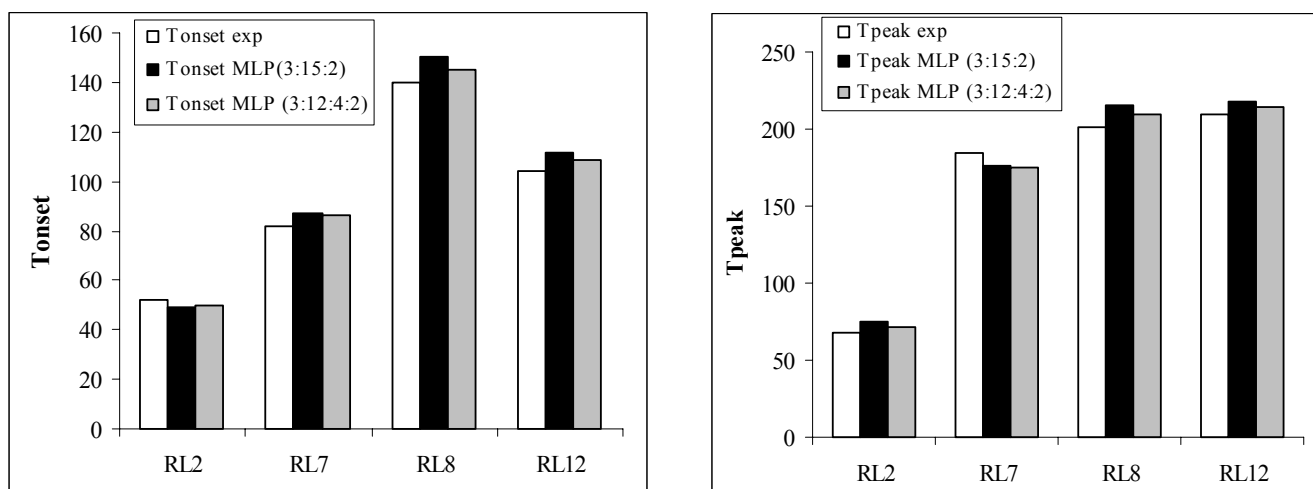


Fig. 3 – The predictions of MLP (3:15:2) and MLP (3:12:4:2) compared to experimental data for the validation stage in direct neural network modeling.

The neural network model with two hidden layers, MLP(3:12:4:2), was used for supplementary predictions. Once a neural network is sufficiently trained, it can be used to predict new results in the same knowledge domain. For obtaining the best prediction accuracy, the neural network was trained with the whole database. New input data sets constructed according to the experimental database were provided to the well trained network for the prediction of the thermal stability. Table 6 presents the predictions of

MLP(3:12:4:2) for a set of pre-established data in order to estimate the thermal stability of new polydimethylsiloxane/silica composites containing complexed La for given ratios of reactants. These results can be a useful guide for the future experiments in order to obtain compounds with good thermal stability.

The direct neural network modeling allows the estimation of thermogravimetric characteristics, even for the situation where experimental data are not available.

Table 6

The prediction of MLP(3:12:4:2) for a pre-established set of data.

Sample	TEOS	LaAc ₃	PDMS	T _{onset}	T _{peak}
P1	33	0.25	0.1	135	478
P2	55	0.25	0.1	135	386
P3	22	0.6	0.05	70	232
P4	22	0.25	0.05	65	85
P5	44	0.5	0.1	134	480
P6	11	0.5	0.1	76	208

By inverse neural network modeling additional information are provided, which can help us to obtain compounds with pre-established thermal stability. This type of neural modeling gives an answer to the following problem: What are the concentration of the PDMS necessary to attain pre-established values for T_{onset} and T_{peak} (that means a compound with pre-established thermal stability) working at imposed values for TEOS and AcLa₃ ?

In this case, neural networks have four input variables (T_{onset}, T_{peak}, TEOS and LaAc₃) and one output variable, PDMS. It was considered that PDMS has the most significant influence on the thermostability.

The best results were obtained with a simple feed-forward neural network with one hidden layer, MLP(4:10:1). The predictions of this

network on training and validation data are presented in Figures 4 and 5.

The MLP(4:10:1) was used for supplementary predictions for a pre-established set of data, as can be seen in Table 7, in order to find out the amount of PDMS that is necessary to obtain new

polydimethylsiloxane/silica composites containing complexed La, with an increased thermal stability.

A special software application – NeuroSolutions – was used in this paper in order to develop and obtain predictions of neural networks.

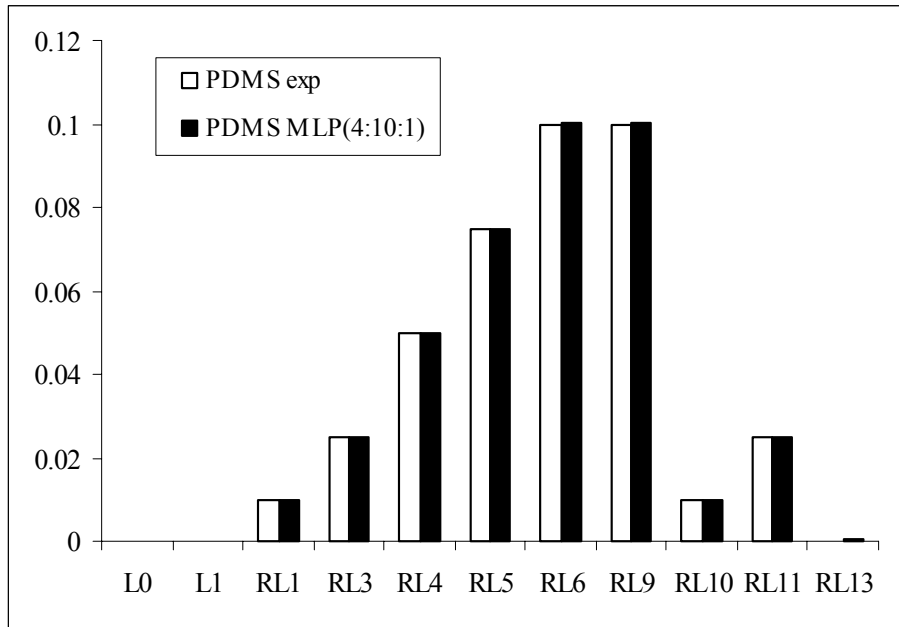


Fig. 4 – Predictions of MLP(4:10:1) compared to the experimental data for the training stage.

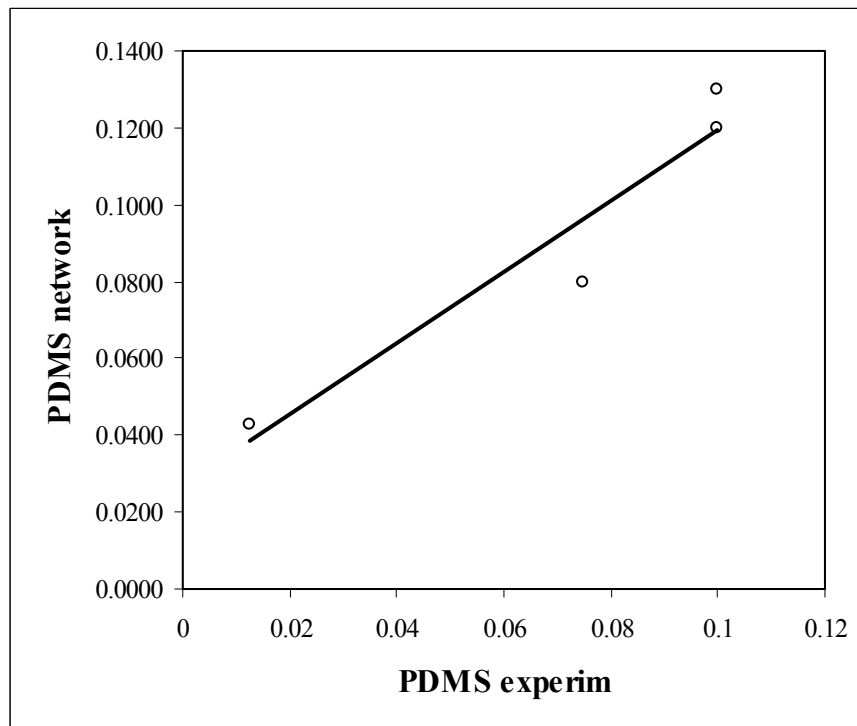


Fig. 5 – Predictions of MLP(4:10:1) compared to the experimental data for the validation stage.

Table 7

The predictions of MLP(4:10:1) for a pre-established set of data

TEOS	LaAc ₃	T _{onset}	T _{peak}	PDMS
11	0.5	90	190	0.0521
22	0.25	140	200	0.0813
22	0.5	130	180	0.0537
44	0.5	130	200	0.0746
44	0.25	140	300	0.0525
55	0.25	130	300	0.0984
66	0.25	140	400	0.006

What must be noted in this paper is the modeling methodology based on direct and inverse neural networks, the setting up of the own data by experiment and thermogravimetric analysis and the selection of the most significant parameters for the considered processes (the synthesis of the composites and their thermal properties). The obtained results, represented by networks with simple structures, provide useful information for experimental practice. Also, developed modeling methodology has a general character and can so be applied to other complex polymerization processes.

EXPERIMENTAL

Materials

Lanthanum acetate, La(CH₃COO)₃ (LaAc₃), purchased from Merck was used as received, M = 316.06.

Tetraethyl-orthosilicate (TEOS), purchased from Fluka (purity > 98 %, b.p.=163 - 167°C, d₄²⁰ = 0.933), was used as received.

3-Aminopropyltriethoxysilane (APT) (Fluka), M = 221.37, bp = 213-216°C, d₄²⁰ = 0.949 was used as received.

2,4-Dihydroxybenzaldehyde (AR) was prepared and purified according to procedure described in literature²¹ (yield: 33%, m. p. 135-137°C).

A polydimethylsiloxane α,ω -diol (PDMS), having an average number molecular mass of about 20000 (determined by GPC), has been synthesized by equilibrium cationic ring-opening polymerization of octamethylcyclotetrasiloxane (D₄), in the presence of Purolite CT 175 as a catalyst and water as a chain transfer agent.²²

Dibutyltindilaurate (DBTDL) was received from Merck-Schuchardt, d₄²⁰ = 1.055.

Tetrahydrofuran (THF), purchased from Fluka (purity \geq 99,0 %, b.p. = 65 - 67°C, d₄²⁰ = 0.887). Solvents: methanol

and acetone (Chimopar, Romania) were freshly dried before using.

Equipments

Thermogravimetric measurements (TGA) were performed on a Mettler Toledo TGA-SDTA851e derivatograph (thermogravimetric analyzer) under a flow of nitrogen (20 ml/min), in the temperature range 25 - 700°C, a heating rate of 10 C/min and 4-6 mg of sample mass. The operational parameters were kept constant to all samples in order to obtain comparable data.

Procedure

A route (Figure 6) that consists in heating all components together was applied to prepare a series of polydimethylsiloxane/silica composites having complexed lanthanum, as was earlier reported.¹¹ TEOS and APT as functionalized silica precursors were mixed in different ratios with PDMS. A homogeneous, colorless, transparent mixture is formed. Then AR dissolved in THF for 0.5 mol/ml as silica modifiers to provide the complexing groups was added and the stirring continued 1 hour at room temperature. LaAc₃ dissolved in water for 0.5 mol/l and acidified with CH₃COOH was added as La supplier to form silica containing complexed La. The mixing continued still 1 hour at room temperature. DBTDL was subsequently added to catalyse the condensation of TEOS/APT hydrolysis products and PDMS Si-OH ending groups. After stirring half an hour, the mixture was poured on Teflon foil and left to evaporate solvent. Thus, a polydimethylsiloxane network is formed, which can be connected to the silica one.

The thermal investigations were performed after the samples were kept in the laboratory environment for about two months. The tests revealed that after this time the mass of the samples is stabilized. The experiments were performed in conditions presented in Table 1.

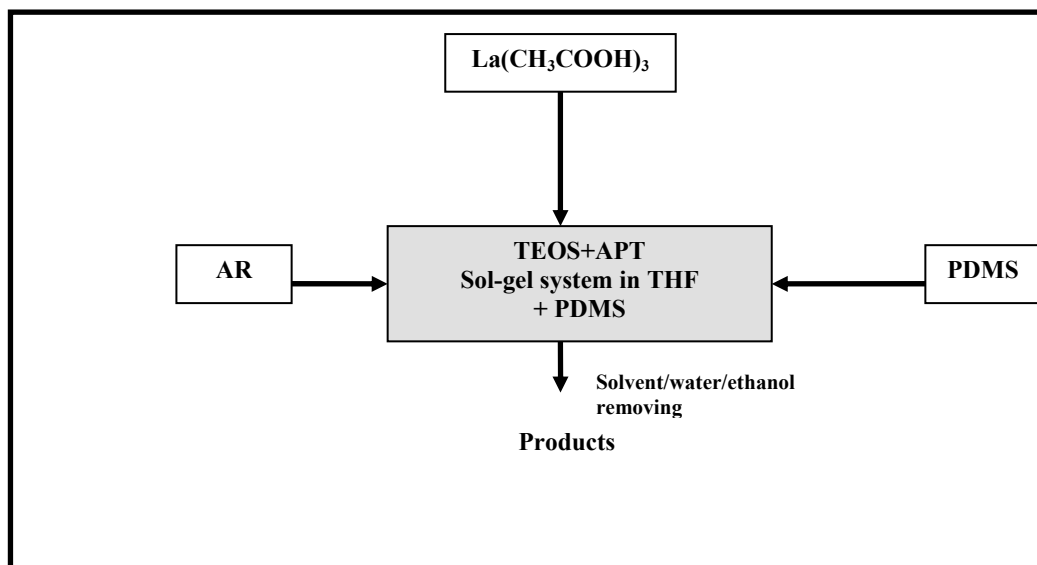


Fig. 6 – Schematic representation of the process for the preparation of the complexed La-containing polydimethylsiloxane/silica composites.

CONCLUSIONS

This paper presents the development of some artificial neural network models for the prediction of thermal stability of complexed La-containing polydimethylsiloxane/silica composites. A series of such materials has been prepared, with different feed molar compositions, providing the input and output parameters for the neural models. The thermostability was estimated by the main parameters of the registered thermogravimetric curves: the temperature when the degradation process starts, T_{onset} , and the temperature corresponding to the maximal degradation rate, T_{peak} , of the first peak.

The best models were multi-layer perceptrons, MLP(3:15:2) and MLP(3:12:4:2) in direct modeling, and MLP(4:10:1) in inverse modeling. These models were correlated with the smallest errors at the end of the training and validation phases. The properties predicted by using neural network modeling were found to be close to the measured values. This revealed the possibility of obtaining accurate results with relatively simple architectures of the networks. The prediction quality can be improved if the database for the training process could be enlarged or the configuration of the network could be further optimized.

Acknowledgements: This work was supported by CNCSIS – UEFISCSU, project number 59 PN II – IDEI 592/2007 and project number ID_600 no. 64/2007.

REFERENCES

1. G. Muller, C. L. Maupin, J.P. Riehl, H. Birkedal, C. Piguet and J. C. G. Bünzli, *Eur. J Inorg Chem.* **2003**, 22, 4065-4072.
2. Q.M. Wang and B. Yan, *J Organometal Chem.* **2006**, 691, 545-550.
3. F. Rocca, F. Monti, A. Kuzmin, A. Dalmaso and D. Pasqualini, *J Synchrotron Rad.*, **1999**, 6, 737-739.
4. M.S. Rao, I.S. Dubenko, S. Roy, N. Ali and B. Dave, *J Am Chem Soc.*, **2001**, 123, 1511-1512.
5. D. C. Lai, B. Dunn and J. I. Zink, *Inorg. Chem.*, **1996**, 35, 2152-2154.
6. J. A. Abdalla, A. Elsanosi and A. Abdelwahab, *J. Franklin*, **2007**, 344, 741-756.
7. R.M.V. Pidaparti and M. J. Palakal, *AIAA Journal*, **1993**, 31, (8), 1533-1535.
8. H. A. Rami and K. Hoan-Kee, *Mech. Mat.*, **2007**, 39, 1035-1042.
9. Z. Jiang, L. Gyurova, Z. Zhang, K. Friedrich and A.K. Schlarb, *Mater Design*, **2007**, 67.
10. Z. Jiang, Z. Zhang, K. Friedrich, *Compos Sci Technol*, **2007**, 67, 168-176.
11. M. Cazacu, A. Vlad, A. Airinei and M. Alexandru, *Polym Int.*, **2008**, 57, 1067-1074.
12. S. Ansari, J.M. Varghese, and K.R. Dayas, *Polym. Adv. Technol.*, **2009**, 20, 459-465.
13. M. Cazacu, A. Vlad, M. Alexandru, P. Budrugaec, C. Racles, F. Iacomi, *Polym. Bull.*, **2009**, DOI 10.1007/s00289-009-0147-7
14. Lv Pin, Z. Wang, Y. Hu and M. Yu, *J. Polym. Res.*, **2009**, 16, 81-89.
15. J. Principe, N. Euliano and C. Lefebvre, *Neural and Adaptive Systems: Fundamentals Through Simulations*. John Wiley and Sons, New York, 2001.
16. S. Curteanu, *Cent. Eur. J. Chem.*, **2004**, 2, 113-140.
17. J. Loboto, P. Cañizares, M. Rodrigo, J. Linares, C. Pulhac and S. Curteanu, *J. Power. Sourc.*, **2009**, 192, 190-194.
18. Y. Tian, J. Zhang and J. Morris, *Chem. Eng. Proc.*, **2002**, 41, 531-538.

19. S. Curteanu, A. Dumitrescu, C. Mihailescu and B. Simionescu, *Polym. Plast. Technol. Eng.*, **2008**, *47*, 1061-1071.
20. A.N. Fernandes and L.M.F. Lona, *Polym. Reaction Eng.*, **2002**, *10*, 181-192.
21. M. Marcu, M. Cazacu, A. Vlad and C. Racles, *Appl Organometal Chem.*, **2003**, *17*, 693-700.
22. M. Cazacu and M. Marcu, *Macromol. Rep. A.*, **1995**, *32*, 1019.