Available online at www.pelagiaresearchlibrary.com

Pelagia Research Library

Advances in Applied Science Research, 2011, 2 (4):147-155

ISSN: 0976-8610
CODEN (USA): AASRFC

Application of artificial neural network technique to predict ultrasonic velocities in binary oxide glasses

K.T. Arulmozhi* and R. Sheelarani

Department of Physics, Annamalai University, Annamalainagar, India

---

ABSTRACT

Accurate measurement of ultrasonic velocities is the essential part of structural characterization of materials. The longitudinal and shear ultrasonic velocities in multicomponent glass systems can be measured experimentally by the conventional pulse-echo technique which needs highly sophisticated instrumentation and so costly. On the theoretical evaluation side the usual statistical simple or multiple regression analysis do not work well to predict the velocities, since the relationship between the characteristic parameters of the components and the ultrasonic velocities are highly non-linear and quite complex. In situations like this artificial intelligence techniques are the best choice to solve the problem. Present work deals with the development of a multiplayer perceptron (MLP) artificial neural network (ANN) to predict the ultrasonic velocities in binary oxide glass systems.

Keywords: Ultrasonic velocity; Binary oxide glasses; Artificial neural network.

INTRODUCTION

Variety of multicomponent oxide glasses are available today with different combinations and compositions of oxides. These find diverse application fields such as electronics, optical communication, solar cells, bioactive materials, etc. The structural properties of the glass are the determining factors to fit to the correct application. As a non-destructive testing (NDT) method, ultrasonic techniques are most commonly used to characterize these glasses. Experimental measurement of ultrasonic longitudinal and shear velocities leads to the determination physical and elastical properties of these materials. As there do not exist any straightforward simple theoretical procedure to compute the ultrasonic velocities in heterogeneous glass systems, regression analysis can help to predict the velocities. Again due to complicated non-linear relationship existing between the velocities and the structural properties of the components a new approach is needed to solve the problem. In this instance artificial neural network (ANN) come in handy as a powerful tool to explore the probability of predicting the ultrasonic velocities. Function approximation (non-linear regression) is one of the important application of ANNs. Good amount of work has been done in this direction to predict certain parameters of materials or systems [1–9]. In this work an attempt has been made to design a feed forward multiplayer

perceptron (FFMLP) artificial neural network to predict the two ultrasonic velocities in binary oxide glass systems.

2. Methodology

The structural property of a multicomponent glass system essentially depends on the characteristics and compositions of the oxides present in the system. In their bond compression model Bridge et al. [10] have considered three important parameters to discuss the structural and elastic properties of the oxide glasses. They are:

n_b – number of bonds per unit volume of glass
$\bar{n}_c$ – average cross-link density per unit glass formula, which includes the number of bridging bonds per cation
F – average stretching force constant, which is a determining factor of bulk modulus.

These three structural parameters are defined by the relations,

$$n_b = \frac{N_a \rho}{M} \sum_i x_i (n_f)_i \qquad \ldots (1)$$

where N_a is Avagadro's number, n_f is the coordination number (the number of density and bonds per unit glass formula), ρ is the density and M effective molecular weight of the glass and x is the mole fraction.

$$\bar{n}_c = \frac{\sum_i x_i (n_c)_i (N_c)_i}{\sum_i x_i (n_c)_i} \qquad \ldots (2)$$

where n_c is the number of cross-link density per cation (equals the number of bridging bonds per cation minus two), N_c is the number of cations per glass formula unit and i represents the i^{th} oxide.

$$F = \frac{\sum_i x_i (n_f)_i f_i}{\sum_i x_i (n_f)_i} \qquad \ldots (3)$$

where n_f is the coordination number and f is the bond stretching force constant and i represents the i^{th} oxide, x being the mole fraction of the oxide.

Makishima and Mackenzie [11,12] proposed the theoretical model to calculate the elastic moduli of oxide glasses, in terms of the packing density (V_T) and dissociation energy (G_T) of the glass. They are given by

$$V_T = \frac{\rho}{M} \sum_i V_i x_i \qquad \ldots (4)$$

where ρ is the density of glass, M the effective molecular weight ($M = \sum x_i M_i$), V_i is the packing factor of the i^{th} oxide and x_i is the molefraction of the i^{th} oxide.

$$G_T = \sum_i G_i x_i \quad \ldots (5)$$

where G_i is the dissociation energy of the i^{th} oxide.

According to Higazy and Bridge [13] the fractional ionic character (FIC) of an oxide is important in deciding the network forming capability in the glass system. The FIC of the glass system as a whole can be computed using the relation

$$FIC_{glass} = \frac{\sum x_i (n_f)_i FIC_i}{\sum x_i (n_f)_i} \quad \ldots (6)$$

where FIC_i is the fractional ionic character of the i^{th} oxide which can be calculated using Pauling's relation.

Finally the molar volume (V_m) of the glass system also has considerable influence on the propagation of ultrasonic waves. V_m is calculated using the relation

$$V_m = M/\rho \quad \ldots (7)$$

where ρ is the density and M is the effective molecular weight of the glass. Even though this molar volume is included while calculating the packing density (V_T) and number of bonds (n_b), it is used as an individual predictor variable in this study.

All these seven characteristic parameters of the glass are used as predictor variables and thus form the inputs to the ANN. The longitudinal velocity (V_L) and shear velocity (V_S) of ultrasonic waves are the two outputs of the ANN.

3. Artificial neural network

3.1. Design concepts

The architecture of ANN is problem dependent. ANNs do not require any specific equation form and thus differ from traditional prediction models. Instead they need enough input-output data pairs. Also ANN can retrain for a new data so that it adapts to predict the new output. When designing an ANN model one has to observe certain considerations. At first the suitable structure of the model must be chosen. Then the activation function need to be determined. Next the training algorithm has to be selected. Most importantly a comprehensive database must be prepared for efficient training of the network.

3.2. Architecture

The first step in designing ANN model is to determine the network architecture. To data there are no established rules to decide the architecture of a back propagation network. Multilayer perceptron (MLP) feed forward networks very popular and successful are being used to variety of tasks such as pattern recognition, function approximation (non-linear regression), dynamic modeling, forecasting, etc. Back propagation algorithm is most commonly used for training the networks. In this, the network propagates the input pattern from layer to layer until the output layer generates the output pattern. If this pattern is different from the desired (target) output an error is calculated and propagated back to the input layer. Based on the error the weights are modified until the desired error between the predicted and target outputs are achieved.

3.3. Deciding factors of topology of MLP NN

There are several factors that should be considered to select the topology of a MLP NN. They are briefly discussed [13].

3.3.1. Input-output parameters

Too many input and output parameters will drastically slow down the learning process. It is essential to optimize the number of input and output parameters.

3.3.2. Layers and neurons

Neurons in the input layer simply accept the inputs and pass them to the first hidden layer and do not perform any computational work. Output neurons produces the predicted outputs. Only the neurons in the hidden layer play the key role of capturing all the features of the input-output pattern. The number of neurons in the input layer equals the number of input parameters *i.e.*, predictor variables. Similarly the number of output neurons equals the number of outputs to be generated. It has been suggested that a single hidden layer with sufficient number of neurons can do the entire job of computing. The number of neurons in the hidden layer drastically affects the output of the network. Too few neurons cannot learn properly and so their response to unseen inputs will be poor. Similarly too many neurons will memorize the input pattern and results in overfitting of data and thus have poor generalization capacity. A parametric study has to be done for fixing the number of neurons in the hidden layer so as to give best prediction capability.

In this study a three layer feed forward neural network trained with back propagation algorithm is used and is shown in Fig. 1.

4. Network training

4.1. Data sets

A database is the essential part of training process. It is a collection of data points, each representing a particular feature of the input-output pattern. The most common practice to train and evaluate the performance of the network is to divide the database into two parts. 80% of the data are used for training and 20% for testing. The training data must be comprehensive. The input-output patterns must cover the lower and upper boundaries for all the parameters and should represent all features of the model. Network training is evaluated by calculating mean square error (MSE).

In the present work 105 data points representing input-output pattern belonging to 26 binary oxide glass systems are used. These data are collected from earlier acoustical studies done by several researchers. All the predictor variables for these systems, other than those taken from references, are computed using relations (1) through (7). 85 data points are used for training and 20 data points for testing the network. The ranges of parameters are shown in Table 1. The binary glass systems and their corresponding characteristics used as predictor variables in the test set are provided in Table 2.

4.2. Epochs

Presenting entire set of training pattern to the network is called an epoch. The number of epochs affects the performance of the network. This number depends on the number of training data and parameters, number of hidden layers and neurons in them, number of output parameters and the error goal to be achieved. If the training is carried out for few epochs the network will not learn all the features of the input-output pattern. For too long training the network overfits the data and losses generalization ability leading to poor predictions of unseen data. Thus the number of epochs should be optimal similar to the selection of number of hidden neurons. The only way to

find these optimum numbers is to carryout a parametric study [14]. To limit the number of epochs to a lower optimal value, the training error goal is set at $1e^{-003}$ in the present work. Further four training algorithms namely, Levenberg Marquardt (trainlm), one-step sequent back propagation (trainoss), scaled conjugate gradient back propagation (trainscg) and Powell-Beale conjugate gradient back propagation (traincgb) are used in this parametric study.

Finally, to get satisfactory training of the network there are some data selection methodologies. Division of the database into sub groups for training, validation and testing is the methodology followed for learning process. The commonly used learning methods for estimating error rates are: Holdout, Random sub-sampling, K-fold cross validation, Leave-one-out and Bootstrap [15].

5. Network performance

The completion of network training is indicated by the reduction in training error. The output generated shows reasonable similarities with the target output. A well trained model should describe a smoother curve through the training data points, missing some, but resisting the effect of noise. To evaluate the function approximation ability of the designed network, the accuracy of the predicted values of ultrasonic velocities is found. It is done by calculating the mean absolute percentage error (MAPE), root means square error (RMS) and absolute fraction of variance (R^2) given by the following relations,

$$\text{MAPE} = \frac{1}{n}\left[\sum_i \frac{|\, t_i - o_i \,|}{t_i} \times 100\right] \quad \ldots (8)$$

$$\text{RMS} = \left[\frac{1}{n}\sum |\, t_i - o_i \,|^2\right]^{1/2} \quad \ldots (9)$$

$$R^2 = 1 - \left[\frac{\sum |\, t_i - o_i \,|^2}{\sum t_i^{\,2}}\right] \quad \ldots (10)$$

where t is the target value, o is the predicted value and n is the number of samples used in the test set.

RESULTS AND DISCUSSION

The predicted values of longitudinal and shear ultrasonic velocity by the four training methods are provided in Table 3. These predicted values are illustrated in Fig. 2(a–h) along with the experimental values. To compare the performance of the network using the four training methods, the calculated error parameters are furnished in Table 4. All these evaluation parameters are separately computed for longitudinal and shear velocities and shown in this Table along with their average values.

It can be seen from Table 4, the trainscg algorithm has good generalization ability. For this method very low values of MAPE (mean) = 4.3916 and RMS (mean) 184.88 are obtained with a high value of R^2 (mean) = 0.9965. The evaluation parameters reveal that the other three methods are more or less equal in their performances.

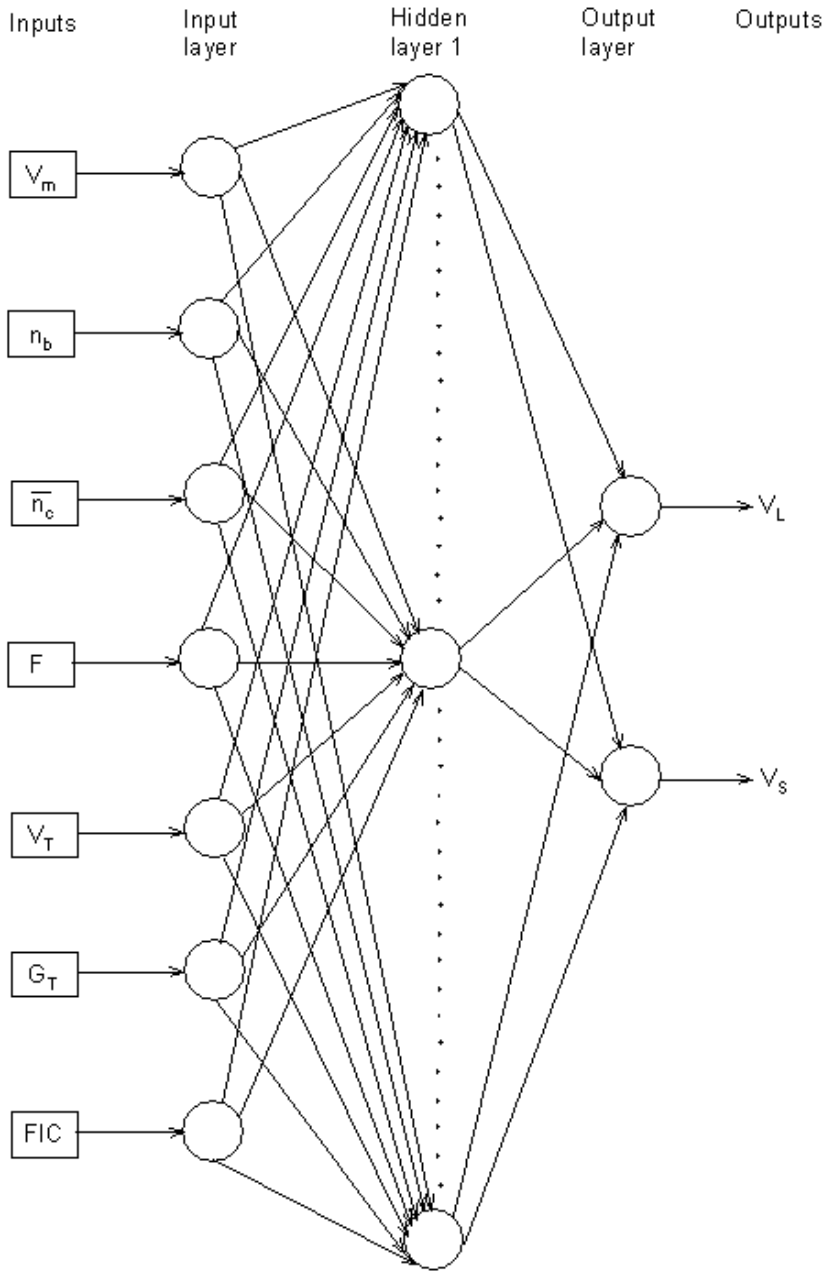

Table 1: Range of values of input and output parameters used in training set and test set

Parameter	Range			
	Training set		Test set	
	Min.	Max.	Min.	Max.
Inputs				
V_m (kg/m^3)	20.2	60.0	21.3	59.6
n_b	4.48	14.3	4.53	12.8
$\overline{n}_c$	1.03	4.00	1.30	4.00
F	198.8	663.6	203	623.8
V_T	0.34	0.88	0.36	0.84
G_T (10^9 kJ/mol)	23.12	61.90	25.38	62.00
FIC	0.3750	0.8122	0.3810	0.7927
Outputs				
V_L (m/s)	2810	6702	3110	6730
V_S (m/s)	1561	3990	1786	3941

Table 2 Glass systems used in training set, their compositions and characteristic parameters used as predictor variables

Sample No.	System (% Mol)	Predictor variables (inputs to ANN)						
		V_m (kg/m^3)	n_b	$\bar{n}_c$	F	V_T	G_T (10^9 kJ/mol)	FIC
1	0.85 TeO_2 – 0.15 BaO	28.3	12.8	4.00	218.3	0.51	51.83	0.4545
2	0.65 TeO_2 – 0.35 B_2O_3	26.72	11.2	2.44	311.7	0.56	43.01	0.4006
3	0.80 TeO_2 – 0.20 B_2O_3	28.5	11.4	3.00	266.0	0.52	47.72	0.3957
4	0.94 Na_2O – 0.06 B_2O_3	35.1	6.77	1.94	246.7	0.36	31.32	0.7927
5	0.10 Li_2O – 0.90 B_2O_3	33.2	6.00	1.30	623.8	0.44	28.13	0.4814
6	0.11 Na_2O – 0.88 B_2O_3	35.5	5.66	1.33	580.7	0.42	23.62	0.4910
7	0.70 TeO_2 – 0.30 MoO_3	31.61	11.4	4.00	218.7	0.53	58.74	0.3810
8	0.70 B_2O_3 – 0.30 Na_2O	28.8	8.16	1.90	464.6	0.50	25.38	0.5822
9	0.73 V_2O_5 – 0.27 PbO	33.1	7.27	2.00	240.2	0.84	57.57	0.4898
10	0.35 Li_2O – 0.65 B_2O_3	24.3	10.1	2.05	541.1	0.54	41.96	0.5909
11	0.90 TeO_2 – 0.76 P_2O_5	31.4	11.4	4.00	207.2	0.53	57.14	0.4100
12	0.24 Ce_2O_3 – 0.76 P_2O_5	59.5	4.53	2.47	157.4	0.55	38.42	0.5067
13	0.25 Ce_2O_3 – 0.75 P_2O_5	59.6	4.56	2.51	156.4	0.55	39.25	0.5757
14	0.30 MnO – 0.70 B_2O_3	23.4	10.10	1.53	534.9	0.64	38.08	0.4926
15	0.40 MnO – 0.60 B_2O_3	21.3	11.9	1.75	503.1	0.69	43.24	0.5100
16	0.70 TeO_2 – 0.30 V_2O_5	36.4	8.93	3.08	229.4	0.57	58.65	0.4278
17	0.75 TeO_2 – 0.25 ZnO	25.6	14.1	4.00	215.7	0.51	52.97	0.4350
18	0.50 TeO_2 – 0.50 V_2O_5	42.7	7.76	3.33	243.8	0.58	62.00	0.4673
19	0.90 TeO_2 – 0.10 Sm_2O_3	30.9	11.9	2.71	203.6	0.51	54.91	0.4302
20	0.90 TeO_2 – 0.10 La_2O_3	31.0	11.9	2.65	203.0	0.51	55.18	0.4325

Table 3 Experimental values of longitudinal and shear velocities and ANN predicted using different training methods

Sample No.	Longitudinal velocity (m/s)					Shear velocity (m/s)				
	Exp.	ANN				Exp.	ANN			
		trainscg	trainlm	traincgb	trainoss		trainscg	trainlm	traincgb	trainoss
1	3179	3178	3202	3227	3210	1786	1791	1785	1823	1805
2	3581	3585	3487	3520	3525	2086	2107	2063	2087	2097
3	3900	3694	3735	3899	3800	2400	2265	2286	2368	2263
4	4207	4199	4203	4151	4215	2322	2318	2314	2279	2329
5	4012	4144	4293	4236	4199	2472	2322	2357	2405	2369
6	4615	4055	4801	4938	4817	2563	2608	3122	2921	3041
7	3190	3291	3226	3193	3310	1823	1825	1830	1772	1856
8	5721	5664	5695	5783	5683	3204	3187	3197	3242	3231
9	3564	3681	3563	3575	3479	1994	1981	1922	1896	1824
10	3564	6618	6561	6561	6632	3941	3920	3919	3896	3852
11	3464	3616	3423	3671	3662	1911	2026	1914	2018	2004
12	4744	4726	4784	4746	4811	2744	2720	2760	2742	2754
13	4723	4786	4712	4713	4692	2688	2757	2697	2720	2691
14	6730	6318	6378	6309	6278	3320	3323	3318	3353	3369
15	6503	6567	6554	6564	6472	3425	3428	3409	3403	3421
16	3110	3113	3044	3124	3111	1800	1722	1736	1759	1769
17	3775	3336	4037	3607	3227	1968	1873	2155	1997	1822
18	3655	3514	4831	2999	3678	1871	1946	2498	1680	1925
19	3446	3085	4026	3116	3156	2175	1840	2343	1796	1852
20	3415	3408	3610	3053	4135	1985	1931	1964	1753	2186

Table 4 Network performance evaluation parameters obtained for the four training algorithms used

Evaluation parameter	Training algorithm											
	trainscg			trainlm			traincgb			trainoss		
	V_L	V_S	Mean	V_L	V_S	Mean	V_L	V_S	Mean	V_L	V_S	Mean
MAPE	3.8126	4.9706	4.3916	4.6381	5.3727	5.0053	3.9167	6.1795	5.0481	4.3367	6.1752	5.2559
RMS	219.87	149.90	184.88	303.47	225.48	264.48	223.80	206.72	215.26	246.31	212.31	229.31
R^2	0.9972	0.9958	0.9965	0.9947	0.9904	0.9925	0.9961	0.9919	0.9945	0.9965	0.9915	0.9940

Fig. 1. A three layer feed forward ANN used in the present work

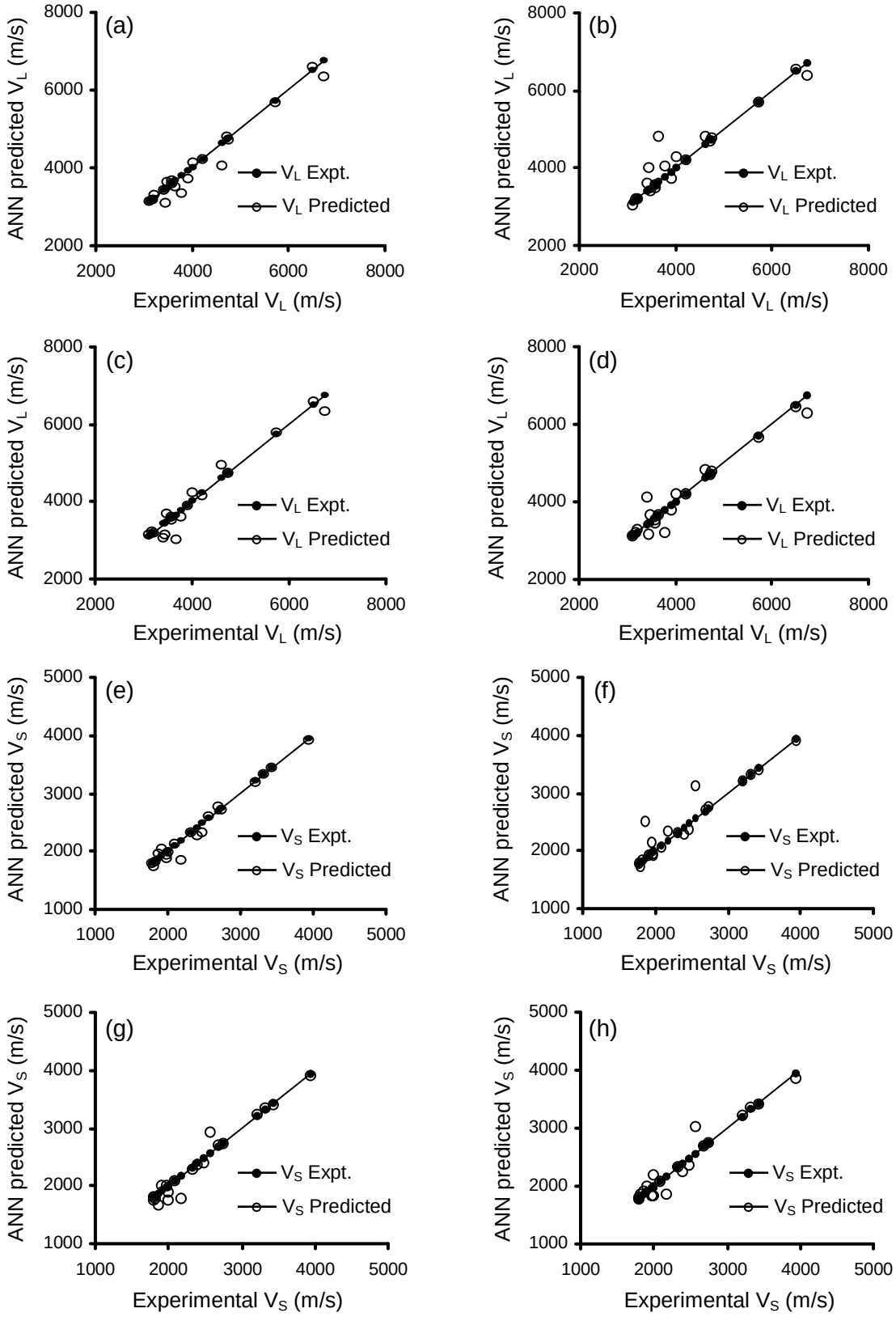

Fig. 2. Linear relationship between a) experimental and predicted V_L (trainscg), b) experimental and predicted V_L (trainlm), c) experimental and predicted V_L (traincgb), d) experimental and predicted V_L (trainoss), e) experimental and predicted V_S (trainscg), f) experimental and predicted V_S (trainlm), g) experimental and predicted V_S (traincgb) and h) experimental and predicted V_S (trainoss)

CONCLUSION

The ability of ANN for function approximation is well utilized in this work. This non-linear regression property of ANN is clearly established from the near perfect predictions of the two ultrasonic velocities in the studied binary oxide glasses. The use of the micro properties of the oxides involved, as predictor variables, is clearly illustrated. However mention should me made that by making the data base more comprehensive with the incorporation of as many as oxide glass systems possible, the ANN modelling will prove as a powerful tool for accurate predictions of ultrasonic velocities in new glass systems without going for the experimental measurements.

REFERENCES

[1] E. Rasa, H. Ketabchi and M.H. Afshar, Trans. A: *Civil Engg*. 16 (2009) 33–42.
[2] O. Onal, A.U. Ozturk, *Adv. Engg. Software* 41 (**2010**) 165–169.
[3] G. Trtnik, F. Kavcic, G. Turk, *Ultrasonics* 49 (**2009**) 53–60.
[4] H. Canakci, M. Pala, *Engg. Geol*. 49 (**2009**) 10–18.
[5] H. Eskandari, M.R. Rezaee, M. Mohammadnia, Application of multiple regression and artificial neural network techniques to predict shear wave velocity from wireline log data for carbonate reservoir, CSEG Recorder, South West-Iran, **2004**.
[6] C. Dreyfus, G. Dreyfus, *J. Non-Cryst. Solids* 318 (**2003**) 63–78.
[7] L.G. Esteban, F.G. Fernandez, P. de Palacios, *Comput. Struct*. 87 (**2009**) 1360–1365.
[8] J. Hola, K. Schabowicz, *NDT & E Intern*. 38 (**2005**) 251–259.
[9] S.B. Kalyanaraman, K.T. Arulmozhi, T. Jayakumari, *Chem. Engg. World* (**2007**) 92.
[10] B. Bridge, N.D. Patel, D.N. Waters, *Phys. Status Solidi*. 77 (**1983**) 655.
[11] A. Makishima, J.D. Mackenzie, *J. Non-Cryst. Solids* 12 (**1973**) 35–45.
[12] A. Makishima, J.D. Mackenzie, *J. Non-Cryst. Solids* 17 (**1975**) 147–157.
[13] A.A. Higazy, B. Bridge, *J. Non-Cryst.l Solids* 72 (**1985**) 81.
[14] M.Y. Rafiq, G. Bugmann, D.J. Easterbrook, *Comput. Struct*. 79 (**2001**) 1541–1552.
[15] M. Alper Selver, E. Ardali, O. Onal, O. Akay, *IEEE* (**2008**) 978-1-4244-2881.