Open Access Library Journal

Use of Artificial Neural Network and Theoretical Modeling to Predict the Effective Elastic Modulus of Composites with Ellipsoidal Inclusions

Anupama Upadhyay, Ramvir Singh*

Thermal Physics Laboratory, Department of Physics, University of Rajasthan, Jaipur, India
Email: *singhrvs@rediffmail.com

Received 25 July 2014; revised 10 September 2014; accepted 12 October 2014

Abstract

In this paper, a possible applicability of artificial neural networks to predict the elastic modulus of composites with ellipsoidal inclusions is investigated. Besides it, based on the general micromechanical unit cell approach, theoretical formula is also developed, for effective elastic modulus of composites containing randomly dispersed ellipsoidal in homogeneities. Developed theoretical model considers the ellipsoidal particles to be arranged in a three-dimensional cubic array. The arrangement has been divided into unit cells, each of which contains an ellipsoid. Practically in real composite systems neither isostress is there, nor isostrain, and besides it due to the effect of random packing of the phases, non-uniform shape of the particles, we are forced to include an empirical correction factor. We are forced to include an empirical correction factor in place of volume fraction which provided a modified expression for effective elastic modulus. Empirical correction factor is correlated in terms of the ratio of elastic moduli and the volume fractions of the constituents. Numerical simulations has also been done using artificial neural network and compared with the results of Halpin-Tsai and Mori-Tanaka models as well as with experimental results as cited in the literature. Calculation has been done for the samples of Glass fiber/nylon 6 composite (MMW nylon 6/glass fiber), Organically mod-ified montmorillonite (MMT)/High molecular weight (HMW) nylon 6 nanocomposite ((HE)$_2$M$_1$R$_1$-HMW nylon 6), Epoxy-alumina composites and MXD6-clay nanocomposite. It is found that both the theoretical predictions by the proposed model and ANN results are in close agreement with the experimental results.

Keywords

Inclusion, Elastic, Composite, Isostress, Isostrain

*Corresponding author.

How to cite this paper: Upadhyay, A. and Singh, R. (2014) Use of Artificial Neural Network and Theoretical Modeling to Predict the Effective Elastic Modulus of Composites with Ellipsoidal Inclusions. *Open Access Library Journal*, **1**: e903.
http://dx.doi.org/10.4236/oalib.1100903

Subject Areas: Applied Physics, Mechanical Engineering

1. Introduction

Engineered composite materials are renowned for their advanced properties. That's why the prediction and estimation of effective mechanical properties of random heterogeneous composite materials are of great interest to researchers and engineers in many science and engineering disciplines. For example, fiber-reinforced composites have superior mechanical properties over their unreinforced matrix. For civilian applications, cost is often a deciding factor in material selection. Compared with continuous fiber composites, short-fiber composites are cost effective because they can be adapted to conventional manufacturing techniques [1]-[6]. However, the application of short-fiber composites has so far been limited primarily to lighter load-bearing components, because of their low strength and toughness. The relatively low strength and toughness of short fiber composites are intrinsic problems caused by two main factors. With respect to interface selection, there exists a tradeoff between the strength and toughness of short-fiber composites: high strength is often obtained at the sacrifice of toughness. For a short fiber composite, a strong interface is desirable to transfer load from matrix to fibers, since relatively stronger interfaces can increase the effective fiber length over which the fiber carries load. The so-called "effective" properties of a heterogeneous composite are obtained by some volume- and ensemble-averaging processes over a "representative volume element" (RVE) featuring a "mesoscopic" length scale which is much larger than the characteristic length scale of particles (inhomogeneities) but smaller than the characteristic length scale of a macroscopic specimen.

One of the simplest approximations is Voigt approximation [1], which is used to evaluate the effective properties of a composite. It was originally introduced to estimate the average elastic constants of poly crystals. Voigt assumed that the strain through the bulk material is always uniform. The inverse assumption to Voigt approximation is the Reuss approximation [2], which assumes that the stress is uniform throughout the phases. Using variational principles, Hashin and Shtrikman [3] [4] established bounds on the materials that could be considered as mechanical mixtures of a number of different isotropic and homogeneous elastic phases, and in bulk, regarded as statistically isotropic and homogeneous. Gusev *et al.* [5] used image analysis to characterize the microstructure of a unidirectional glass/epoxy composite which was found to be transversely randomly packed. Monte Carlo procedure was employed to generate periodic computer models with unit cells comprising of random dispersion of a hundred non-overlapping parallel fibers of different diameter. An ultrasonic velocity method was used to measure elastic constants. On the basis of periodic three-dimensional meshes, the composite elastic constants of the Monte Carlo models were calculated numerically. It was shown that the randomness of the composite microstructure had a significant influence on the transverse composite elastic constants while the effect of fiber diameter distribution was small and unimportant.

Lusti *et al*. [6] predicted the thermo elastic properties of misaligned short glass fibre reinforced composites, using the finite-element-based numerical approach. Characterization of the microstructure of the two injection-moulded materials chosen for examination, in particular the fibre length and fibre orientation distributions, were used to ensure that the computer models were built with the same microstructure as the "real" materials. Agreement between the measurements, in particular for the longitudinal Young's modulus E_{11} and the longitudinal and transverse thermal expansion coefficients, α_1 and α_2, and the numerical predictions was found to be excellent.

Segurado and Llorca [7] developed a numerical approximation to the elastic properties of sphere-reinforced composites. The elastic constants of the ensemble of spheres embedded in a continuous and isotropic elastic matrix were computed through the finite element analysis of the three-dimensional periodic unit cells, whose size was chosen as a compromise between the minimum size required to obtain accurate results in the statistical sense and the maximum one imposed by the computational cost. Jweeg *et al*. [8] did the experimental work and studied theoretically, modulus of elasticity for long, short, woven, powder, and particle reinforcement of composite materials types with difference volume fraction of fiber. The results show the best modulus of elasticity for reinforcement composite is unidirectional fiber types in longitudinal direction and the woven reinforcement fiber types for transverse direction. More recently Upadhyay and Singh [9] modified Hashin-Shtrikman bounds using nonlinear volume fraction dependence of dispersed phase using the concept of microstructure and interconnectivity of phases at the interface. Modniks and Andersons [10] employed the finite element method to evaluate the elastic properties of a unit cell of a composite reinforced with short-fiber. For prediction of the stiffness of short-flax-fiber-reinforced polymer matrix composite, the orientation averaging approach is used. Ji and Wang [11] used cell model to analyze the effect of micro structural factors on the mechanical response of short fibers or particles-reinforced metal-matrix composites. Based on the cell model, the plastic constitutive relation of fiber or particle reinforcement composites was established. Koker *et al*. [12] investigated the effect of various training algorithms on learning performance of the neural networks on the prediction of bending strength and hardness behavior of particulate reinforced composites. The basic consideration of this study is to predict the result of the bending and hardness experiments of Al_2O_3/SiC reinforced composites. Sha *et al*. [13] described the use of artificial neural network method to study, in the field of materials science and engineering research. The Halpin-Tsai theoretical model is well known model that provides good agreement with the experimental data in case of long, random fibres for fibre reinforced composite materials, Halpin and Tsai developed a well known composite theory for predicting the stiffness of unidirectional composites as a function of aspect ratio [14]-[16]. The Mori-Tanaka average stress theory has also received considerable attention in the literature [17]. It was derived on the principles of Eshelby's inclusion model for predicting an elastic stress field in and around an ellipsoidal particle in an infinite matrix [18]. To account for finite filler concentrations, Mori and Tanaka [17], however, considered a non-dilute composite consisting of many identical spheroidal particles that cause the matrix to experience an average stress different from that of the applied stress; to satisfy equilibrium conditions the volume average over the entire composite was forced to equal the applied stress.

This paper proposes a theoretical model that predicts the elastic modulus of short-fiber composites or we can say composite reinforced with ellipsoidal particles. The overall goal of the research is to deduce the theoretical formula to predict the effective elastic modulus of composite injected with ellipsoidal fillers and compare its results with results of other theoretical models, results of artificial neural network ANN approach and finally to validate these with experimental predictions as given in literature. Some real ellipsoidal injected composites invariably have disoriented fibers of highly variable length; we focus here on composites having aligned ellipsoidal particles/fibers with uniform length and mechanical properties. The modeling of composites with effect of distributions of fiber orientation is improved with the inclusion of correction term in place of volume fraction. All of the models use the same basic assumptions: the fibers and the matrix are linearly elastic, the matrix is isotropic, and the fibers are either isotropic or transversely isotropic. The fibers are axisymmetric, identical in shape and size. The fibers and matrix are well bonded at their interface, and remain that way during deformation. Thus, we do not consider interfacial slip, fiber-matrix debonding or matrix microcracking. Examples of heterogeneous particles or fibrous composites are abundant, such as graphite/epoxycomposites, ceramic matrix composites, porous and cracked media, concrete and cementitious composites, polymer-blended soils, and rocks, etc. The experimental data of following composite materials are used in this study.

1) Glass fiber—MMW (medium molecular weight) nylon 6 composites, (Glass fiber/MMW composite);

2) $(HE)_2M_1R_1$—HMW (high molecular weight) nylon 6 composites (MMT/HMW composite);

Or Organically modified montmorillonite (MMT)/nylon 6 nanocomposites-Organoclay $[(HE)_2M_1R_1]$ = Bis (hydroxyethyl)-(methyl)-rapeseed quaternary ammonium organoclay, where R = Rapeseed, HE = Hydroxyethyl, M = Methyl.

Rapeseed is natural product composed predominantly unsaturated C_{22} alkyl chains (45%).

3) MXD6/clay nanocomposites, where MXD6 is poly (m-xylylene adipamide);

4) Epoxy composites reinforced with 200 nm thick alumina platelets.

The elastic properties of these composites are given in **Table 1**. The present approach is simple and provides

Table 1. Elastic properties of composite materials used in this study.

Composite	Filler	Elastic Modulus of Filler (GPa)	Matrix	Elastic Modulus of Matrix (GPa)
Glass Fiber/MMW Nylon 6 Composites	Glass Fiber	72.4 [19] [20] [23]	MMW Nylon 6	2.82 [19] [20] [23]
MMT/HMW Nylon 6 Composites	MMT	178 [21] [22] [24] [25]	HMW Nylon 6	2.75 [19] [20] [23]
MXD6/Clay Nanocomposites	Clay	84 [26]	MXD6 Nylon	4 [26]
Epoxy/Alumina Platelets Composites	Alumina Platelets	375 [27]	Epoxy	3.82 [27]

wider applicability to ellipsoidal model and enhances its ability to predict correctly the effective elastic modulus of composites system.

2. Theoretical Modeling

Here first we propose a theoretical model to evaluate the effective mechanical behavior in terms of effective elastic modulus of a matrix reinforced with a random and homogeneous distribution of ellipsoids by the unit cell approach and also computed numerically with artificial neural network (ANN).

According to our model the arrangement has been divided into unit cells each of which contains an ellipsoid. However, in real systems, the packing and the shape of the particles are random. In order to incorporate the effect of deformed reinforcement particles, varying individual geometries and non-linear stress and strain, a correction term in place of the physical volume fraction has been introduced. Expressions for the volume fraction correction term have been obtained empirically by simulating experimental data reported in the literature. In this paper, all particles are assumed to be non-intersecting (impenetrable) and embedded firmly into a homogeneous matrix material, *i.e.*, perfect interfacial bonding is assumed. Further, we assume that statistical homogeneity holds. Therefore, effective (averaged) material properties remain the same for arbitrary averaging domains inside a composite medium. As a consequence, heterogeneous composites can be represented by equivalent homogeneous continuum media with appropriately defined effective properties.

2.1. Ellipsoidal Inclusion Unit Cell Model

While exploring the problem, here we consider that the filler particles be ellipsoidal having principal axes $2a$, $2c$ and $2a$ ($a < c$). We assume the distribution where these filler particles to be positioned at the corners of a simple cube of side $2b$ each, as shown in **Figure 1(a)**. The geometry of a unit cell is shown in **Figure 1(b)**. We consider the origin of coordinate axes is located at the centre of the ellipsoid. The unit cell can be divided into thin sections or slices by planes perpendicular to the x-axis. Let us take one such section which is bounded by two planes at x and $x + \mathrm{d}x$ distances. In **Figure 1(c)**, the section is shown, which is subdivided into four quadrants. One such section is shown in **Figure 1(d)**. This section is further divided by planes perpendicular to the z-axis. Thus it results in the section of rectangular bars. In **Figure 1(e)**, one such bar is shown. Let the length of the bar be b. Its cross-sectional area will be $\mathrm{d}x\mathrm{d}z$. The shaded portion of the element in **Figure 1(d)** represents the filler phase and the non-shaded portion represents the matrix phase.

The volume fraction of the solid phase will be

$$\left(y\mathrm{d}x\mathrm{d}z\right)/\left(b\mathrm{d}x\mathrm{d}z\right) = y/b \tag{1}$$

Similarly, the volume fraction of the filler phase will be

$$\left(b-y\right)\mathrm{d}x\mathrm{d}z/\left(b\mathrm{d}x\mathrm{d}z\right) = \left(1-y/b\right) \tag{2}$$

The terms (y/b) and ($1 - y/b$) are equivalent to the one-dimensional volume fraction. Therefore, using the Voigt model, the Elastic modulus of the bar will be:

$$E' = E_1\left(y/b\right) + E_2\left(1-y/b\right) \tag{3}$$

where E_1 and E_2 are the Elastic moduli of the filler and matrix phase respectively. With reference to **Figure 1(d)**, the elastic modulus of the section will be

$$\begin{aligned} E'' &= \frac{ab\mathrm{d}x}{b^2\mathrm{d}x}E'_{av} + \frac{\left(b-a\right)b\mathrm{d}x}{b^2\mathrm{d}x}E_2 \\ E'' &= \left(a/b\right)E'_{av} + \left(1-a/b\right)E_2 \end{aligned} \tag{4}$$

where

$$E'_{av} = \left(1/a\right)\int_0^a E'\mathrm{d}z \tag{5}$$

Combining Equations (4) and (5) yield the following result:

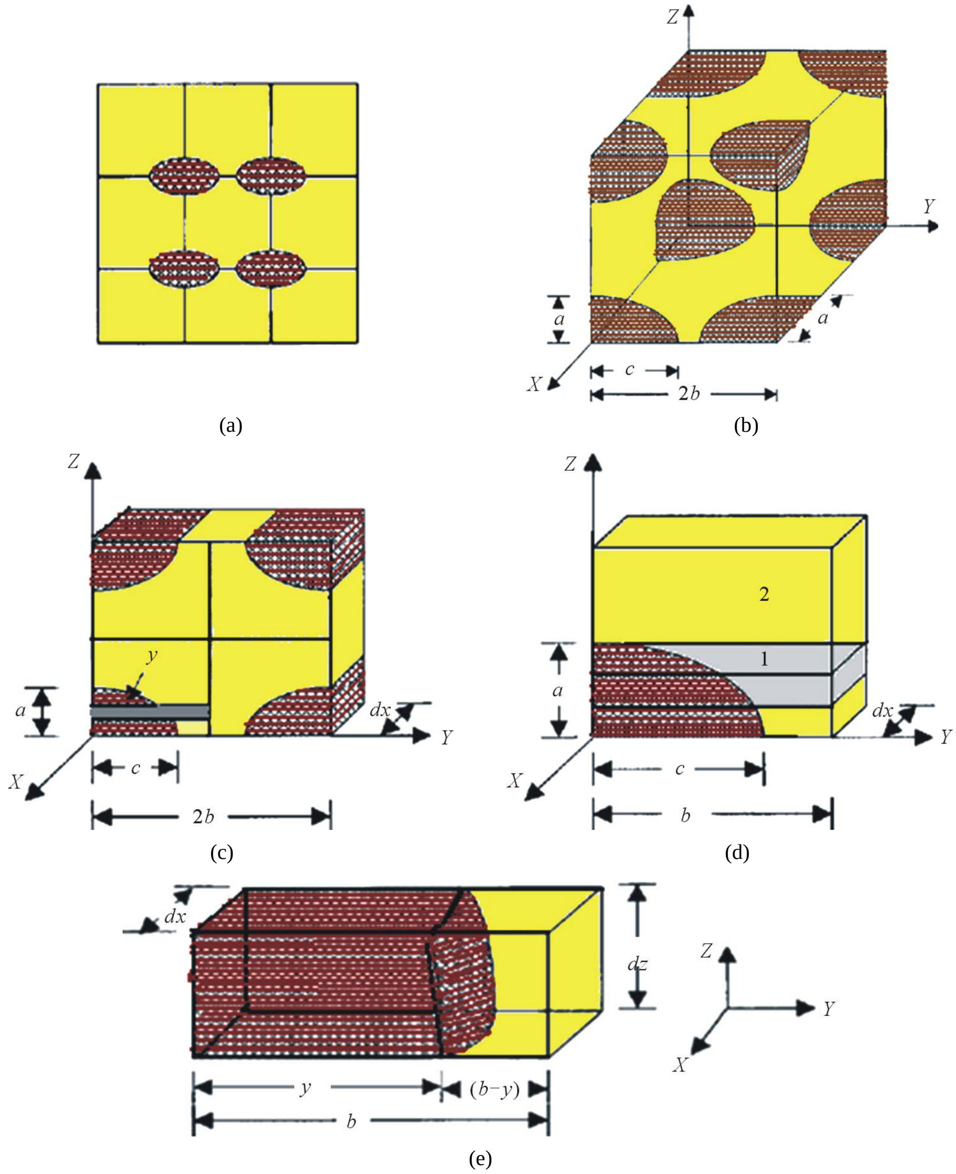

Figure 1. The unit cell model for two-phase systems with ellipsoidal particles: (a) Particles distribution in two dimensions; (b) Geometry of a unit cell; (c) One section of unit cell; (d) One part of the section and (e) Rectangular bar.

$$E'' = (1/b)\int_0^a E'\mathrm{d}z + (1 - a/b)E_2 \tag{6}$$

With reference to the **Figure 1(d)**, we have:

$$\text{Volume fraction of portions numbered 1} = (ab\mathrm{d}x)/(b^2\mathrm{d}x) = (a/b) \tag{7}$$

$$\text{Volume fraction of portions numbered 2} = \{(b^2 - ba)\mathrm{d}x\}/(b^2\mathrm{d}x) = (1 - a/b) \tag{8}$$

Therefore, the effective elastic modulus (E_{eff}) of the unit cell for isostress case from Reuss model will be

$$\frac{1}{E_{eff}} = \frac{(a/b)}{E''_{av}} + \frac{(1 - a/b)}{E_2} \tag{9}$$

Therefore E'' varies as x changes from 0 to a then, on averaging, we get

$$E''_{av} = (1/a)\int_0^a E''\mathrm{d}x \tag{10}$$

Combining Equations (6) and (10) yield the following result

$$E''_{av} = (1/a)\int_0^a \left[(1/b)\int_0^a E'\mathrm{d}z + (1-a/b)E_2\right]\mathrm{d}x \tag{11}$$

Combining Equations (3) and (11) yield the following result

$$E''_{av} = (1/a)\int_0^a \left[(1/b)\int_0^a \left\{E_1(y/b) + E_2(1-y/b)\right\}\mathrm{d}z + (1-a/b)E_2\right]\mathrm{d}x$$

Therefore:

$$E''_{av} = \left\{(E_1 - E_2)/(ab^2)\right\}\int_0^a\int_0^a y\,\mathrm{d}x\mathrm{d}z + E_2 \tag{12}$$

For an ellipsoidal particle we have

$$\left(x^2/a^2\right) + \left(y^2/c^2\right) + \left(z^2/a^2\right) = 1 \Rightarrow y = c\sqrt{\left\{1-\left(x^2/a^2\right)-\left(z^2/a^2\right)\right\}} \tag{13}$$

By combining (12) and (13), we get the following result

$$E''_{av} = \left\{(E_1 - E_2)/(ab^2)\right\}\left\{(\pi a^2 c)/6\right\} + E_2$$

therefore

$$E''_{av} = \left\{(E_1 - E_2)(\pi ac)/(6b^2)\right\} + E_2 \tag{14}$$

By combining (9) and (14), we get the following result

$$\frac{1}{E_{eff}} = \frac{(a/b)}{\left\{(E_1 - E_2)(\pi ac)/(6b^2)\right\} + E_2} + \frac{(1-a/b)}{E_2}$$

Therefore,

$$E_{eff} = \frac{E_2\left[(E_1 - E_2)\left\{(\pi ac)/(6b^2)\right\} + E_2\right]}{\left[(1-a/b)(E_1 - E_2)\left\{(\pi ac)/(6b^2)\right\}\right] + E_2} \tag{15}$$

The unit cell contains one ellipsoid inside. Therefore, fractional volume of the solid phase will be

$$\phi_1 = \frac{\left\{(4/3)(\pi a^2 c)\right\}}{8b^3} \tag{16}$$

Putting the limiting condition into Equation (16), if $c = b$, then we get

$$\phi_1 = \frac{\pi a^2}{6b^2} = (\pi/6)\left(a^2/b^2\right)$$

therefore

$$(a/b) = \left\{\sqrt{(4/\pi)}\right\}\phi_1^{1/2} \tag{17}$$

Combining Equations (15) and (17) we get the following result:

$$E_{eff} = \frac{E_2\left[(E_1 - E_2)\left\{\sqrt{(\pi/6)}\right\}\phi_1^{1/2} + E_2\right]}{\left[\left(1-\left\{\sqrt{(6/\pi)}\right\}\phi_1^{1/2}\right)(E_1 - E_2)\left\{\sqrt{(\pi/6)}\right\}\phi_1^{1/2}\right] + E_2} \tag{18}$$

For cubic packing of ellipsoidal inclusions the maximum value of the packing fraction will be <0.52 (because $a < b$). In the limiting case, it can be seen that, when ϕ_1 tends to 0, E_{eff} approaches E_2 and when ϕ_1 tends to 0.52, E_{eff} leads to the arithmetic mean of the phases. Considering that (18) is based on rigid geometry and it does not represent the true state of affairs of a real two-phase system. The effective elastic modulus depends upon the various characteristics of the system, most prominent amongst them being the volume fraction and elastic modulus of the constituent phases. Thus, for practical utilization, we have to modify the expression (18) by incorporating a correction term. It should be a function of the ratio of the elastic modulus of the constituent phases, as well as of the volume fraction of the filler phase. Considering random packing of phases, non-uniform shape of particles and anisotropy in stress and strain, the composite constituents are not restricted to be in isostress or in isostrain arrangement, we here replace physical volume fraction of filler phase by the correction term, F. F in general should be a function of the volume fraction of the filler phase and the ratio of the elastic modulus of the constituent phases. Therefore, Equation (18) may be written as

$$E_{eff} = \frac{E_2\left[(E_1 - E_2)\left\{\sqrt{(\pi/6)}\right\}F^{1/2} + E_2\right]}{\left[\left(1-\left\{\sqrt{(6/\pi)}\right\}F^{1/2}\right)(E_1 - E_2)\left\{\sqrt{(\pi/6)}\right\}F^{1/2}\right] + E_2} \tag{19}$$

Rearranging Equation (19) we get:

$$AF + BF^{1/2} + C = 0 \tag{20}$$

where

$$A = \left[E_{eff}(E_1 - E_2)\right],$$

$$B = \left\{\sqrt{(\pi/4)}\right\}(E_1 - E_2)\left(E_2 - E_{eff}\right)$$

and

$$C = E_2\left(E_2 - E_{eff}\right)$$

2.2. Applications of the Artificial Neural Networks-Three-Input ANN Model

In the present paper, we have also employed the application of artificial neural networks (ANN) to predict the elastic modulus of the composite materials. Here, we will see that the results obtained to predict the elastic modulus of the composite materials are encouraging. First, we prepared a database to train and test the models developed here. Three input neural networks architecture is developed. The effective elastic modulus of composites depends on the properties of its constituents, so the trained ANN is composed of three input neurons (filler elasticity modulus, matrix elasticity modulus, filler volume fraction) and one output neuron (effective elasticity modulus of the composite) as to satisfy the following relation

$$E_{eff} = f\left(E_f, E_m, v_f\right)$$

we obtained the closest results using 10 optimum number of neurons, in hidden layers and with the training function "Trainlm". The three inputs ANN model is built, trained and tested by the feed forward back propagation algorithm, to obtain the effective properties of the composite materials from the properties of their components. Feed forward networks consist of a series of layers. The first layer has a connection with the network input. Each subsequent layer has a connection with the previous layer. The final layer produces the network's output. Feed forward networks can be used for any kind of input to output mapping. A feed forward network with one hidden layer and enough neurons in the hidden layers can fit any finite input-output mapping problem. Feed forward back propagation neural network structure includes an input layer, a hidden layer and an output layer. The number of neurons in the input layer is equal to the number of input parameters, and the number of neurons in the output layer is equal to the output parameters.

The number of neurons in the hidden layer depends on the number of input and output parameters and of training dataset used. Here, we determined the optimal number of neurons in the hidden layer, by trying different networks. The best outcome is for 10 numbers of neurons in the hidden layer. The ANN model is found capable of predicting elastic modulus of composites well within the ranges of the input parameters considered. The results for elastic modulus predicted by ANN are then compared to those obtained using ellipsoidal model and other theoretical models.

3. Results and Discussion

In our opinion micro-macro mechanical approaches offer new insights in the material behavior of such spatially distributed particle reinforced composites and may result in new procedures to develop realistic material models for design and optimization purposes. In this paper, we focused on the evaluation of effective material properties of randomly distributed ellipsoidal particle reinforced composites. However, in real systems, the packing and the shape of the particles are random. In order to incorporate varying individual geometries and considering that the strain and stress are not uniform throughout the phases because of the difference in elastic properties of constituent phases, a correction term in place of the volume fraction of filler-phase has been introduced. An expression for the correction term for theoretical predictions has been obtained empirically by simulating experimental data reported in the literature for Glass fiber/MMW Nylon 6 *i.e.* (MMW/glass fiber) composites [28], Organically modified montmorillonite (MMT)/HMW nylon 6 nanocomposites *i.e.* ($(HE)_2M_1R_1$/HMW nylon 6 or MMT/HMW) composite [28], epoxy composite reinforced with alumina platelets [27] and MXD6-clay nanocomposite [26] etc. Elastic properties of the constituent phases of composites are given in **Table 1**. Without any correction term, Equation (18) exhibits large deviations from the experimental results. This prompted the introduction of a correction in volume fraction. The correction term introduced for each sample has been computed using (20) and plotted with $\phi_1^{1/2}\exp(E_2/E_1)$. For all four composite samples, $F^{1/2}$ increases roughly, linearly with increasing $\phi_1^{1/2}\exp(E_2/E_1)$.

One of these plots of $\phi_1^{1/2}\exp(E_2/E_1)$ versus $F^{1/2}$ for MMT/HMW nylon 6 nanocomposites is shown in **Figure 2**, where squares denote the experimental data and straight line indicates the theoretical simulation. From **Figure 2** we can observe, that $F^{1/2}$ increases roughly, linearly with increasing $\phi_1^{1/2}\exp(E_2/E_1)$.

We have used the curve fitting technique and found that the following expression

$$F^{1/2} = C_1\left\{\phi_1^{1/2}\exp(E_2/E_1)\right\} + C_2 \tag{21}$$

optimum fits the curve obtained in **Figure 2**, where C_1 and C_2 are constants. These constants are different for different type of materials. The values of these constants for MMW/glass fiber, MMT/HMW nylon 6 nanocomposites, epoxy composite reinforced with alumina platelets and MXD6-clay nanocomposite systems are given in **Table 2**.

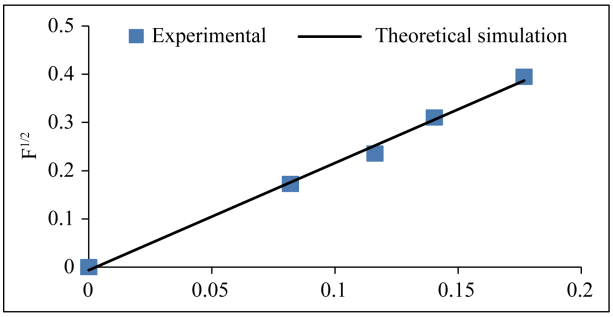

Figure 2. The variation of volume fraction correction term $F^{1/2}$ v/s $\phi_1^{1/2}\exp(E_2/E_1)$.

Table 2. Values of constants C_1 and C_2 for given samples.

Composite sample	C_1	C_2
Epoxy/Alumina	1.1	0
Glass Fiber/MMW nylon 6	1.887	−0.202
MXD6/Clay	3.422	−0.393
MMT/HMW nylon 6	2.222	−0.006

On putting (21) as the volume fraction correction term in (19) we have calculated values of EEM for many of samples reported in the literature. **Tables 3(a)-(d)** show a comparison of experimental results of EEM and calculated values from (19). Thus, the correction term depends purely on the elastic properties of the constituent phases and the volume fraction of the filler phase. Developed relation is found to depend on nonlinear contribution of volume fraction of constituents as well as ratio of elastic properties of individual phases. This relation is

Table 3. Elastic modulus data, experimentally and theoretically predicted using developed Ellipsoidal model and artificial neural network (ANN) for various volume fractions of filler phase. (a) Epoxy-alumina composites; (b) Glass Fiber/MMW nylon 6 composite; (c) MXD6-clay nanocomposite; (d) MMT/HMW nylon 6 composite.

(a)

Filler Vol. fraction	Experimental (GPa)	Theoretical (GPa)	ANN (GPa)
0	3.82	3.82	3.829284
0.005	4.04	4.206909	4.026671
0.01	4.55	4.422214	4.549224
0.05	6.03	5.658323	6.776822
0.1	6.79	7.165182	6.788372

(b)

Filler Vol. fraction	Experimental (GPa)	Theoretical (GPa)	ANN (GPa)
0	2.84	2.034051	2.840033
0.023	2.96	3.076102	2.846745
0.0475	3.88	3.759054	3.880004
0.0734	4.93	4.617962	4.93
0.101	5.89	5.80625	5.889999
0.161	9.6	10.77567	9.536906

(c)

Filler Vol. fraction	Experimental (GPa)	Theoretical (GPa)	ANN (GPa)
0.007304	1.5988	2.500496	1.602362
0.013565	2.9692	4.037053	2.977182
0.038609	5.2532	6.18543	5.311692
0.045391	7.0804	7.056479	6.634082
0.051652	9.136	8.034228	9.132238
0.065217	9.8212	11.08888	9.819519

(d)

Filler Vol. fraction	Experimental (GPa)	Theoretical (GPa)	ANN (GPa)
0	2.75	2.758749	2.830263
0.0065	3.49	3.509905	3.490001
0.0131	3.92	4.0508	4.933519
0.0191	4.59	4.54403	4.589997
0.0303	5.7	5.570141	5.699856

applied for the calculation of effective elastic modulus for Epoxy/Alumina, GlassFiber/MMW nylon 6, MXD6/Clay, and MMT/HMW nylon 6, composite materials. **Table 3** cites experimental data reported in literature for EEM and proposed theoretical results, as well as ANN predictions. The predicted results of elastic modulus using composite theories of Halpin-Tsai and Mori-Tanaka are also employed to validate and compare our theoretical predictions. Our Theoretical predictions using developed relations are compared with the experimental data, and results of Mori Tanaka and Halpin-Tsai theoretical models as shown in **Figures 3-6**. It is found that the predicted values of effective elastic modulus using modified relations are quite close to the experimental results. To predict the theoretical results using both the well known Halpin-Tsai equations and the Mori-Tanaka theory, we have to consider many conditions for simplicity *i.e.* many assumptions are inherent to both approaches like the filler and matrix are linearly elastic, isotropic, and firmly bonded. The filler is perfectly aligned, asymmetric, and uniform in shape and size. Particle-particle interactions are not explicitly considered. Of course, for all composite theories the properties of the matrix and filler are considered to be identical to those of the pure components. Therefore, we also have developed our theory considering the above mentioned same assumptions.

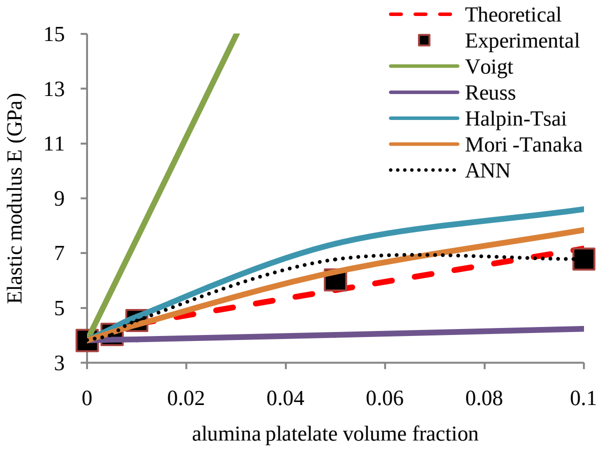

Figure 3. Experimental and predicted results of the effective elastic modulus for epoxy composite reinforced with alumina platelets, with various alumina platelets contents, based on proposed theoretical model, ANN and other models, like Voigt, Reuss, Halpin-Tsai and Mori-Tanaka model.

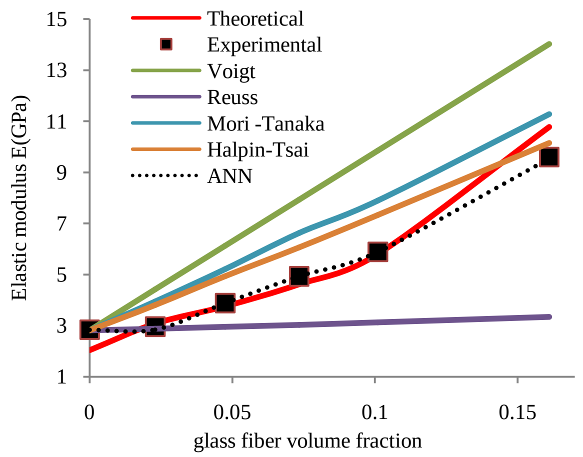

Figure 4. Experimental and predicted results of the effective elastic modulus for Glass Fiber/MMW nylon 6 composite, with various glass fiber contents, based on proposed theoretical model, ANN and other models, like Voigt, Reuss, Halpin-Tsai and Mori-Tanaka model.

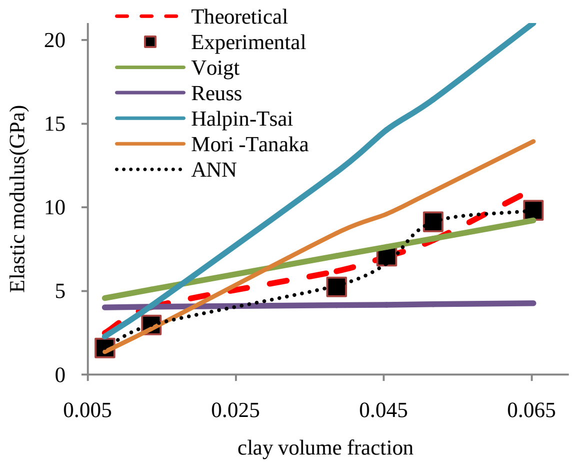

Figure 5. Experimental and predicted results of the effective elastic modulus for MXD6/clay nanocomposite, with various clay contents, based on proposed theoretical model, ANN and other models, like Voigt, Reuss, Halpin-Tsai and Mori-Tanaka model.

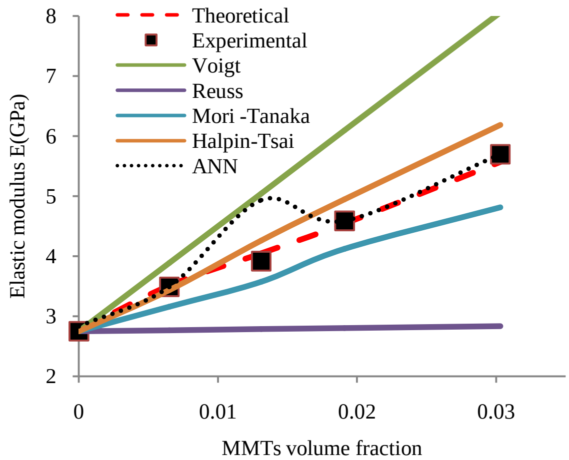

Figure 6. Experimental and predicted results of the effective elastic modulus for MMT/HMW nylon 6 composite, with various MMT contents, based on proposed theoretical model, ANN and other models, like Voigt, Reuss, Halpin-Tsai and Mori-Tanaka model.

Tables 3(a)-(d) show a comparison of experimental results of effective elastic modulus and calculated values including the correction term for all above mentioned composites. The deviation between the hypothetically predicted values from our model, and the experimental values is comparatively lower than other models, because in our model, we have used the actual ellipsoidal shape of the filler phase.

Table 3 also refers to the ANN predictions. The results of ANN computation show that ANNs have strong potential as a feasible tool for predicting the elastic modulus. Here, we used the multilayered feed-forward neural network with back propagation algorithm, because it can be trained to recognize any arbitrary mapping from an input to output by a gradient-descent based learning algorithm (*i.e.* Adaption learning function-LEARNGDM). However, it also has its boundaries, especially, slower convergence speed, which affects its practical application to a large extent. In this work, somewhat different neural network architecture is used in which, the multilayered feed-forward neural network and the recurrent neural network were combined. It's referred to as an internally recurrent neural network, which is composed of an input layer of nodes, a hidden layer and an output layer of sigmoid neurons. Unlike the ordinary feed-forward neural network, it adds an additional unit to the input layer of the above network, called a context or state layer. Two bias nodes are separately added to the hidden and the output layer. Cross validation was used as the stop criterion during the training of algorithms, when the set of data was divided into training set and test set. To determine for which internal architecture of ANN, we may obtain the closest results, two hidden layers were used and tested for 10 neurons, with bias and sigmoid activation in the hidden neurons and linear activation in the output neuron. Here, MATLAB R2010bSP1 was used to apply the ANN. We can realize by our computations that this "three input ANN model" show results closer to the experimental data analyzed, except some values which may be regarded as experimental errors.

Further **Figures 3-6** show the comparison between the experimental and the theoretical values of the elastic modulus for Epoxy/Alumina, Glass Fiber/MMW nylon 6, MXD6/Clay, and MMT/HMW nylon 6 composite materials, respectively, as a function of filler content. It is seen from the **Figures 3-6**, that with the increase in the filler concentration, the effective elastic modulus increases with the increase of filler concentration. We can observe from figures, that the predicted values of effective elastic modulus using modified relations are quite close to the experimental results.

These **Figures 3-6** include ANN predictions too. Thus ANN results and theoretical predicted results are compared with the experimental data, Mori Tanaka and Halpin-Tsai theoretical models. The ANN Architecture is used for different numbers of input neurons and different mixed models (Training function-TRAINLM, Number of Layers 2). **Tables 3(a)-(d)** show the comparison of the results obtained using different ANN architectures with optimum number of neurons in the hidden layer for all considered samples.

We observe that for three input ANN architecture, best results are obtained with 10 neurons. Besides this statistical comparison, the graphical comparison, as shown in **Figures 3-6** reveals that the predictions of ANN are very close to the experimental data and appear as a good option. In reality, the composite materials have been the complex structured materials. Therefore, it may not be practical to describe all details of the internal structure accurately. As the effective mechanical properties depend on various characteristics of the material, accounting for all these is a complex affair. The complexity of geometry encountered, along with the large difference in elastic properties of the constituents makes it difficult to predict the effective mechanical properties.

For this reason, we have used artificial neural networks (ANNs) for the prediction of effective mechanical properties of composite materials. In a simplified mathematical model of the neurons, the effects of the synapses are represented by connection weights that modulate the effect of the associated input signals, and the non-linear characteristic exhibited by neurons is represented by a transfer function. The neuron impulse is then computed as the weighted sum of the input signals, transformed by the transfer function. The learning capability of an artificial neuron is achieved by adjusting the weights in accordance to the chosen learning algorithm. The learning purpose in artificial neural networks is to update weights, so that with presenting set of inputs, desired outputs are obtained. ANN is identified and learns correlated patterns between input data sets and corresponding target values. After training, ANNs are used to predict the outcome of new independent input data. Training is a process that finally results in learning. During this process, the connecting weights between layers are changed until the difference between predicted values and the target (experimental) is reduced to the permissible limit.

Weights interpret the memory and knowledge of a network. With the aforementioned conditions, learning process takes place and trained ANN is used for prediction of outputs of new unknown patterns. For learning this network, back propagation (BP) learning algorithm is used. In the case of BP algorithm, the first output layer weights were updated. A desired value exists for each neuron of output layer. The weight coefficient was updated by this value and learning rules. During training the network, calculations were carried out from input of network toward output and error was then propagated back through the network to prior layers, updating the individual weights of the connections and the biases of the individual neurons. Output calculations were conducted layer to layer so that the output of each layer was the input of next one. Thus error is minimized and best output results are achieved. The main advantage of the ANN approach is that the predictions do not depend upon empirical parameters and is easy to perform.

The aim of the ANN is to predict as accurately as possible the desired output corresponding to an input value. This is realized by training the network, *i.e.* changing the weight values until satisfying results are obtained for given number of training data. After training the network it is expected that the network will also give a correct output response for other data from the data set. Now, we can conclude that the predicted results for elastic modulus using three input ANN model, show good results in the qualitative and quantitative analysis. Therefore, its use is practical for the region analyzed with an elevated training set.

4. Conclusions

The comparison between the experimental data and the proposed model's predictions is made in the present study. Composite materials have been assumed to contain ellipsoidal particles, arranged in a regular three-dimensional cubical geometry. It shows some dependence on the micro structural characteristics and the interconnectivity of each phase and the bonding characteristics of an interface may also affect the elastic modulus of the composite. The elastic properties of the composite materials depend strongly on the elastic properties of their individual phases, and their concentration. This dependence is considered by putting a correction factor in the place of the volume fraction in the derived expression, to calculate the effective elastic modulus. Experimental results of four composites (Epoxy/Alumina, Glass Fiber/MMW nylon 6, MXD6/Clay, and MMT/HMW nylon 6) are used to validate the modified relations. Additionally to compare, theoretical results of Mori Tanaka and Halpin-Tsai models are also used. One may observe that here as $E_1 > E_2$, the effective elastic modulus increases, with the increase in the filler concentration. Thus the additional merits of the proposed theoretical model are as follows:

1) The proposed model for prediction of the EEM of systems holds not only for systems for which the EEM of the constituent phases is comparable, but also for systems having a high EEM ratio of the filler and matrix phases, whereas one may find that other models give higher deviations in those situations.

2) This model enables one to avoid the introduction of sphericity or any other factor in the expression of EEM, making the model simple but powerful enough without compromising on the results.

3) This model can also be used with generalization conditions for three-dimensional cubicarray with spherical particles. The generalization to ellipsoidal particles is a useful one, since the ellipsoid can be used to model a variety of particle shapes, including discs and fibers in limiting cases.

The theoretically calculated values of the elastic modulus are in good agreement with the experimental values for all the composite materials. In the present paper, application of artificial neural networks to predict the elastic modulus is investigated. This work shows a possible applicability of ANN to predict the elastic modulus of composites with ellipsoidal inclusions. An ANN model is trained and tested using the available test data collected from the literature. The ANN model is found to predict elastic modulus of the composites well within the ranges of the input parameters considered. The elastic modulus results predicted by ANN are also compared to those obtained using results of the developed ellipsoidal theoretical model as well as Mori Tanaka and Halpin-Tsai models. These comparisons show that ANNs have strong potential as a feasible tool for predicting elastic modulus of composites with ellipsoidal inclusions within the range of input parameters considered. Thus, application of ANN provides us with an additional option to predict the effective properties of the composites and the results obtained using optimum architecture of ANN are reasonably compatible with the experimental data.

Acknowledgements

A Junior Research fellowship awarded by CSIR-UGC to one of the authors (AU) is gratefully acknowledged.

References

[1] Voigt, W. (1889) Ueber die Beziehung zwischen den beiden Elastizita tskonstanten isotroper Korper. *Annalen der Physik*, **38**, 573-587. http://dx.doi.org/10.1002/andp.18892741206

[2] Reuss, A. (1929) Berechnung der Fliessgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle. *ZAMM—Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, **9**, 49-58. http://dx.doi.org/10.1002/zamm.19290090104

[3] Hashin, Z. (1962) The Elastic Moduli of Heterogeneous Materials. *Journal of Applied Mechanics*, **29**, 143-150. http://dx.doi.org/10.1115/1.3636446

[4] Hashin, Z. and Shtrikman, S. (1963) A Variational Approach to the Theory of Elastic Behaviour of Multiphase Materials. *Journal of the Mechanics and Physics of Solids*, **11**, 127-140. http://dx.doi.org/10.1016/0022-5096(63)90060-7

[5] Gusev, A.A., Hine, P.J. and Ward, I.M. (2000) Fiber Packing and Elastic Properties of Transversely Random Unidirectional Glass/Epoxy Composite. *Composites Science and Technology*, **60**, 535-541. http://dx.doi.org/10.1016/S0266-3538(99)00152-9

[6] Lusti, H.R., Hine, P.J. and Gusev, A.A. (2002) Direct Numerical Predictions for the Elastic and Thermo Elastic Properties of Short Fibre Composites. *Composites Science and Technology*, **62**, 1927-1934. http://dx.doi.org/10.1016/S0266-3538(02)00106-9

[7] Segurado, J. and Llorca, J. (2003) A Numerical Approximation to the Elastic Properties of Sphere-Reinforced Composites. *Journal of the Mechanics and Physics of Solids*, **50**, 2107-2121. http://dx.doi.org/10.1016/S0022-5096(02)00021-2

[8] Jweeg, M.J., Hammood, A.S. and Al-Waily, M. (2012) Experimental and Theoretical Studies of Mechanical Properties for Reinforcement Fiber Types of Composite Materials. *International Journal of Mechanical & Mechatronics Engineering*, **12**, 62-75.

[9] Upadhyay, A. and Singh, R. (2012) Elastic Properties of Al_2O_3-NiAl: A Modified Version of Hashin-Shtrikman Bounds. *Continuum Mechanics and Thermodynamics*, **24**, 257-266.

[10] Modniks, J. and Andersons, J. (2010) Modeling Elastic Properties of Short Flax Fiber-Reinforced Composites by Orientation Averaging. *Computational Materials Science*, **50**, 595-599.

[11] Ji, B. and Wang, T. (2003) Plastic Constitutive Behavior of Short-Fiber/Particle Reinforced Composites. *International Journal of Plasticity*, **19**, 565-581. http://dx.doi.org/10.1016/S0749-6419(01)00041-9

[12] Koker, R., Altinkok, N. and Demir, A. (2007) Neural Network Based Prediction of Mechanical Properties of Particulate Reinforced Metal Matrix Composites Using Various Training Algorithms. *Materials and Design*, **28**, 616-627. http://dx.doi.org/10.1016/j.matdes.2005.07.021

[13] Sha, W. and Edwards, K.L. (2007) The Use of Artificial Neural Networks in Materials Science Based Research. *Materials and Design*, **28**, 1747-1752. http://dx.doi.org/10.1016/j.matdes.2007.02.009

[14] Halpin, J.C. (1969) Stiffness and Expansion Estimates for Oriented Short Fiber Composites. *Journal of Composite Materials*, **3**, 732-734.

[15] Halpin, J.C. and Kardos, J.L. (1976) The Halpin-Tsai Equations: A Review. *Polymer Engineering & Science*, **16**, 344-352. http://dx.doi.org/10.1002/pen.760160512

[16] Ashton, J.E., Halpin, J.C. and Petit, P.H. (1969) Primer on Composite Materials Analysis. Technomic Publishing Company, Stamford.

[17] Mori, T. and Tanaka, K. (1973) Average Stress in Matrix and Average Elastic Energy of Materials with Misfitting Inclusions. *Acta Metallurgica*, **21**, 571-574. http://dx.doi.org/10.1016/0001-6160(73)90064-3

[18] Eshelby, J.D. (1957) The Determination of the Elastic Field of an Ellipsoidal Inclusion and Related Problems. *Proceedings of the Royal Society A*, **241**, 376-396. http://dx.doi.org/10.1098/rspa.1957.0133

[19] van Es, M., Xiqiao, F., van Turnhout, J. and van der Giessen, E. (2001) Chapter 21: Comparing Polymer-Clay Nanocomposites with Conventional Composites Using Composite Modeling. In: Al-Malaika, S. and Golovoy, A.W., Eds., *Specialty Polymer Additives*: *Principles and Applications*, Blackwell Science, CA Malden, 391-414.

[20] Hui, C.Y. and Shia, D. (1998) Simple Formulae for the Effective Moduli of Unidirectional Aligned Composites. *Polymer Engineering & Science*, **38**, 774-782. http://dx.doi.org/10.1002/pen.10243

[21] Van Olphen, H. (1977) An Introduction to Clay Colloid Chemistry: For Clay Technologists, Geologists and Soil Scientists. 2nd Edition, Wiley, New York.

[22] Clark, S.P., Ed. (1966) Handbook of Physical Constants, Geological Society of America. Memoir 97, The Geological Society of America, Inc., New York, 50-89.

[23] Kohen, M.I. (1995) Nylon Plastics Handbook. Hanser, New York.

[24] Alexandrov, K.S. and Ryshova, T.V. (1961) The Elastic Properties of Rock-Forming Minerals. II: Layered Silicates. *Bulletin USSR Academy of science*, *Geophysics Series* 9, **12**, 1165-1168.

[25] McNeil, L.E. and Grimsditch, M. (1993) Elastic Moduli of Muscovite Mica. *Journal of Physics*: *Condensed Matter*, **5**, 1681-1690. http://dx.doi.org/10.1088/0953-8984/5/11/008

[26] Sheng, N., Boyce, M.C., Parks, D.M., Rutledge, G.C., Abes, J.I. and Cohen, R.E. (2004) Multiscale Micromechanical Modeling of Polymer/Clay Nanocomposites and the Effective Clay Particle. *Polymer*, **45**, 487-506. http://dx.doi.org/10.1016/j.polymer.2003.10.100

[27] Shukla, D.K. and Parameswaran, V. (2007) Epoxy Composites with 200 nm Thick Alumina Platelets as Reinforcements. *Journal of Materials Science*, **42**, 5964-5972. http://dx.doi.org/10.1007/s10853-006-1110-8

[28] Fornes, T.D. and Paul, D.R. (2003) Modeling Properties of Nylon 6/Clay Nanocomposites Using Composite Theories. *Polymer*, **44**, 4993-5013. http://dx.doi.org/10.1016/S0032-3861(03)00471-3