CHAPTER 3

MATERIALS AND METHODS

3.1 FUNCTIONALIZATION AND DISPERSION OF MWCNTs

3.1.1 Introduction

In order to make use of carbon nanotubes effectively and utilize their extraordinary properties, they should be functionalized and well dispersed within the reinforced matrix. Functionalization is a significant aspect in the chemistry of carbon nanotubes, these chemical exploitations being necessary for many of the applications of CNTs. Multi-walled carbon nanotubes (MWCNTs) have been functionalized by both covalent and non-covalent chemical treatments (Rao & Govindaraj 2005). This technique is extensively used for chemical treatment of the surface of CNTs.

The chemical treated CNTs will facilitate in improving the efficiency of dispersion and the bonding between the CNTs and with the material matrix. Dispersion of CNTs means scattering the nanotubes separately within the matrix by separating the agglomerations and bundles. In this study, dispersion of CNTs within the epoxy was the major part in controlling the tribological properties of the epoxy/MWCNTs nanocomposites. Poor dispersion of these MWCNTs within the epoxy matrix will not improve the nanocomposites properties, similarly it significantly degrade and deteriorate the matrix properties. Multi wall Carbon nanotubes in dry conditions forms a bundle together due to the Van Der Waals forces.
These interfacial forces at the nano level are strong and sufficient to pull the nanotubes stick together, even after being dispersed in an aqueous solution. Chemical surfactants that give non-covalent bonds have been used to decrease the surface tension of the solution and maintain the CNTs suspension and it is unbundled within the solution after they have been dispersed by mechanical dispersion.

3.1.2 Chemical treatment of MWCNTs

The chemical treatment techniques are widely used for the surface treatment of CNTs. Several different approaches have been used for chemical treatment (functionalization) of CNT surfaces, and many of them exhibit good results in effectively dispersing CNTs within the matrix and improve the bonding between the CNTs and host matrix. There are two main functionalization namely, covalent and non-covalent functionalization.

Covalent functionalization is extensively used in the nanocomposites preparation in the recent development. It is one of the extensive tools for CNT and CNF dispersion and also opened the way to many applications of different nanocomposites by improving the reactivity and bonding between functionalized CNTs and the hosting matrix. Covalent functionalization has effectively utilized these CNTs into usable composite materials.

Numerous approaches have been used to functionalize CNTs for epoxy nanocomposites, like acid treatment, oxygen treatment, ozone treatment and plasma oxidation. The main purpose of these processes is to provide a functional group at the side surface of CNTs to enhance dispersion and increase the reactivity and bonding strength between functionalized CNTs and the matrix by covalent bonds. The most common functional groups used
in epoxy/MWCNTs nanocomposites are the oxygen groups, which include hydroxyl, carboxyl, carbonyl, and ester side groups.

The development of carbon nanotubes reinforced with epoxies could be made via chemical functionalization of CNTs with multifunctional amines. The enhancement of the bonding to the matrix as well as a better dispersion of the CNTs could be observed by Zhu et al (2003). A schematic illustration of functionalization process is shown in Figure 3.1 (Schulte et al 2005). In the first step, an oxidative treatment of the nanotubes was used to develop carboxylic groups. This guides to an opening of the CNT cap, which would facilitate to direct bonding of the carbon nanotubes and end to the matrix via the carboxylic groups. In the second step, the carboxylic groups would react with multifunctional amines and form bonds either ionic or covalent to these amines via an acid-base reaction.

In the third step, with the addition of the epoxy resin, the free suspended amino functions on the surface of CNTs will react with the epoxy molecules forming equivalent bonds, which lead to an improved nanotubes matrix bonding. The effect of functionalization to attain bonding between the matrix and the nanotubes was shown by Frankland et al (2002) via molecular dynamics simulation. The acid treatment enables steady aqueous solution of catalytically produced MWCNTSs to be prepared (Shaffer et al 1998). Solution based methods have also been used to produce CNTs/polystyrene composites. Both SWNTs and MWCNTSs were solubilized by functionalizing with a polystyrene (PS) copolymer (Hill et al 2002).

This was attained by acid treatment of the carbon nanotubes and then carrying out etherification of the surface bound carboxylic acid. The polymer modified carbon nanotubes were shown to be soluble in common organic solvent. The polymer modified carbon nanotubes were shown to be soluble in common organic solvent. The chemical functionalization of
MWCNTs improves the compatibility with the epoxy matrix due to the formation of an interface with stronger interconnections. This, in turn, causes a substantial decrease in the electrical conductivity with respect to the untreated MWCNTs which can be described in terms of tunnelling resistance between interacting nanotubes (Guadagno et al 2011).

Figure 3.1  Functionalization processes of CNTs showing the steps from the oxidation to the composite manufacturing

In the non-covalent functionalization, the commonly used chemical surface etchant’s was used during sonication process. The highest purpose of these chemical surfactants is to decrease the surface tension of the water, thereby helping to separate the carbon nanotubes and keep them suspended and separated within the solution. The non-covalent functionalization approach offers the least amount of damage to the CNT surfaces since no defects are caused by the chemical surfactant to the surface of the CNTs and the only impairment will be due to excessive sonication power induced.
Although it is very inspiring to obtain good dispersion within epoxy composites, it is more exciting to estimate quantitatively the level of dispersion of carbon nanotubes within many matrices, especially within epoxy nanocomposites. However, some researchers assessed the dispersion of CNTs experimentally, SEM and TEM imaging can give some impression on how CNTs are qualitatively dispersed within the host matrix.

3.1.3 Mechanical Dispersion of MWCNTs

Mechanical dispersion can be carried out using ultrasonic wave mixer without any chemical surfactants. However, the ultrasonic wave mixer is sufficient to break the Van Der Waals forces between the CNTs and detach them in the aqueous solutions. The ultrasonic wave mixer as shown in Figure 3.2, induces high energy into the solution with high frequency vibrations, causing vacuum bubbles i.e micro and nano cavitation to be formed among the solution molecules.

![Figure 3.2 Dispersion of MWCNTs using ultrasonic wave mixer](image-url)
These micro and nano vacuum bubbles will detonate when they touch the CNT surfaces. The detonate bubbles will cause a massive vacuuming force that will pull out the nanotubes away into the solution. Hence, the CNTs will be separated from each other and in used in the solution, the suspended CNTs will start to agglomerate and bundle again. In order to disperse the CNTs effectively, adequate energy and sonication time should be applied. If excessive amounts of sonication energy, sonication time and both are introduced into the CNT solution, the huge forces from detonate micro bubbles will fracture the nanotubes. Optimizing the sonication process will require the optimum combination of sonication energy, duration, volume of solution, concentration of nanotubes, temperature, amount, and type of chemical surfactant like anionic, cationic and non-ionic used in the solution.

3.1.4 Fundamental aspects of Dispersion

Liu & Wagner (2005) from his investigation, functionalization of carbon nanotubes is not always essential to prepare a polymer composite. A good dispersion not only makes more filler surface area, but also prevents aggregation of the filler action as stress concentrators as well as slippage of CNTs during composites loading, which all decrease the performance of the composites greatly. Since nanofillers have an extremely high surface area, only a few polymer molecules can penetrate between them while reinforced with matrix.

Now, if the CNTs should equally distribute in the matrix polymer, some challenges should be faced like volume fraction, length of the tubes, their entanglement and the high matrix viscosity. With increasing CNT length, the resulting interactive forces are similar to the influence of the molecular weight that (chain length) hinder the separation of the tubes. The shear forces introduced into the suspension in order to split the agglomerates and to disperse the CNTs are controlled during manufacturing process.
Dispersion of the nanotubes can be done through various methods like stirring, calendaring and sonication.

Sonication method is only suitable for very low viscous matrix materials and small volumes because ultrasonic devices produce high impact of energy, but introduce small portion of shear forces. The effectiveness of the dispersion is limited as the local introduction of the energy leads to a rupture and damage of CNTs reducing the overall aspect ratio (Lu et al 1996). In his report MWCNTs were sonicated for 20 min at 30% amplitude, mixed with the epoxy resin and again sonicated for 10 min. After that, agglomerates are still remained as shown in Figure 3.3.

![Image of TEM images of sonicated Epoxy/MWCNTs composites](image)

**Figure 3.3 TEM images of sonicated Epoxy/MWCNTs composites**

A reduction in the agglomerate size can be attained with a functionalization process (Gojny et al 2003). Similarly, an appropriate procedures to apply the sonication technique to produce CNT–polymer
nanocomposites is to disperse them in a suitable solvent like acetone, ethanol etc., In which the first allows the agglomerates to be separated due to vibrational energy. The suspension can later be mixed with the polymer and the solvent can simply be evaporated by heating. Morphology and physical properties of poorly dispersed without solvent and well-dispersed in ethanol, CNTs/epoxy composites have been analysed by Seok & Ryoun (2004).

He revealed that superior tensile strength, electrical conductivity and thermal conductivity are observed from well dispersed CNTs/epoxy composites over poorly dispersed one. The combination of sonication and an oxidative process where the functional groups, increase the surfaces of the CNTs, which lead to electrostatic interactions with the solvent, and it results an enhanced distribution of CNTs in the matrix.

Stirring is a common method to disperse nanoparticles. The dispersion result can be controlled by the shape and size of the propeller and the mixing speed. After vigorous stirring of MWCNTs in epoxy resin, a relative fine dispersion can be attained (Sandler et al 1999). However, the re-agglomeration of MWCNTs is mainly caused by frictional contacts and elastic interlocking mechanisms (Schmid & Klingenberg 2000).

Calender is another method to disperse carbon nanotubes and nano-particles into the host matrix. It is a promising approach to reach an excellent state of dispersion (Gojny et al 2004). A major benefit of this method is, that besides the improved dispersion results, efficient manufacturing of larger quantity of nano-composites can be achieved. Alternatively, insufficient dispersion may be represented by discontinuities at the boundaries between mixing regions containing various concentrations of dispersed MWCNTSs (Andrew et al 2002). High shear mixing to disperse MWCNTSs may result in tube breakage.
The investigation depicts that some breakage occurs and it is meant that tube length is reduced with increasing energy input. The rate at which mean tube length decreases as the material and it is dispersed and tube separation increases. Therefore, tube breakage is not a serious problem and the aspect ratio of the tubes remains very high reducing from one by fourth. Good dispersion can be achieved at the expense of an acceptable reduction in tube length.

3.2 MIXING MWCNTs IN AN EPOXY TO MAKE THE NANOCOMPOSITES

3.2.1 MWCNTs material

The COOH functionalized multi-walled CNTs used in this study were provided by Bottom Up Technologies Corporation. The MWCNTs were produced using the chemical vapor deposition (CVD) process. Typically to perform a reflux in sulfuric / nitric acid to functionalize the surfaces of these nanotubes which is resulted in the attachment of carboxyl (-COOH) groups on the nanotubes surface by chemical bonding. Amide (NH₂) functionalized nanotubes are a derivative of COOH functionalized nanotubes.

Generally COOH group is reacted with SOCl₂ (thionyl chloride) will form an Acyl chloride, and then it reacts with dimethylamine to functionalize these nanotubes. Amine functionalization is strongly recommended for polymer based nanocomposites formulation with CNT and for making biocompatible Carbon nanotubes for numerous applications. The SEM image (Figure 3.4) and physical properties provided by the manufacturer are listed table 3.1.
Figure 3.4 SEM image of supplied MWCNTs

Table 3.1 Physical properties of MWCNTs – COOH treated

<table>
<thead>
<tr>
<th>Description</th>
<th>MWCNTs-COOH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purity</td>
<td>&gt;92%</td>
</tr>
<tr>
<td>Diameter</td>
<td>20-30nm</td>
</tr>
<tr>
<td>Length</td>
<td>10-15 micron</td>
</tr>
<tr>
<td>Specific surface area</td>
<td>&gt; 200 m²/g</td>
</tr>
<tr>
<td>No. of walls</td>
<td>7-8</td>
</tr>
<tr>
<td>Metallic impurities</td>
<td>&lt;5%</td>
</tr>
<tr>
<td>Colour</td>
<td>Black</td>
</tr>
<tr>
<td>State</td>
<td>Amorphous powder</td>
</tr>
</tbody>
</table>
3.2.2 MWCNTs Solution Preparation

The solution preparation process of the epoxy-MWCNTs nanocomposites mixture is started by weighing the required quantity of the CNTs using electronic weighing machine with the least count of 0.01mg. The necessary quantities of the acetone and the surfactant were measured and added together with the CNTs into a water jacketed beaker with a capacity of 100ml and 250 ml as shown in Figure 3.5.

The dispersion process was carried out using an ultrasonic mixer. The high frequency of the ultrasonic waves produced the vibration, and its transferred through the 13 mm titanium alloy probe to the acetone medium with a maximum power that could reach 450 - 500 W and a frequency of 10 kHz. It provided a uniform dispersion of the CNT filaments in the solution. Under sufficient ultrasonic wave power and for a certain period of sonication time, the high energy put into the mixture broke the agglomerations and bundle of the CNTs by breaking the chemical bonding of the Van Der Waals forces between the nanotubes.

![Figure 3.5 Water jacketed beakers](image-url)
The high ultrasonic wave power develops the heat into the solution resulting small amount of acetone and it is getting evaporated from the solution. In order to decrease the solution temperature, the water flow from inlet to outlet in the water jacket beaker and it is helped to maintain the temperature less than 45° C and reduced the excessive evaporation throughout the dispersion process.

The amount of ultrasonic wave power and time length of dispersion were a critical phenomena for achieving a good dispersion of CNTs. Less energy and time could not guarantee a good dispersion, while adequate energy and time would dissolve and break the nanotubes. The sonication power for all the different weight fraction of MWCNTs solutions was 40W and the power per solution volume was 0.8 W/ml of the solution. The sonication period for the different MWCNT weight fraction is 30 min.

3.2.3 Mixing of MWCNTs solution with Epoxy

The necessary amount of sonicated MWCNTs solution was taken into Speed mixer DAC 150.1 FV-K dual asymmetric centrifuge as shown in Figure 3.6(a). The required quantity of epoxy resin and MWCNTs are filled into a small cup with the capacity of 100 ml. The cup is inserted into the speed mixer with a 30° inclination angle as shown in Figure 3.6(b). During the mixing process, the cup rotates in its z-axis and the base plate rotates in vertical axis in opposite direction. The mixing process is based on a kind of high-power shaking. Due to the centrifugal forces, only minimum amount of air is entrapped in the mixture. This mixing process lasted 5 min at 1500 rpm.

After stirring was done, the mixture was evacuated and aerated by turns until no more bubbles were generated. In the earlier step, the pure epoxy was kept in another beaker with required quantity. The blender was stated with dispersion solution and then the pure epoxy was added gradually
to the MWCNTs solution. When increasing the speed of mixer, the solution spread, split and stuck on the jar. To avoid this low and medium speed was maintained during processing.

![SpeedMixer](image)

**Figure 3.6** (a) Speed mixtures machine (b) cup titled into 30° angle.

### 3.2.4 Casting the epoxy-MWCNTs nanocomposites into the Molds

Epoxide-MWCNTs nanocomposites mixing were done, the nanocomposites solution was poured into another beaker. The hardener, araldite HY 951 was mixed with epoxy-MWCNTs in the ratio of 10:1 and the sonication continued for another 30min. Hardener is a substance which thermally reacts in room temperature to convert epoxy resin to epoxy plastic. The reaction is called exothermic, which means that the heat is dissipated. The reaction between an epoxy resin and hardener is an irreversible poly addition. The products are formed and the epoxy composites are decomposed into epoxy, MWCNTs and hardener.
Immediately after mixing the epoxy-MWCNTs nanocomposites are poured into the acrylic plastic molds of 100mm length and 6mm diameter for wear test. Similarly, nanocomposites are poured into acrylic plastic molds size of 85X 25X10 mm as shown in figure 3.7 (a & b) for wear and erosion test respectively.

![Figures 3.7](image)

**Figure 3.7 Acrylic plastic moulds for (a) wear and (b) erosion samples**

The acrylic plastics molds were chosen for their smooth surfaces and small dimensional tolerances. The process was repeated for all the samples of epoxy/MWCNTs of 0.1wt.%, 0.5wt.%, 1.25wt.%, 2.5wt.% and 5wt.%. The moulds were kept in the oven at 110°C for 8 hours for curing. The cured specimens were cut into pins of 30mm length for wear test as shown in figure 3.8. Similarly, rectangle specimen was cut into the size of 25 X 25 X 10mm (figure 3.9) for erosion test. The specimen surface was cleaned before and after testing.
3.2.5 Epoxy/MWCNTs nanocomposites

Six different epoxy-MWCNTs nanocomposites samples were produced during the course of investigation. The first sample was the pure epoxy as reference sample and other five samples contain different weight fraction of MWCNTs in the pure epoxy. The five different weight fraction are
0.1wt.%, 0.5wt.%, 1.25wt.%, 2.5wt.% and 5wt.% of MWCNTs into the pure epoxy. Each weight fraction nearly three or four specimens were made to get a representative average value from wear and erosion testing. Similarly, nearly 20 to 25 specimens were made and tested on both end and nearly 40 to 50 experimental results were obtained for developing computational numerical results in Artificial neural network using Matlab software.

3.3 EXPERIMENTAL WORK

3.3.1 Wear and Friction

The pin on disc machine as shown in Figure 3.10 was used to observe the wear and friction behavior of the pure epoxy and epoxy/MWCNTs nanocomposites. The pin shaped pure epoxy and proposed nanocomposites specimen were held against a high speed rotating steel disc of EN8 material with hardness 60HRc and surface roughness Ra1.6. A fixed track diameter of 50mm was used with constant speed of 200rpm for 942m with the time span of 30min. The tests were conducted in the room temperature for all the samples without changing the operating conditions.

The sliding load of 30N, 60N and 90N was applied to evaluate the wear and friction behavior of pure epoxy and proposed nanocomposites. The machine was connected with the hardware unit to initialize and set the parameter of disc speed, time and load. The schematic illustration of pin on disc, load and wear track as shown in Figure 3.11.

Basically, the wear process removes some materials from the sample. The pin sample was initially weighed to an accuracy of 0.1mg in an electronic balance. The difference between the initial and final weight is the measure of slide wear loss. For each condition, at least three tests were performed and the mean value of the weight losses is reported.
The contact surface was polished with an emery paper of 600 grit size to ensure the uniform contact with the rotating disc. The frictional coefficient was recorded and calculated by the ratio between the tangential force and normal load. The surface of both disc and samples were cleaned with a soft paper which is soaked in acetone and thoroughly dried before the test.

Figure 3.10 Pin on disc machine experimental setup

Figure 3.11 Schematic illustration of Pin on disc machine, load and wear track
\[ W_s = \frac{\Delta m}{F_N l \rho \left( \frac{mm^3}{Nm} \right)} \]  

where \( \Delta m \) = mass of worn specimen (g), \( F_N \) = normal force (N), \( l \) = sliding distance (m) and \( \rho \) = specific gravity of composite (g/cm\(^3\)). The same procedure was adopted for all specimens. After completing the wear test, the worn surface of the pin material was examined by field emission scanning electron microscopy [JEOL JFM 6701F]. The technical specification of pin on disc machine listed in Table 3.2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample Size</td>
<td>mm</td>
<td>Ø 3</td>
<td>Ø 12</td>
</tr>
<tr>
<td>Disk Size</td>
<td>mm</td>
<td>Ø 160</td>
<td></td>
</tr>
<tr>
<td>Disk Thickness</td>
<td>mm</td>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>Wear Track</td>
<td>mm</td>
<td>Ø 20</td>
<td>Ø 145</td>
</tr>
<tr>
<td>Disk Rotation</td>
<td>RPM</td>
<td>200</td>
<td>2000</td>
</tr>
<tr>
<td>Normal Load (in step of 5 N)</td>
<td>N</td>
<td>5</td>
<td>200</td>
</tr>
<tr>
<td>Wear</td>
<td>Micrometer</td>
<td>0</td>
<td>2000</td>
</tr>
</tbody>
</table>

### 3.3.2 Erosion Test

The erosion test rig as shown in Figure 3.12 was used to evaluate the erosive performance of epoxy/MWCNTs nanocomposites. The test rig consists of a particle feeder, air drying unit, air compressor, accelerating chamber and air particle mixing unit. The irregular silica sand particles with
the size of 100±20µm are mixed with compressed air in mixing unit and then accelerated by passing the mixture through a convergent brass nozzle of 2.5mm internal diameter.

The erosion test was carried out in room temperature. The rotating disc method is used to determine the velocity of eroding particles. The mass flow rate and average particle velocity distribution throughout the flow cross section were obtained from pressure at various distances from the nozzle tip. It was found that the average uniform velocity at higher pressure is attained at 12mm distance from nozzle tip around the flow axis. This setup has the capacity of developing erosive situation for assessing erosion resistance of the nanocomposites samples.

Figure 3.12 Schematic diagram of erosion test machine
Table 3.3 Erosion test parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Erodent</td>
<td>-</td>
<td>Silicon Sand Particles</td>
</tr>
<tr>
<td>Erodent Size</td>
<td>μm</td>
<td>100 ± 20</td>
</tr>
<tr>
<td>Erodent Shape</td>
<td>-</td>
<td>Irregular</td>
</tr>
<tr>
<td>Impingement Angle</td>
<td>Degree</td>
<td>30°, 60° &amp; 90°</td>
</tr>
<tr>
<td>Nozzle Diameter</td>
<td>mm</td>
<td>2.5</td>
</tr>
<tr>
<td>Sample Size</td>
<td>mm</td>
<td>25 X 25 X 10</td>
</tr>
<tr>
<td>Erosion Time</td>
<td>min</td>
<td>5</td>
</tr>
<tr>
<td>Nozzle to Sample Distance</td>
<td>mm</td>
<td>12</td>
</tr>
</tbody>
</table>

The erodent particles impact the samples which can be mounted on in the specimen holder. The sample size is approximately 25 X 25 X 10 mm. The mounted specimens were subjected to three impingement angles between 30° and 90° with the increment of 30°. Wear was measured by weight loss of the specimen. Electronics balancing with sensitivity of 0.1mg was used to measure the weight loss before and after the erosion test. The eroded surface morphology of some specimens was examined by the field emission scanning electron microscope to understand the mechanism of material removal. The samples were gold-sputtered to reduce electrostatic charging of the surface. The erosion test parameters are listed in Table 3.3.

3.3.3 Tensile Test

Tensile test was performed using Instron tensile test machine at a crosshead speed of 0.1 mm/min, according to ASTM D638. The selection of this quite low loading rate is to compare later with the results of more brittle and more rigid materials. Schematic illustration of dog bone shaped tensile specimen and machine setup are shown in Figure 3.13 and Figure 3.14. Extensometer with a gauge length of 12.5±2.5 mm was used to measure the
tensile strain. The displacement was measured by high resolution encoder with the accuracy of 0.6μm. Young’s modulus was calculated from the tensile stress–strain curve. Tensile test specimen of pure epoxy and 0.1wt.%, 0.5wt.%, 1.25wt.%, 2.5wt.% and 5wt.% of epoxy/MWCNTs nanocomposites are shown in Figure 3.15.

The specimens were tested under the condition at a temperature of 33±2°C and a relative humidity of 47±5%. The machine is connected with data acquisition system connected with the hardware unit to initialize the parameter of loading rate, gauge length, width and thickness of the specimen. The cross pitch scares gripping jaws are fitted to the top and bottom head of the machine. The dog bone shaped specimen with length of

Figure 3.13 Schematic illustration of dog bone shape tensile test specimen

Figure 3.14 Schematic illustration of tensile test machine
165mm, width 19mm, gauge length 57.15 mm and the thickness of sample after polishing is between 6 and 7 mm were fitted in the machine and loads are applied gradually with the increment of 0.1KN. The data reported are the average of the results for 3 specimens.

3.4 NUMERICAL SIMULATIONS

3.4.1 Artificial Neural Networks

Artificial neural networks are computational systems that simulate the microstructure of a biological nervous system. Inspired by the nerves system, this ANN technology is being used for variety of complex engineering and scientific problems. The ANN has emerged as good candidate to solve wide range of material science engineering problems.
Figure 3.16 A schematic illustration of an ANN architecture

The ANN should only be used in the dataset, which satisfies the following criteria (Jiang et al 2007):

1. A large datasets with more than one dependent parameter.
2. Datasets with incomplete, complex and noisy values.
3. Datasets where it is difficult to find an accurate solution by existing mathematical equations.
4. Datasets with non-linear type of data and mathematical equations is not possible to form.

The properties of polymer composites i.e., wear, creep, erosion, corrosion and fatigue meet all of these conditions. The ANN architecture is shown in Figure 3.16. The sequences of layers are input, hidden (intermediate) and the output layers, hidden layers which are constructed with
one or several layers for its practical applications. Each layer has different number of neurons in the elements. As in nature, the interconnection between these elements can be largely determined by the network functions. In this computational study the input data contains information about the testing conditions (load, sliding time, material composition) and the output identifies the specific wear rate of the specimen.

### 3.4.2 Network Training and Testing

In practical application for composite material investigation, it is necessary to collect a large enough experimental dataset that is resulted to develop an ANN with a good performance. The training algorithm, architecture and transfer function and other parameters should be carefully chosen during the ANN design. Thus, the well trained ANN can be used to obtain the solution of new input dataset in the same experimental domain. This process can be summarized in term of the following stages.


2. Training the ANN: this includes training algorithm, architecture and transfer functions.

3. Evaluate the trained network: test the network performance.

4. Using the trained ANN for simulation and prediction.

In this present computational study, material composition load and sliding load were selected as input variables and specific wear rate were chosen as output parameters. Sigmoid function is the most effective activation function in ANN architecture, because it combines constant, linear and curvilinear behavior depending on the input.
\[ f(x) = \frac{1}{1 + e^{-x}} \]  

(2)

The transform function \( f(x) = x \) served between the last hidden layer and the output layer is to minimize the output value to a small range. The phenomina of ANN with an appropriate number of hidden layer and neurons is able to approximate any functional relationship between input variable and output parameters. The number of neuron in the intermediate layer was calculated from the equation.

\[ N_n = \frac{1}{2} (Inputs + Outputs) + \sqrt{Number\ of\ training\ data} \]  

(3)

Feed forward, radial basis, pattern recognition and general regression neural network are used to solve the problems and the ANN was programmed and executed in MATLAB language. The experimental dataset was divided into two parts. One set of datasets are used for training and the other sets for testing the ANN. The wear performance of epoxy/MWCNTs nanocomposites has quite complex relationship with the input parameters. The more number of training data definitely improve the predictive quality as well. The current investigation proves that 80 experimental data sets were used to construct fully developed ANN network. Out of these, 68 datasets were used as training data and the residuals 12 were used in testing process (LiuJie et al 2007).

To obtain desired error level, the interconnections between the neurons are modified in the first dataset. Then the network was examined and evaluated by the second dataset. These values are compared to the measured values for evaluating the ANN prediction quality. The quality of the prediction can normally be characterized by the widespread identification of
root mean square error (RMSE). The high predictive quality is calculated by the following formula.

$$RMSE = \sqrt{\frac{\sum (Q_e - Q_p)^2}{\sum Q_e}}$$  \hspace{1cm} (4)

where, $Q_e$ is the experimental value of wear and $Q_p$ represents ANN predicted wear value.