International Journal of General Engineering and Technology (IJGET)
ISSN(P): 2278-9928; ISSN(E): 2278-9936
Vol. 3, Issue 1, Jan 2014, 1-10

International Academy of Science, Engineering and Technology
Connecting Researchers; Nurturing Innovations
IASET

FRACTURE TOUGHNESS ANALYSIS BY EXPERIMENTAL AND SIMULATION OF SWCNTs – RESOLE NANOCOMPOSITES

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ABSTRACT

Fracture toughness analysis for resole reinforced with single wall carbon nanotubes (SWCNTs) has been studied, in terms of mechanical properties, which are subject to changes in SWCNTs volume fraction. Simulation program for the fracture propagation was built up to comparison the experimental results with that simulation results. The nanocomposites candidates for this study were pure matrix resole and SWCNTs - resole nanocomposites. Hot press technique was used to prepare the nanocomposites as well resole specimens using flash mold at standard conditions. The impact testing machine type pendulum hammer was used in Charpy impact mode to calculate the fracture toughness according to ISO79. Simulation program of fracture propagation of the specimens was carried out using finite difference method.

Fracture toughness results show that the toughness values were increased progressively by succession of volume fraction of SWCNTs. Fracture toughness results showed a linear dependence with the SWCNTs volume fraction. These linear relationships are strongly influenced with the reinforced condition and they are attributed to the response of the nanocomposites to the impact test conditions. Such responses were appeared as plastic deformation associated with the damage observed. The experimental observation of the failure specimens are in good agreement with fracture mechanism, which concerned with debonding mechanism, which related to SWCNTs nanocomposites failure mechanism. The failure could be explained by two processes. The first is concerned with the interlaminar effects, which increase the surface energies, and the second is related to the work required for forming plastic zone. The elastic strain energy released, which represented the physical meaning of fracture toughness, was calculated by simulation program using the experimental data. Simulation results values coming higher than experimental results values. This could be explained, as the interface affect of SWCNTs – nanocomposites, which had high strength and strong bond force. Hardness and densities values coupled with optical microscopy were evidenced to the results.

KEYWORDS: Toughness, Fracture, Resoles SWCNTs, Simulation, and Nanocomposites

INTRODUCTION

Since their discovery in 1991 by Sumio Ijima [1], carbon nanotubes have been the focus of much research and many publications. Their tremendous mechanical properties have been proven and measured many times, especially for single-walled nanotube (SWCNT) that exhibits calculated values as high as (200 GPa) for tensile strength and more than 1.4 TPa of modulus [2,3]. The electronic structure of these SWCNTs is also unique. According to their chirality, they could have a metallic or a semiconductor character. Studies have been undertaken to understand, model and measure these phenomena by computer simulations and electrical and thermal properties measurements.

Even though the results currently published are not in good consistency, all studies show their excellent electrical and thermal properties [4].

Carbon nanotubes can be described as a sheet of carbon graphite rolled into a tube. An ideal nanotube can be thought of as a hexagonal network of carbon atoms that has been rolled in a cylinder. This cylinder can be several microns long and covered at each end with a cap that has the structure of a half-fullerene molecule. Some nanotubes are composed of several nanotubes assembled together in a concentric pattern. These nanotubes are called multi-walled carbon nanotubes (MWCNTs), in opposition to single walled carbon nanotubes (SWCNTs), commonly referred as nanotubes in this paper. MWCNTs and SWCNTs have different properties. However, the electronic properties of perfect MWCNTs are theoretically rather similar to those of perfect SWCNTs, because the coupling between the cylinders is weak in MWCNT [5, 6].

The main objective of this paper is to measure and understand the fracture behavior of SWCNT-reinforced resole nanocomposites. The focus selected for this paper is, in two parts. The first includes empirical impact strength test of (SWCNT) nanocomposites, and the second is to develop a finite element modeling capability that can accurately simulate crack growth in composite material shell structures. To accomplish this, a crack growth criterion based on fracture mechanics energy concepts is used. This research is particularly interested in using the energy release rate as a crack growth criterion.

THEORETICAL APPROACH

When a force is applied to material is work done in the sense that a force moves through a distance (the deformation of the material) this work is converted to elastic (recoverable) energy absorbed in the material. The original work on fracture mechanics done by Griffith and the proposed that unstable crack growth (fracture) would occur if the incremental change in the net energy (work done – elastic energy) exceeded the energy which could be absorbed in the creation of the new surface:

$$\frac{\partial}{\partial a}(w-u)\rangle\gamma\frac{\partial A}{\partial a}. \tag{1}$$

Where *w*, work done on the surface, *u*, elastic energy, *γ*, is surface energy per unit area, *A*, is a plane crack extension and *a*, is crack length. When the applied force loses not work, there is no overall change in length of the material then *w* = 0 and eq. (1) becomes:

$$\frac{\partial u}{\partial a}\rangle\gamma\frac{\partial A}{\partial a} \tag{2}$$

For through crack propagation in a sheet of material of thickness, *B*, it can be written:

$$\partial A = 2B\partial a \tag{3}$$

So eq. (1) becomes:

$$\frac{\partial}{\partial a}(w-u)\rangle 2\gamma B. \tag{4}$$

Up to now, it can be had used a local approach to fracture, by focusing on the vicinity of the crack tip. This was not the case of the original approach of Griffith, who postulated that crack propagation will occur if the energy release rate during crack growth exceeds a critical level, given by the rate of increase in surface energy associated with the formation of new crack surfaces. It can be defined the energy release rate (G_c) as the energy released per unit of crack area extension. In the specific case of thin plates, an alternative definition is possible, recurring to integration over the thickness and considering the unit length of the crack. In this way (G_c) is seen to be the energy supplied per unit length along the crack edge, and used in creating the new fracture surface. In context of fracture mechanics, the term (2 γ) is replaced by the (G_c), so that the condition for fracture is written as [7]:

$$\frac{1}{B}\frac{\partial}{\partial a}(w-u)\rangle G_C. \tag{5}$$

G_c is a material property which is referred to as the toughness, critical strain energy release rate or crack extension force, it is the energy required to increase the crack length by unit length in apiece of material of unit width. Its units (J /m^2).

Now consider apiece of material of thickness *B*, subjected to a force *F*, and the elastic stored energy, (*u*) may be expressed as:

$$u_1 = \frac{1}{2}F\delta. \tag{6}$$

Where, δ , is deflection due to force or the crack tip opening displacement. If the crack extends by small amount (∂a) then the stiffness of the material changed and there wick be small change in stiffness of the material changes and there will be small change in both load ∂F and deflection ($\partial\ \delta$). So the elastic stored energy would be [8]:

$$u_2 = \frac{1}{2}(F+\partial F)(\delta+\partial\delta). \tag{7}$$

From eq. (6) and (7) the change in stored energy as result of the change in crack length ($\partial\ a$) would be given by:

$$\partial u = u_2 - u_1 = \frac{1}{2}(F\partial\delta + \delta\partial F + \partial F\partial\delta). \tag{8}$$

The work done (∂w), as result of the change in crack length (∂a) is given by:

$$\partial w = F\partial\delta + \frac{1}{2}\partial F\partial\delta. \tag{9}$$

Using eq. (8) and (9) in eq. (5):

$$\frac{1}{2B}\left[\frac{F\partial\delta}{\partial a} - \frac{\delta\partial F}{\partial a}\right] = G_c. \tag{10}$$

If we consider the compliance (*C*) of the material this in the reciprocal of stiffness and are given by:

$$C = \frac{\delta}{F}. \tag{11}$$

$$\partial\delta = F\partial C + C\partial F$$

And using this in eq. (10) it can be got:

$$G_c = \frac{F_c^2}{2B}\frac{\partial C}{\partial a}. \tag{12}$$

F_c: is the applied force at fracture .and this can be written as :

$$u = G_c.B.\frac{C}{(\frac{\partial C}{\partial a})}. \quad (13)$$

So it can be can calculated (u) energy of fracture for different crack length (a) if we know the geometrical for factor (ϕ) which depends on compliance:

$\phi = \dfrac{C}{\partial C / \partial (\frac{a}{D})}$, where (D): thickness of material. So eq. (13) can be written as:

$u = G_c \,.\, BD\phi$. Where, $\dfrac{u}{BD\phi}$ is straight line with slop = G_c

Irwin determined fracture mechanism in materials and showed that the arrange stresses near the crack would depend on crack length (a) so the tensile stress may be defined as, fracture occurs when the applied stress level exceeds some critical value of stress strength, σ_c. Similarly ,since the stresses in the vicinity of a crack tip can be defined in terms of the stress intensity factor, a critical value of (K) exists that may be used to specify the conditions for brittle fracture; this critical value is termed the fracture toughness (K_c), and is defined by:

$$K_c = \frac{3FSY}{4w^2B}\sqrt{\pi a} \quad (14)$$

Now it can be represented (Y) as function of both crack length (a) and component width (w), as $Y\ (a\ /\ w)$. By definition, fracture toughness is a property that is the measure of a materials resistance to brittle fracture when a crack is present. Its units are the same as for the stress intensity factor ($MPa\sqrt{m}$). It can be summarized the relationship between K_c , G_c , and γ as follow [9, 10]:

$G = G_c = 2\gamma$ …………. (15)

$K_c^2 = E\ G_c$ …………… (16)

Where, E, is young modulus in GPa.

EXPERIMENTAL APPROACH

Phenol – formaldehyde resin material (resole type) designed by (PFR) in form of solid manufactured by F.C.F. was used as a matrix in preparation of composite materials. Single wall carbon nanotubes (SWCNTs) from (Hoechst, Germany) of diameter between 30 to 50 nano meters are used as reinforced resole nanocomposites. The volume fraction of (SWCNTs) included in the resole are (0.2, 0.4, 0.6, and 0.8) Vol. %. Well mixing of constituent SWCNTs and resole is done before molding for all specimens to ensure homogeneity. Molding of specific mixing ratio is carried out in flash mold using (Hot – press) technique.

The impact testing machine (pendulum type hammer) model THRCO (MT 220) was used in the Charpy impact mode. The machine has four energy scales (5J, 15J, 30J, and 45J). Requirements of Charpy test need the adjustment of the level of the machine, the transverse location at center of the pendulum, the pendulum arm for straightness the zero position of pointer, and finally measuring the vertical distance of fall of the pendulum striking edge from the trip high to its lowest point. The specimen was supported as a horizontal simple beam and was broken by a single swing of the pendulum with the impact line mid way between the supports. The energy scale was accurately corrected for frictional and resistance losses and scale errors.

SIMULATION APPROTCH

The object of fracture mechanics is to describe the behavior of a body with crack under loading. Thereby a crack is a partial or complete macroscopic separation of a body. Pre-existing cracks are very common and virtually impossible to avoid in large structures. An important question is whether a pre-existing crack will grow for a given loading. Cracks are also frequently formed during manufacturing of the material or as the result of mechanical processes during manufacturing structural parts. Based on fracture mechanics investigations the safety and reliability of a body is estimated. Modeling of fracture processes in structures and its simulations are challenging problems in mechanics as well as mathematics. Its understanding is important for the construction of structures and the development of new materials [11].

Several techniques have been developed for evaluating energy release rate in finite element analysis [12]. One of the most well-known techniques is an application of the Irwin crack closure integral described in Reference [13] where springs are placed between coincident node pairs ahead of a crack tip. The integral has the physical interpretation of being the amount of work needed to close an extension of crack. The work is defined as a product of spring forces and displacement of node pairs in the vicinity of the crack tip. This method has been widely used for modeling crack extensions with recent applications to composite materials. An advantage of this method is that it does not require stress to be computed in order to evaluate the energy. However, the very stiff springs between the crack tip nodes will likely cause a reduction of time step size for explicit time integration. Another popular approach is the so-called virtual crack extension method. The method is based on an evaluation of the change in stiffness matrix leading to the change in energy due to crack extension. This method has been extensively applied to a wide range of material responses including visco-elastic, visco-plastic and composite materials [14, 15]. Expressions for the energy release rate integral using the virtual crack extension method have disadvantages for applications with the finite element method. The energy release rate is a function of stresses and strains that are most accurately known at element integration points [16]. While the use of an integration path that passes through integration points is possible for the line integral, other inconveniences are associated with this such as evaluation of the volume integrals required in the domain integration. Therefore, the most convenient integration path is along element boundaries. In order to calculate energy release rate along element boundaries, the stresses and strains have to be computed at various locations (points/nodes) on the travel path of the integration. This requires interpolation and/or extrapolation of stresses and strains at nodes, thus reducing accuracy. Recent work described in References [17–19] using the so-called extended finite element method with level sets for modeling arbitrary crack growth also offers a promising analysis method for the class of problems of interest in this paper.

RESULTS AND DISCUSSIONS

Results of fracture toughness and its evidence were shown in Figures 1, 2 and 3. Experimental and simulation influence of SWCNTs vol. % and its directions on the fracture toughness of PFR was shown in Figure 1. From the Figure it can be seen that the behavior of experimental fracture toughness curve of PFR nanocomposites similar to that simulation curve. But the highest value it was for experimental random direction (EXP. RAN. dir.) comparing with simulation random direction (Simu. RAN. dir.). Besides, Figure 1 shows the influence of (SWCNTs) vol. % and the direction of (SWCNTs) by simulation; simulation parallel direction (Simu. PAR. dir.), simulation perpendicular direction (Simu. PER. dir.), and simulation random direction (Simu. RAN. dir.), on the fracture toughness of nanocomposites and its comparison experimental random direction (EXP. RAN. dir.) results. From the Figure it can be seen, that the values of experimental random direction results (EXP. RAN. dir.) were located between simulation perpendicular direction and simulation random direction of (SWCNTs) nanocomposites with respect to impact load direction. That can be explained as; experimentally most of (SWCNTs) were aligned in perpendicular direction with respect to impact load supplied which is led to high value of fracture toughness.

It can be explained Figure 1 by using Figures 2 which shows load distributions when the specimens were fractured by simulation operation. From the Figure, it can be seen load distribution regions, which can be explained by using crack propagation mechanism; the fracture toughness of a nanocomposite depends on a number of factors, and there is currently much speculation as to what micromechanical mechanisms contribute to the total work of fracture. The situation can be summarized in the following way. In SWCNTs nanocomposites the situation is often slightly clearer because the ends of many SWCNTs must inevitably be nearer to a crack face than half the critical transfer length and these ends will therefore be pulled from the matrix as the nanocomposite separates into two or more pieces. In such a situation, the work of pulling the SWCNTs out against the interface friction can account for a large part of measured fracture energy. In a nanocomposite in which brittle SWCNTs are very strongly bonded to a brittle matrix; cracks can propagate almost without hindrance through both SWCNTs and matrix, and the fracture energy will be little higher than that of the matrix itself. On the other hand, as it have seen, if the bond is weak, lateral tensile stresses ahead of the advancing crack tip can cause the SWCNTs to become debonded from the matrix and shearing forces at the interface can then cause these debonded regions to spread even further along the SWCNTs. Work is done when debonding occurs, because the SWCNTs and matrix move relative to one another. The debonded SWCNTs will be loaded in tension to its fracture points as the crack proceeds and it may break in the resin well away from the crack planes. In order, for the specimen to be broken into two parts these broken SWCNT ends must then, be pulled from their holes in the matrix. Figure 3 and 4 shows scanning electron microscopically (SEM) how these processes occur in the fracture region in PFR matrix.

The evidence of scanning electron microscopically results Figure 3 can be explained for the matrix and reinforcements (SWCNTs) as: when a crack propagates in a brittle material like PFR, second phase in homogeneities act as obstacles, which can be impeded the moving crack. This effect can often be directly observed by studying fracture surface features. During fracture, steps can be formed on the fracture surface as different sections of the crack front propagate on different parallel planes. As the crack propagates the crack front tends to move onto a single plane and the steps coalesce to form characteristic (river) markings. The steps so formed are perpendicular to the moving crack front and by using the pattern of the river markings on a fracture surface. The general effect of crack pinning can be extended to filled brittle polymers. A crack, pinned by a row of in homogeneities will bow out between them until the bowed-out segments meet and join beyond the in homogeneity and the crack continues its movement.

The evidence of explanation of fracture toughness shown in Figure 3 and 4, can be explained the results using the phenomenon of crack pinning as the basis of a model to explain the increase in fracture toughness of two-phase brittle materials, can be seen from another view; The elastic energy stored in a solid under stress is increased by the presence of a crack. It can be argued that the increase in energy associated with the crack as a whole could also be directly related to the crack front. Thus in principle an expression can be derived for the elastic energy associated with unit length of crack front. As a crack begins to propagate in a stressed solid, the crack front bows out between the second-phase dispersion, while remaining pinned at all positions where it encounters the dispersion. During this initial stage, new fracture surface is formed and the length of the crack front is increased due to its change in shape. Energy is therefore required both to create new fracture surface and to supply energy to the newly formed length of crack front, which possesses a line tension.

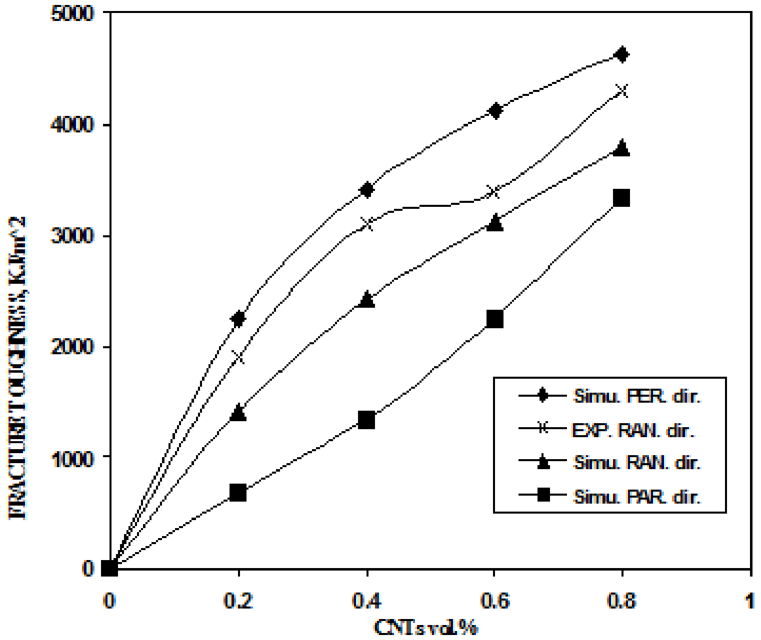

Figure 1: Influence of SWCNTs Vol % and Direction on the Fracture Toughness of Resole of Simulation Results and its Comparison Experimental Random Direction Results

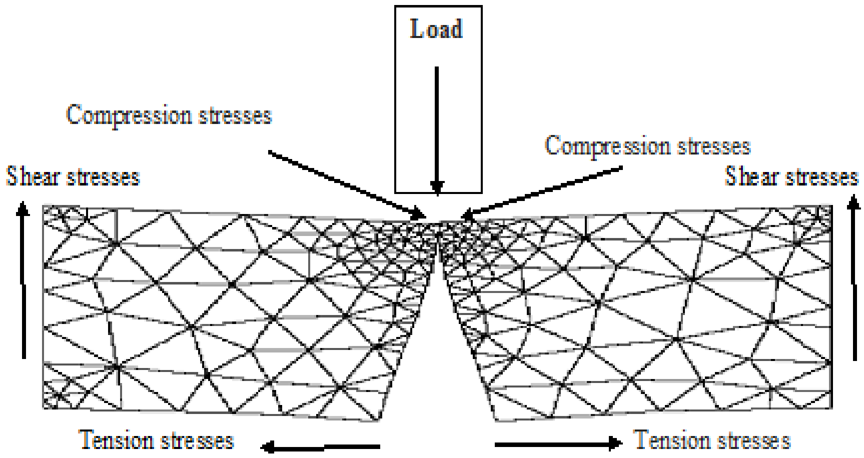

Figure 2: Simulation Load (n) Distribution in SWCNTs Resole Nanocomposite Specimen before Fractured

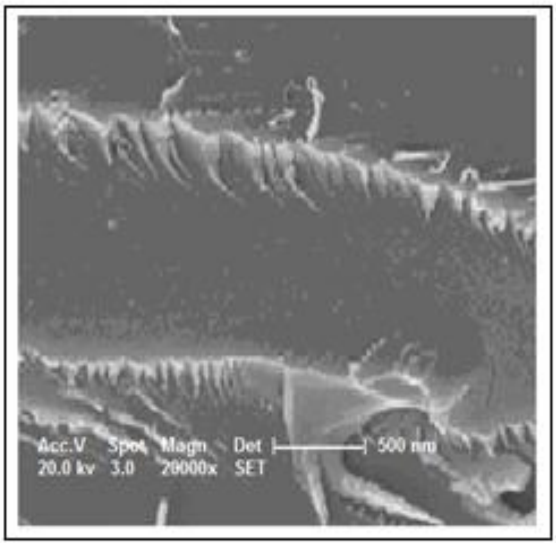

Figure 3: Fracture Surface of Pure Resole Resin Matrix without Reinforcements

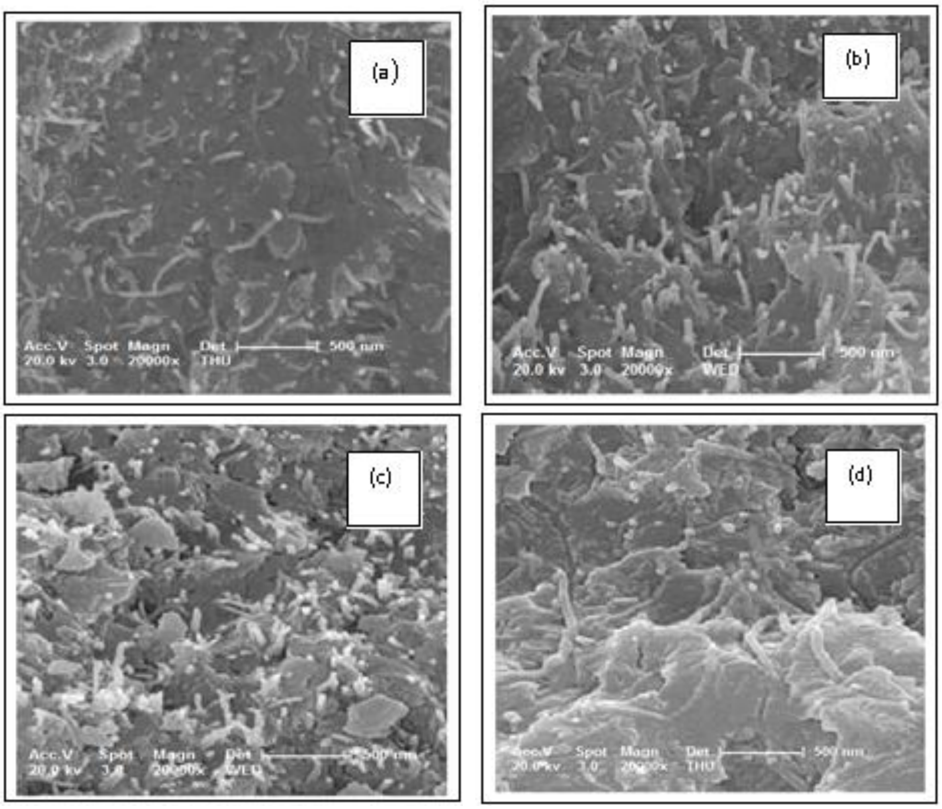

Figure 4: Scanning Electron Microscopy (SEM) of Fracture Region for Different of Fracture Region for Different SWCNTs Volume Fractions in PFR Matrix at Mag. 20000X: (a) 0.2 Vol.%, (b) 0.4 Vol.%, (c) 0.6 Vol.%, and (d) 0.8 Vol.%

CONCLUSIONS

Fracture toughness has increased with increment of volume fraction of SWCNTs. Experimental results SWCNTs nanocomposites had higher values of fracture toughness comparison with simulation results. From the fracture toughness results, it can be concluded, that the failure takes place by pull-out and pining mechanisms.

According to the simulation results, it has obtained three sets of values; represent arrangement direction of SWCNTs with respect to impact load direction. And it was concluded that the experimental results were fallen in between the perpendicular direction and random direction simulation values, evidence to the nearest arrangement of SWCNTs to the perpendicular direction more than randomly direction with respect to impact load direction.

ACKNOWLEDGEMENTS

This work was supported by The University of Mustansiriah, Ministry of Sciences and Technology, The University of Technology, and Baghdad University, Iraq.

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