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Investigation and Simulation by a Metaheuristic Algorithm of the Effect of Carbon Nanotubes Fibers on the Improvement of the Properties of Nanocomposite Material

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In this article, we investigated and studied the effect of carbon Nanotubes fibers on the improvement of the mechanical and thermal properties of our epoxy matrix composite material. Our calculations were based on a heuristic optimization algorithm. The results show that the level of the damage is related to the concentration of the mechanical and thermal stresses, for the three materials studied carbon/epoxy, Graphite-epoxy and carbon nanotubes/epoxy, the calculations also show that carbon nanotubes have greatly improved the mechanical and physical properties of our material, and that this material is more resistant than the other carbon/epoxy composite materials and graphite-epoxy nanocomposite. The numerical simulation shows a good agreement with the real behavior of the three materials studied. This means that the mechanical and physical properties have been greatly improved after the use of carbon nanotubes fibers. Finally, we can say that our model has worked well in relation to the phenomenon of damage of composites and nanocomposites materials. It would be interesting to see, thereafter, the effect of carbon nanotubes fibers on the damage of the fiber-matrix interface of a bio-nanocomposite.

Keywords: carbon nanotubes, damage, interface, nanocomposite, epoxy, graphite-epoxy.

1. Introduction

The carbon nanotubes are an allotropic form of carbon belonging to the fullerene family. They are composed of one or more layers of carbon atoms wound on themselves forming a tube. The tube may or may not be closed at its ends by a half-sphere. One can distinguish the single-walled carbon nanotubes (SWNT or SWCNT, for Single-Walled (Carbon) Nanotubes) and multi-sheet (MWNT or MWCNT, for Multi-Walled (Carbon) Nanotubes) [1-3].

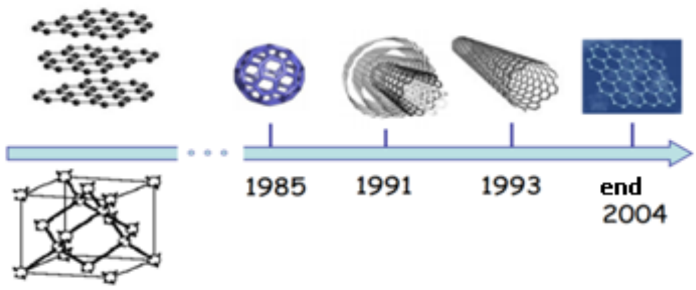

Figure 1 The history of carbon nanotubes (1985-2004)

The electrical conductivity, thermal conductivity and mechanical strength of the carbon nanotubes are remarkably high in their longitudinal direction. They are part of the products of nanotechnologies currently used and marketed in various fields [2].

In 1981 a group of Soviet scientists published the results of the chemical and structural characterization of carbon nanoparticles produced by thermocatalytic dissociation of carbon monoxide. Using MET and X-ray images, the authors suggested that their "multi-layer carbon crystals" were formed by rolling layers of graphene into cylinders. Moreover, they assumed that during this winding several layers of the hexagonal network of graphene were possible. They considered two possibilities: a circular arrangement ("armchair" type nanotubes) and a spiral arrangement (chiral nanotubes) [4-9].

In 1993, Sumio Iijima and Donald S. Bethune of IBM in California independently succeeded in synthesizing single-walled nanotubes [10, 11]. If Iijima obtains its single-walled nanotubes in the gas phase, Bethune uses a technique of covaporization of carbon and cobalt.

The Young's modulus of carbon nanotubes was calculated theoretically via simulations by different research teams using different methods. The theoretical values in the literature range from 1 to 1.5 Tpa [12, 13]. Experimentally, the Yu et al team attached MWNTs at the forefront of an AFM to measure their Young's moduli. Values ranging from 270 to 950 GPa were measured. The rupture mechanism has been demonstrated for MWNT [14].

The very high stiffness and wide deformability give them energy absorption properties that surpass those of existing materials such as Kevlar and spider silk. Such fibers could be incorporated into high-performance and lightweight protective materials (bumpers, bulletproof vests, etc.) [15, 16].

Our work is devoted to the study by a genetic approach of the effect of the carbon nanotubes fibers on the improvement of the mechanical and physical properties of the nanotubes carbon/epoxy material. This genetic modeling is based on the model of the Cox and the two probabilistic damage models of Weibull. Our new results will be compared by other results obtained by the same model on other graphite-epoxy and carbon/epoxy composite and nanocomposite materials.

2. The analytical simulation models

2.1. *Thermal stresses*

The field of thermal stresses resulting from differential expansion of the fibers and matrix during cooling after preparation of the composite at high temperature. It is given by the following equations Lebrun:

$$\sigma_f^T = E_f \frac{a}{1+a} \left(M_2 - M_0\right) \tag{1}$$

with:

$$M_0\left(T\right) = \int_{T_0}^{T_e} \left(\alpha_m - \alpha_f\right) dT$$

$$M_2\left(T\right) = \int_{T_e}^{T} \left(\alpha_m - \alpha_f\right) dT$$

T_0 room temperature, the temperature Te of development, T the test temperature and finally α_f α_m and expansion coefficients of the fiber and matrix [17, 18].

2.2. *The analytical model of Cox*

For the interface their damage based on the model of Cox [19] that is defined by the following relation:

$$\tau = \frac{E_f a \varepsilon}{2} \beta th(\beta l/2) \tag{2}$$

$$\beta^2 = \frac{2G_m}{E_f r_f^2 \ln(\frac{R}{r_f})}$$

with:

G_m – shear modulus of the matrix,
E_f – Young's modulus of fiber,
ε – the deformation,
a – radius of the fiber,
R – The half distance,
τ – The shear stress of the interface.

2.3. *The probabiliste models of Weibull*

When the stress is uniform, damage to the matrix is given by formula (3) de Weibull [20]:

$$D_m = 1 - \exp\left\{-V_m \left[\frac{\sigma + \sigma_m^T}{\sigma_{0m}}\right]^{m_m}\right\} D_m = 1 - \exp\left\{-V_m \left[\frac{\sigma + \sigma_m^T}{\sigma_{0m}}\right]^{m_m}\right\} \tag{3}$$

with:

σ – the applied stress,

σ_m^T – the thermal stress,

V_m – the volume fraction of the matrix,

$m_m et \sigma_{0m}$ – the Weibull parameters.

A broken fiber is discharged along its entire length [20]. That is, it can only break once. The rupture obeys a law similar to that described for the matrix.

$$D_f = 1 - \exp\left\{-A_f * L_{equi} \left[\frac{\sigma_{\max}^f}{\sigma_{0f}}\right]^{m_f}\right\} D_f = 1 - \exp\left\{-A_f L_{equi} \left[\frac{\sigma_{\max}^f}{\sigma_{0f}}\right]^{m_f}\right\} \tag{4}$$

with:

$\sigma_{\max}^f$ – the maximum stress applied,

$Lequi$ – the length that the fibers would have for the same break under uniformly distributed.

2.4. *Dissemination mechanisms*

The epoxy resin absorbs water from the atmosphere through its surface layer until reaching equilibrium with the environment. This step is reached quickly and is allowed by the diffusion of the water in the material. Two approaches [20, 21] allow to describe this phenomenon: The theory of free volumes: The diffusion of the penetrating molecules is determined by the number and the size of the holes of the polymer network on the one hand and by the forces of attraction between the penetrating molecules and the polymer on the other hand [22]. The presence of holes is determined by the structure of the material and by its morphology (density of cross linking, rigidity of the molecular chains, etc.). The water molecules migrate by capillary action along the free spaces of the material. These cavities are present in the composite either between the macromolecules entangled in the polymer or in the interfacial charge/resin zones. During the molding of our samples, the resin completely coats the silica because of its low viscosity. However, cross linking and the difference in coefficient of expansion of the two components may result in shrinkage and thus create detachments between the filler and the resin. The distribution of water depends on the quantity of cavities and their size. During the diffusion, the water molecules move from one site to another with an activation energy (Fig. 2). Water is then considered as liquid or free water (Fig. 3), [23, 24-27].

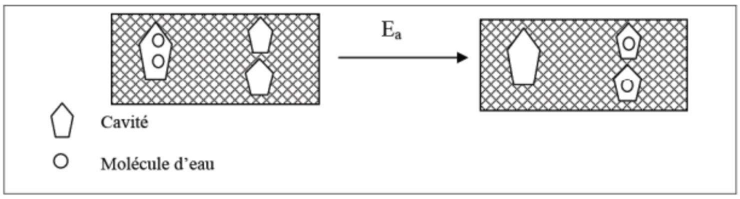

Figure 2 The theory of free volumes [25]

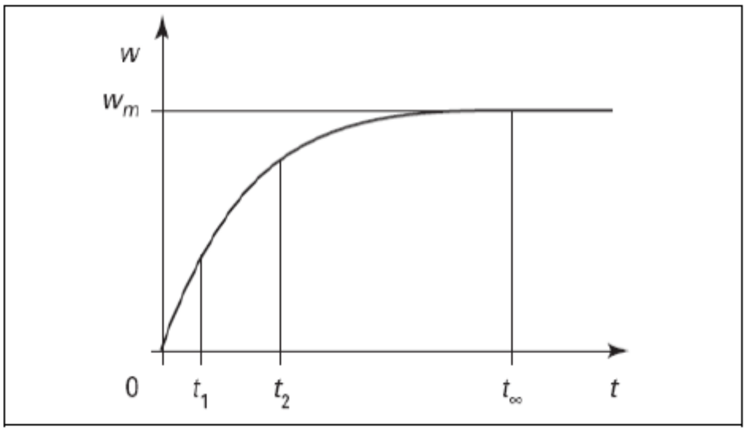

Figure 3 The kinetics of water diffusion in a polymer material [26,27]

To simplify dissemination analyzes, the following assumptions have been made:
– The diffusion coefficient D is independent of the water concentration C.
– The diffusion profile is considered plane and in the direction x. [26, 27].
The following equation is then determined: $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$ (5)

3. The properties of the materials studied

3.1. *The physical properties of carbon nanotubes*

In Tab. 1, we describe the physical properties of carbon nanotubes that we will use in our simulation model [28].

Table 1

Designation	Young's Module	Stress at breakage	Density g/cm^3	Thermal stability
Carbon nanotubes	1 Tpa	45 Gpa	1.3-1.4	2800°C under vacuum 700°C to the air

3.2. *The properties of Graphite- Epoxy*

In this study, we will use the experimental results on the graphite-epoxy nanocomposites found by Yasmine et al. [29] to validate our genetic approach (see Fig. 4).

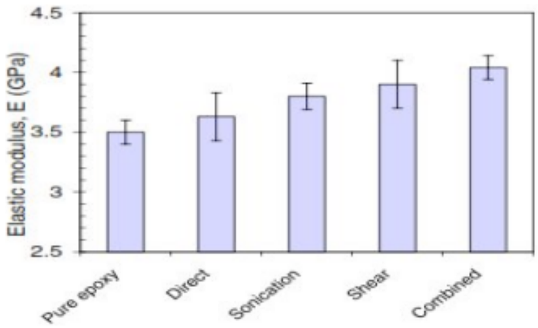

Figure 4 Influence of different processing techniques on the value of the elastic modulus of a graphite-epoxy nanocomposite

3.3. *The properties of the epoxy resin*

The physical properties of the epoxy resin are shown in Tab. 2.

Table 2

Density	Compressive strength [MPa]	Tensile strength in bending [MPa]
1.3 ± 0.05	> 70	25

4. Numerical simulation by metaheuristic algorithm

4.1. *Development*

The objective of this study is to show the effect of carbon nanotubes fibers on the resistance of the fiber-matrix interface of the three composite materials and nanocomposites studied carbon/epoxy, graphite-epoxy and carbon nanotubes/epoxy. Our genetic simulation consists in using the values of each of the mechanical and physical properties to calculate the damage level of the interface each time using the Weibull equations (2, 3) and the Cox equation (4). To see the effect of the thermal stress and moisture on this damage, we will use the equation 1 of Lebrun and equation 5 of diffusion profile. The damage to the interface is determined by the intersection of the two; carbon fiber and carbon nanotubes damage and the epoxy matrix damage. The evaluation of each generation is carried out by an objective function based on the Cox model, which includes all the variables defined at the beginning of the algorithm (mechanical properties of each composite component, Young's modulus,...). Finally, we determine the damage to the fiber length of the interface for the three materials used (carbon/epoxy, graphite-epoxy and carbon nanotubes/epoxy). The numerical calculations are carried out using the software Matlab R2012b. [30].

4.2. *The flowchart*

In this flowchart, we will present the steps followed in our genetic simulation. The main operators of a genetic algorithm are selection, crossing and mutation. In our study, the selection is based on the choice between the two best values of the two matrix and fiber damage calculated from the two Weibull equations (3, 4). The crossing is calculated by Dm and Df. The construction of the new generation was obtained from maximum population generator which is 120 in our program.

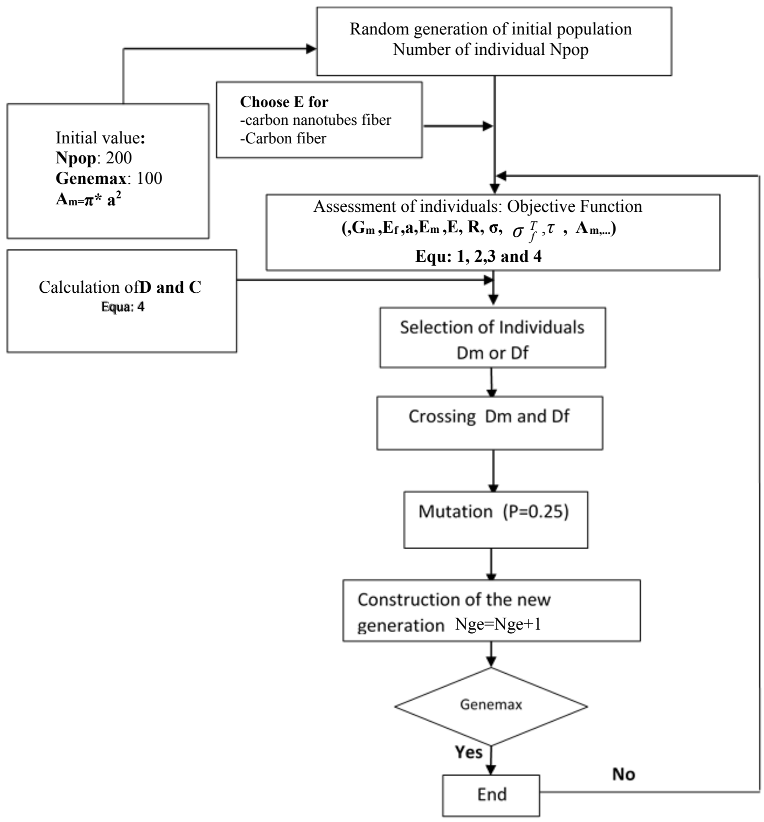

Figure 5 The flowchart of our genetic modeling

5. Results and discussions

To validate our model, we calculated the damage level of the fiber-matrix interface on three types of composite and nano-composites materials: carbon/epoxy, graphite-epoxy and carbon nanotubes/epoxy. From the simulation results by a genetic algorithm, we examined the strength of materials after application a tensile stress ranging from ($\sigma = 95$ to $\sigma = 115$ N/m^2) and we show the influence of the thermal stress on the damage to the interface for the three materials studied, we also calculated the damage of the fiber matrix interface as a function of moisture content. Figures 5, 6 and 7, 8 and 9, 10 show the level of damage to the interface as a function of the length of the fiber and as a function of the moisture content for the three carbon/epoxy materials, graphite-epoxy and carbon nanotubes/epoxy.

5.1. *Carbon/epoxy*

The Figs. 6 and 7 show that the "D" interface damage begins at 0.28 ($\sigma = 95$ N/m^2 and T = 40°C) and then increases to a maximum value of 0.38 for $\sigma = 15$ N/m^2 and T = 80°C), and when the moisture content increases, the damage increases and reaches its maximum after 60% of the humidity. It can also be said that the increased level of damage meant the concentration of mechanical and thermal stresses that give a strong degradation of the interface in the wet environment.

5.2. *Graphite-epoxy*

The Figs. 8 and 9 show that the "D" interface damage begins at 0.22 ($\sigma = 95$ N/m^2 and T = 40°C) and then increases to a maximum value of 0.29 of ($\sigma = 115$ N/m^2 and T = 80°C), and when the moisture content increases, the damage increases and reaches its maximum after 60% of the humidity. It can also be said that the increased level of damage meant the concentration of mechanical and thermal stresses that give a strong degradation of the interface in the lower wet environment compared to the carbon/epoxy composite material.

5.3. *Carbon nanotubes/epoxy*

The figure 10 and 11 show that the "D" interface damage begins at 0.08 ($\sigma = 95$ N/m^2 and T = 40°C) and then increases to a maximum value of 0.19 of ($\sigma = 115$ N/m^2 and T = 80°C), and when the moisture content increases, the damage increases and reaches its maximum after 60% of the humidity. It can also be said that the increase in level of damage meant the concentration of mechanical and thermal stresses that give a much deeper interface degradation in the wet environment much lower compared to the graphite-epoxy nanocomposite material.

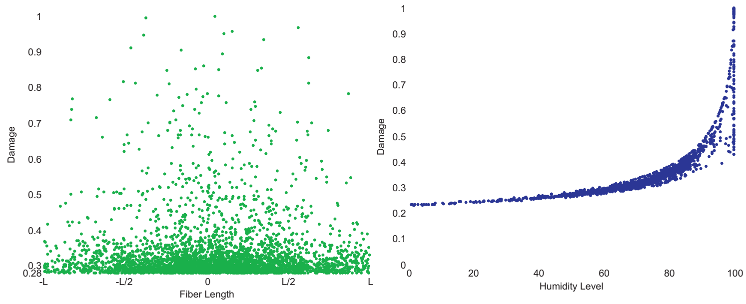

Figure 6 The influence of moisture and thermal stress on the damage of the interface

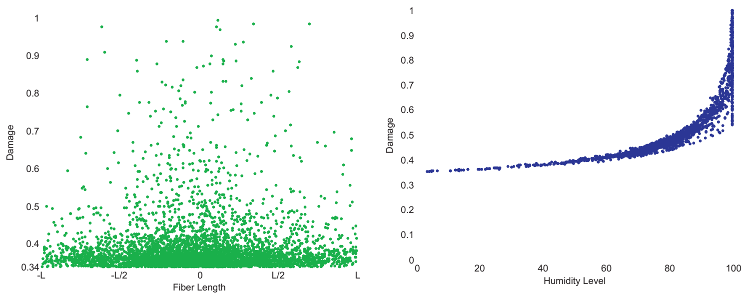

Figure 7 The influence of moisture and thermal stress on the damage of the interface

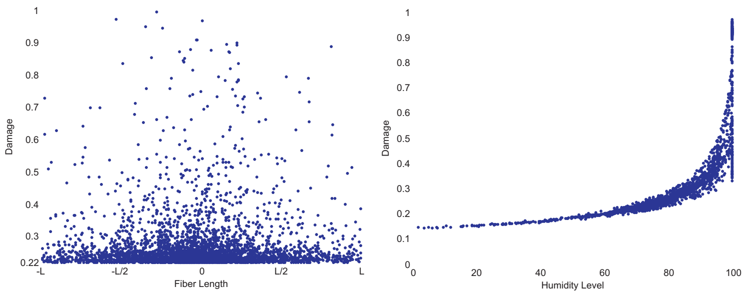

Figure 8 The influence of moisture and thermal stress on the damage of the interface

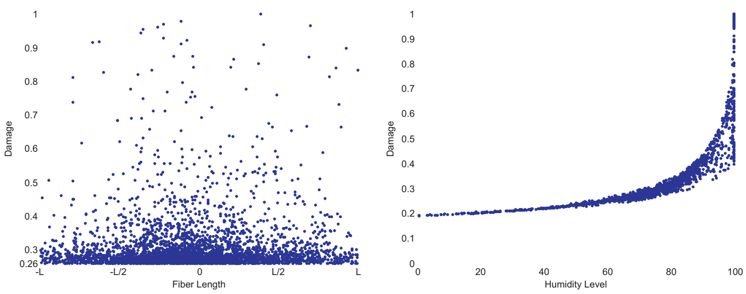

Figure 9 The influence of moisture and thermal stress on the damage of the interface

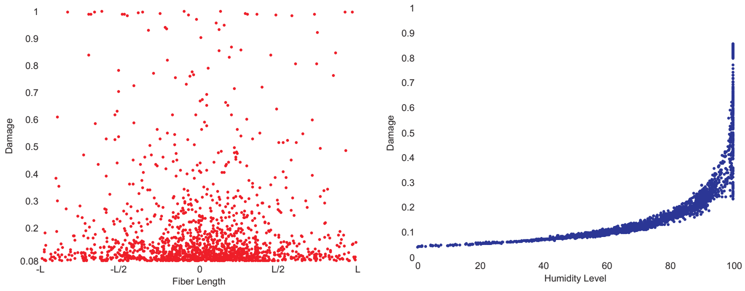

Figure 10 The influence of moisture and thermal stress on the damage of the interface

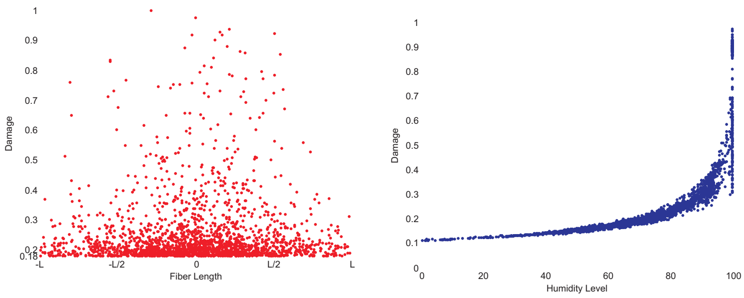

Figure 11 The influence of moisture and thermal stress on the damage of the interface

6. Conclusion

In conclusion, we recall that the materials studied are carbon/epoxy, graphite-epoxy and carbon nanotubes/epoxy, the calculation was based on a genetic algorithm, the results show that the level of damage is related to the concentration of mechanical and thermal stresses, for the three materials studied. Numerical simulation also shows a concordance with the actual behavior of the three materials studied. The results of numerical simulation show that carbon nanotubes have greatly improved the mechanical and physical properties of our epoxy matrix composite material and that this material is more resistant than the other carbon/epoxy composite materials and nanocomposite Graphite-epoxy. This means that the carbon nanotubes have altered the mechanical and physical properties of the epoxy matrix and transform it into a matrix that is more resistant to mechanical and thermal stresses applied. Finally, we can say that our model has worked well in relation to the phenomenon of damage of composites and nanocomposites. It would be interesting to see, subsequently, the effect of carbon nanotubes on the damage of the fiber-matrix interface of a bio-nanocomposite.

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