Computational simulation of a diffusion process of carbon nanotubes in aluminium to improve the mechanical properties of a composite material

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Abstract. A computational thermo-mechanical insertion model was implemented considering the incorporation of carbon nanotubes (CNTs) into semisolid aluminium. A shell surface of CNTs within an aluminium matrix was obtained using the Particles Dynamic Method (PDM). Also, energy absorption simulations were performed through computational impact tests in order to characterize the behaviour of the nanocomposite under high strain rates. Theoretical results are useful in the design of nanocomposites and the experimental processing of Al/CNTs nanocomposites for different applications.

1. Introduction
Matter diffusion processes in which diffusion coefficients are mainly dependent on temperature and other transport and substance-specific properties such as viscosity, size and shape of solute, have been reported extensively [1]. Many reports in this topic involve modelling of phenomena related to substances with well-known physicochemical properties [1]. On the other hand, reports of diffusion processes involving nanomaterials are much more unusual.

In this paper, a computational mathematical model that describes the diffusion of carbon nanotubes into aluminium in semisolid state is presented and diffusion coefficients are introduced to allow consideration of the translational and rotational effects, as well as other geometric parameters of nanotubes in mixture [2,3]. In this way, modelling of diffusion and dispersion of CNTs is attainable, allowing for far more realistic physical conditions [2-4].

Computational tests for ballistic impact energy absorption were developed on Al/CNT nanocomposites with the goal of estimating the improvement of the material’s mechanical properties by the contribution of the CNTs [5-7].

2. Mathematical modelling and computational simulation
Diffusion of CNTs in Al was mathematically modelled following Fick’s law in transient state [2]. Random movement of particles that complied with thermodynamic principles was guaranteed by addition of physical interactions for different relations of CNTs to Al.

Additional parameters such as rotational coefficient, translational coefficient, static flexion persistence length, static bend radius, intrinsic viscosity and mean spatial distance were included in the diffusive coefficient with the in order to have an appropriate representation of the behaviour of thermo-mechanical diffusion processes [2,3].
The results of concentration functions for mixture in transient state were achieved following the implementation of a numerical model in Matlab®. Simulations of the composite material were executed in order to determine mechanical resistance and overall contribution of nanotubes to composite material. Boundary conditions related to impact energy on Al/CNTs composite were also implemented.

2.1. Mathematical descriptions and constitutive laws

Rotational effects of CNTs were determined using equation (1) [3]:

\[ D_r = \left( \frac{kT}{n_s} \right) \left( \frac{2}{L_p^2} \right) \left[ 0.253 \left( \frac{L}{4L_p} \right)^{\frac{1}{2}} + 0.159 \ln(2L_p) - 0.387 + 0.160 \right] \]  

In (1), \( L \) is the contour length of CNTs, \( T \) is the temperature at which diffusion occurs, \( k \) is the number of static flexion points, \( n_s \) is the viscosity of the solvent, \( L_p \) is the spacing between friction elements along the contour and \( l_p \) is the length of persistent dynamic flexion.

Equation (2) was used to denote translational effects of CNT’s [3]:

\[ D_t = \left( \frac{kT}{3\pi Ln_s} \right) \left[ 1 + \ln(2l_{ap}) - 2.431 + 1.843 \left( \frac{N}{2l_{ap}} \right)^{\frac{1}{2}} + 0.138 \left( \frac{N}{2l_{ap}} \right)^{\frac{1}{2}} - 0.305 \left( \frac{N}{2l_{ap}} \right)^{-1} \right] \]  

In (2), \( N \) is the number of friction elements and \( l_{ap} \) is the apparent persistence length.

Fick’s law mathematical model was applied [1] (see Equation 3) to represent diffusive flux on insertion of Al/CNTs. Random movement of CNTs reached homogeneity when equilibrium between forces related to concentration gradient and friction forces related to medium viscosity was achieved [1].

\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad ; \quad 0 \leq x \leq L \land t \geq 0 \]  

In (3), \( C \) is the concentration of CNTs in aluminium; \( D=f(D_r, D_t) \) is the diffusion coefficient. Boundary and initial conditions in the diffusion system were defined by:

\[ \frac{\partial C}{\partial x}(0,t) = K(C_s - C) \rightarrow K = g(D, A_{r, t}) \quad ; \quad x = 0 \land t \geq 0 \]  

\[ \frac{\partial C}{\partial x}(L,t) = 0 \quad ; \quad x = L \land t \geq 0 \]  

\[ C(x,0) = C_0 = 0 \quad ; \quad 0 < x \leq L \land t \geq 0 \]  

Schematically, the process can be represented as seen in Figure 1.
For the implementation of computational tests on the material exposed to projectile impact, Al/CNTs was configured by means of generalized Hooke’s model for anisotropic materials [7] and Johnson-Cook’s model was used to determine material failure and propagation of energy [7,8].

In Hooke’s model, composite density was calculated from mass proportions [7]:

\[
\rho_c = \frac{1}{\frac{m_{AL}}{\rho_{AL}} + \frac{m_{NTC}}{\rho_{NTC}} + \frac{V_c}{\rho_C}}
\]

\(m_{NTC}, m_{AL}\) are the mass proportions of the constituent and \(V_c\) is the proportion in void volume.

Johnson-Cook’s Constitutive Model describes the relationship between stress, strain, strain rate and visco-elastic material temperature. This model is appropriate for situations in which strain rate varies between \(10^{-2} \text{s}^{-1}\) and \(10^{6} \text{s}^{-1}\) and temperature varies according to plastic deformation caused by thermal softening. Stress flux model is represented as in (8) [8,9]:

\[
\sigma = (A + B \varepsilon^p)(1 + C \ln \dot{\varepsilon}^p)(1 - T^m)
\]

In (9) \(T\) is the system temperature, \(\dot{\varepsilon}^p\) is the velocity of equivalent plastic deformation, \(\varepsilon\) is the equivalent plastic deformation, \(A\) is the initial cadence stress (MPa), \(B\) is the hardening module, \(n\) is the strain hardening exponent, \(C\) is the strain-rate dependent coefficient and \(m\) is the thermal softening coefficient.

The materials’ properties values used during diffusion process and ballistic computational tests for Al/CNTs composite with a material type Al 1100 and for CNTs were given a stiffness module of \(1.8 \times 10^{12}\) and a Poisson ratio of 0.45 [9-11].

2.2. Numerical-computational description

Fick’s law was modelled through progressive divided differences approximation for transient behaviour applications. General scheme is described in (10) [12]:

\[
\frac{C_i^{(n+1)} - C_i^{(n)}}{\Delta t} = D \frac{C_i^{(n)} - C_{i-1}^{(n)} + C_{i+1}^{(n)}}{(\Delta x)^2}
\]

Numeric mesh size in time interval \(\Delta t\) should guarantee:

\[
\Delta t \leq \frac{0.5 \Delta x^2}{D}
\]
In (10) $D$ is the diffusion coefficient, $\Delta t$ is the time interval or step and $\Delta x$ is the spatial interval.

During computational tests, finite elements analysis (FEA) was used to study the behaviour of Al/CNTs composite. A flat plaque with an area of 20x20cm and thickness of 5.2mm was elaborated to represent the composite material. A mesh was elaborated in order to determine the behaviour of the plaque when subjected to dynamic impact force. Uniform quadrilateral elements were used to develop the mesh (Figure 2).

![Figure 2. Lattice of a flat-surface plaque with uniform elements.]

In the same way, another numerical mesh for the 7.62mm-caliber projectile was elaborated. This projectile impacted the flat plaque, Figure 3.

![Figure 3. Framework of the 7.62mm-caliber projectile with controlled numerical elements.]

Based on international standards for shielding and ballistic testing [13], criteria and reference data for computational tests were determined. Projectile speed equalled 847m/s±9.1m/s, dimensions and geometric characteristics were selected as show the Figure 4.

NOM-166-SCFI-2005 [13] was the main guideline for the development of simulations and the determination of ballistics-specific characteristics such as: protection level, gun type, projectile calibre, work velocity, dimensions of target and others.
Using the Particles Dynamic Method (PDM.), a computational algorithm was implemented with the goal of analysing behaviour of dissipation and propagation of energy in a domain comprised of elastic Al and CNTs point particles. Newton’s laws and elastic laws were specifically used in this case [14,15].

\[ \rho \partial^2 u_i = \sum f \]  

P.D.M was designed according to the structure presented in Fig. 5.
3. Results

Functions of flux diffusion of CNTs in Al were obtained, with a tendency to homogenize concentration and temperature (Figure 6).

![Figure 6. Molecular diffusion behaviour of Al/CNTs (functions indicate level of concentration in a specific time and space).](image1)

Mechanical tests performed on the impact-subjected Al/CNTs composites indicated that reinforcement material favour the composite’s mechanical properties, achieving energy dissipation-absorption and effectively stopping the projectile trajectory. Impact plaque was 5.2mm thick with 13 layers of Al 1100 and 12 insertions of CNT layers (Figure 7).

Results were validated through PDM simulations. Algorithms implemented with PDM were developed in Matlab’s programming language, allowing for modification of different particulate layers, and mechanical properties, projectile velocity, and orientation. In this case, an initial simulation of a particulate surface (plaque) was made using point particles of Al. This surface was impacted by a spherical projectile (Figure 8). Later, an impact subjected plaque, consisting of three different layers of point particles of CNTs and Al 1100 (Figure 9) was simulated. In general, the results showed the composite exhibited kinetic energy dissipation modes and a capacity to diminish impact damage.

![Figure 7. Laminate plaque with 5.2mm thickness made of AL1100 and CNTs.](image2)
4. Conclusions

Initially, a computational algorithm was developed with the purpose of simulating concentration gradient of CNTs on Al matrix. Simulations indicate appropriate distribution of CNTs with respect to the depth achieved during diffusion. Thermal conditions and media concentration can affect the degree of perforation of reinforcement material and the upgrade of the mechanical properties of the matrix.

Several simulations were executed on an Al 1100/CNTs plaque subjected to dynamic impact load until the perforated surface didn’t pass the security limit defined by NOM-166-SCFI-2005 guidelines. Simulations considered a solid projectile in order to grant the design a higher safety factor. The most favourable result was achieved using a lamina made of 13 plaques of Al 1100, on which CNTs were deposited. Maximum deformation achieved was 1.5cm deep. Fragmentation of the material was observed in areas close to impact zone.

Modelling of the impact behaviour of a spherical projectile on particulate Al/CNTs surface was also performed. Each particle was characterized using singular mechanical properties of Al and CNTs in order to simulate specific characteristics of materials with continuous constitution. Impact dynamics of elastic particles were considered and fragmentation of the material was observed as the projectile perforated the particulate surface.

This research offers insight on how perforation of composite materials subjected to ballistic impact is generated. Incidence of damage to wearer, as well as possibility of reinforcement improvement and diffusion/dispersion of CNTs in Al is also discussed.
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