A multi-objective optimization approach for design of blast-resistant composite laminates using carbon nanotubes

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Article info

A B S T R A C T

A reliable process for the design of blast-resistance composite laminates is needed. We consider here the use of carbon nanotubes (CNTs) to enhance the mechanical properties of composite interface layers. The use of CNTs not only enhances the strength of the interface but also significantly alters stress propagation in composite laminates. A simplified wave propagation simulation is developed and the optimal CNT content in the interface layer is determined using multi-objective optimization paradigms. The optimization process targets minimizing the ratio of the stress developed in the layers to the strength of that layer for all the composite laminate layers. Two optimization methods are employed to identify the optimal CNT content. A case study demonstrating the design of five-layer composite laminate subjected to a blast event is used to demonstrate the concept. It is shown that the addition of 2% and 4% CNTs by weight to the epoxy interfaces results in significant enhancement of the composite ability to resist blast.

Keywords:
A. Carbon-carbon composites (CCCs)
B. Impact behavior
C. Laminate mechanics
D. Blast-resistant composites

1. Introduction

Structural fiber reinforced plastic (FRPs) composites have been used extensively in several high performance structural applications (e.g., vehicles, airplanes, etc.) for their significantly high strength-to-weight ratio. Other plausible features of FRPs include their manufacturing flexibility, which allows composites to achieve material properties that are difficult to attain using single-phase materials. However, typical structural composites exhibit limited ductility, which limit their ability to absorb energy under impact loading and ultimately leads to their failure [1]. This limited energy absorption is related to the lack of plasticity mechanisms and dominant debonding at weak interfaces [2]. The dominant failure mechanism in composite laminates subjected to impact-loading is a complex combination of delamination predominantly caused by mode II shear, matrix cracking caused by transverse shear, and translaminar fracture in terms of fiber fracture and kinking [3]. There are several factors that dictate the above fracture processes, such as the material variables, loading and environmental conditions and the source of impact. Amongst the material variables, the mechanical properties of fiber and matrix, particularly the failure strains, interface properties, fiber configuration and stacking sequence in angle-ply laminates play important roles in determining the impact damage resistance of composites [4].

Significant efforts for developing blast-resistant composites have been conducted in the last three decades. Brennan and Prewo [5] reported a composite made of a glass–ceramic matrix reinforced with silicon carbide fibers that exhibited exceptional mechanical strength and toughness. Toughness measurements of new silicon carbide fiber composites were reported to be 50 times that of typical ceramic composites. Much interest was directed to examine the impact strength of carbon/epoxy composites [6]. Kang and Lee [7] reported a significant improvement in energy absorption of multi-laminate carbon composites by chain and plain stitching. More recently, Tekalura et al. [8] investigated the advantages of using polyurea and E-glass vinyl ester layered composites as a sandwich material for shock mitigation structures.

Research was also devoted to developing computational tools to simulate composite behavior under impact loads and to quantify damage in laminated composites (cf. [9]). Riccio and Tessitore [10] demonstrated the strong dependence of composite behavior on the loading conditions using nonlinear finite-element modeling. Batra and Hassan [11] also used a continuum damage mechanics approach in their characterization of damage due to blast loading of unidirectional fiber reinforced composites. Moreover, Donadona et al. [12] successfully implemented and validated a 3D continuum damage mechanics finite-element modeling approach for composite laminates subjected to low-velocity impact. Such investigations provided a roadmap to identify the desired characteristics of composites to resist blast events. Here we suggest the addition of carbon nanotubes to enhance blast resistance of structural composites and we discuss below a numerical approach to determine the optimal carbon nanotubes content to enhance blast resistance.
2. Carbon nanotubes

Carbon nanotubes (CNTs) have drawn significant attention from the research community for their attractive mechanical properties. CNTs represent a unique form of carbon that can be visualized by considering a single graphene sheet representing a lattice of carbon atoms distributed in a hexagonal pattern [13]. A single wall carbon nanotube (SWCNT) is 1–3 nm in diameter [14]. The attractive properties of SWCNTs might be attributed to their unique nanostructure. SWCNTs possess exceptional mechanical [15] properties and superior thermal and electric properties compared to macroscale fibers such as graphite, Kevlar, SiC and alumina. The strength, elastic modulus and the fracture properties of carbon nanotubes are an order of magnitude higher than those of most common composite materials. The properties of CNTs are presented in Table 1 after [16]. A schematic representation of a SWCNT is shown in Fig. 1(a) and a transmission electronic microscope (TEM) image of several SWCNTs is shown in Fig. 1(b).

Numerous experiments have been reported on the enhanced mechanical properties of SWCNTs. Of interest here is the significantly high stiffness (Young’s modulus of elasticity) of SWCNTs measured experimentally, researchers [19] found that absorbed energy to failure of a composite based on polyvinyl-SWCNTs was 18 times higher than Kevlar fibers and 48 times higher than graphitic fibers. Various methods have been successfully utilized to synthesize CNTs, such as arc discharge, laser ablation pyrolysis and chemical vapor deposition [20]. Researchers reported successful inclusion of CNTs in polymer matrices using various techniques to avoid the difficulty of uniformly dispersing CNTs in polymer [21] including the use of magnetic fields [22]. We suggest here that CNTs can be dispersed in epoxy forming the interface of the composite laminate. CNTs at concentrations of 2–5% in epoxy can significantly enhance the tensile strength and tensile modulus of the composite interface. We suggest that using classical Voigt’s mixture rule [23]; we can approximately predict the properties of CNT strengthened epoxy. We hypothesize that such a change of strength and stiffness of the interface will play a major role in blast resistance as it alters the stress to strength distribution inside the composite laminate.

3. Stress waves propagation in composite laminates

To simulate this effect, we adopt a simplified approach for stress wave propagation in bounded elastic media after Kolsky [24] and Al-Haik and Almyadmeh [25]. The velocity of longitudinal waves $C_0$ in a medium of density $\rho$ and bulk modulus $K$ can be computed as

$$C_0 = \sqrt{\frac{K}{\rho}}$$

This method allows computing reflection and refraction of both dilation and distortion waves at free boundaries and at an interface between two media. We limit our discussion here to the propagation of longitudinal waves at the interface to predict the normal stresses at both sides of an interface in the composite laminate due to an incident pressure. However, the proposed approach can be extended to include torsional and flexural stress waves [24]. Considering a limited width $\Delta x$ of the composite layer as shown in Fig. 2 with the applied stress $\sigma_{\text{xx}}$ and the transmitted wave producing the stress at the other side of the interface $\sigma'_{\text{xx}}$, one can write the following differential equation

$$\rho \frac{\partial^2 u}{\partial t^2} = E \frac{\partial^2 u}{\partial x^2}$$

This equation can be solved by considering a linear displacement time function $u(t)$. This leads us to realize the fundamental relationship of the stress with particle velocity as

$$\sigma_{\text{xx}} = \rho C_0 \frac{\partial u}{\partial t}$$

The term $\rho C_0$ is known as the characteristic impedance. Defining the particle velocity $V = \partial u / \partial t$ we can re-write Eq. (3) to relate the particle velocity to the stress as
The transmitted stress can be computed by considering the continuity of velocity across the interface plane $V_I = V_T + V_R$ where $V_I$ is the incident particle velocity, $V_T$ is the reflected particle velocity and $V_R$ is the transmitted particle velocity. This is shown schematically in Fig. 3. Relating the incident stress to the incident particle velocity at the first layer before the interface $V_I$ can be computed as

$$V_I = \sigma_I \rho_I c_I$$

Equilibrium at the interface also requires that

$$(\sigma_I + \sigma_R)A_1 = \sigma_A A_2$$

where $A_1$ and $A_2$ are areas of Layers 1 and 2, respectively. By substituting Eq. (5) in Eq. (2) and solving Eq. (6) one can deduce the transmitted stress $\sigma_T$ and the reflected stress $\sigma_R$ as

$$\sigma_T = \frac{2A_1 \rho_1 c_1}{A_1 \rho_1 c_1 + A_2 \rho_2 c_2} \sigma_I$$

$$\sigma_R = \frac{A_2 \rho_2 c_2 - A_1 \rho_1 c_1}{A_1 \rho_1 c_1 + A_2 \rho_2 c_2} \sigma_I$$

For the composite laminates considered in the current investigation, all the areas will be assumed identical; $A_1 = A_n, n = 1, \ldots, N$ where $N$ is the total number of layers. It becomes obvious from Eqs. (7) and (8) that direction of the reflected pressure $\sigma_R$ is a function of the characteristic impedance of each layer. The stress distribution can therefore be altered by optimally distributing the impedance (stiffness) of the composite layer. By adding CNTs to the epoxy interface, one will increase the characteristic impedance of the layer and alter the reflected and transmitted pressure. It is important to realize that the final stress in each layer is the algebraic sum of both the reflected and transmitted stress waves occurring in the layer at different time steps. Therefore, a step-by-step in-time analysis is required to account for all the stress propagation in the laminate. A computer code is thus developed after [25] to perform the step-by-step in-time analysis to obtain the stress pulse time history.

4. Multi-objective optimization

The above simulation method can predict the stresses at the different composite layers due to an incident pressure applied to the composite laminate. We suggest that adding CNTs to the epoxy interface can alter the stress distribution in the composite layers. Moreover, adding CNTs to epoxy will also enhance the ultimate tensile strength of the interface and thus might alter the failure mode to occur in the composite fiber instead of the interface. However, CNTs are expensive materials and therefore one shall optimize the amount of CNTs to be added such that the composite strength against blast is enhanced while limiting the cost. Furthermore, if more than one interface exists (which is the case in most composite laminates), nonlinear behaviors can be observed with alternating the impedance of the interface layers by using different CNT content in each layer.

Classical optimization approaches have always considered a single-objective function while dealing with all other objectives as constraints. The fundamental difference between single-objective and multi-objective optimization is the ability of multi-objective optimization to avoid the artificial fixes needed for single-objective optimization methods in order to address tradeoffs between the two different objectives. For instance, we might need to limit failure of all interface layers, the optimal CNT contents of the layers are those needed to distribute the stress in the composite laminate such that the maximum stress in each interface layer does not exceed its strength, which is also a function of the CNT content. We suggest that such a design can be achieved by getting candidate designs to lie in the Pareto front, typically known as Paretto-optimal solutions after Pareto [26]. De Kruifj et al. [27] reported successful microstructural optimization to handle the tradeoffs between alternative microstructures to achieve desired conductivity and stiffness in composite materials.

Two categories of multi-objective optimization methods are identified in the literature (cf. [28]). The first category utilizes classical single-objective optimization methods while reformulating the problem to address multi-objectives considering preferences between the different objective functions [29]. Methods in the first category include techniques such as the weighted sum method, the $\varepsilon$-constraint method and the hierarchical optimization method [29]. In the hierarchical optimization method the top priority objective function is initially optimized and then the second priority function is optimized subject to the constraint that the top priority is not adversely affected. This procedure repeats itself for all priority functions. In this paper, weighted sum method is used due to its ability and relative simplicity in demonstrating different optimization alternatives. The second category of multi-objective optimization methods establishes an optimization method that is multi-objective in nature by using evolutionary optimization such as non-sorted genetic algorithms [30].

5. Case study

Here we present a case study to demonstrate the integration of the above methods for designing a blast-resistant structural composite using carbon nanotubes. The composite of interest here is a five-layer carbon fiber composite shown schematically in Fig. 4. The properties of the materials used for the five composite layers are presented in Table 2. We simulated a blast event, using scaling laws after Smith and Hetherington [31]. This blast is aimed to produce an incident pressure of 140 MPa at the surface of the composite to assure the failure of the composite before the addition of
CNT. Using the stress wave propagation approach described above, the stresses in the structural composite layers at different time steps were simulated using the step-by-step in-time analysis. The stress at each layer was then compared to the material strength of that layer. Carbon nanotubes were then assumed to be added to the epoxy interface at Layers 2 and 4. Addition of carbon nanotubes increased the interface strength and altered the stiffness distribution in the composite, and therefore, the stress propagation in the composite.

We implemented an optimization method to identify the Pareto-optimal design front. Two objective functions representing the maximum tension and compression stress to strength ratios in the composite denoted as \( f_1 \) and \( f_2 \) are defined as

\[
 f_1 = \max_{1 < m < N} \left( \frac{\max(s_{m}^{T})}{\sigma_{m}^{T}} \right) \\
 f_2 = \max_{1 < m < N} \left( \frac{\max(s_{m}^{C})}{\sigma_{m}^{C}} \right)
\]

In this formulation, \( f_1 \) is the maximum tensile stress to strength ratio in all individual layers and \( f_2 \) is the maximum compressive stress to strength ratio in all individual layers. \( N \) is the total number of layers in the composite; \( \sigma_{m}^{T} \) is the maximum tensile stress observed in the \( m \)th layer due to the applied stress wave; \( \sigma_{m}^{T} \) is the ultimate tensile strength of the \( m \)th layer; \( \sigma_{m}^{C} \) is the maximum compressive stress observed in the \( m \)th layer due to the applied stress wave; \( \sigma_{m}^{C} \) is the ultimate compressive strength of the \( m \)th layer.

The optimization problem is formulated as a multi-objective nonlinear unconstrained optimization that targets minimizing the combined objective function \( f \) defined as

\[
 \min f = w_1 f_1 + w_2 f_2
\]

where \( w_1 \) and \( w_2 \) are the \( j \)th set of weights of the objective functions \( f_1 \) and \( f_2 \) such that \( w_j = 1 - w_i \) and \( j = 1, 2, 3, \ldots, J \) where \( J \) depends on the weight increment. The CNT content in Layers 2 and 4, denoted by \( x_1 \) and \( x_2 \), are defined as the design variables subject to the following bounds

\[
 0 \leq x_1 \leq x_{\text{max}} \quad \text{and} \quad 0 \leq x_2 \leq x_{\text{max}}
\]

\( x_{\text{max}} \) is the maximum CNT ratio, which is set at 5% for practical reasons.

Two optimization methods (denoted here as OPT1 and OPT2) were used to find the optimal values of \( x_1 \) and \( x_2 \). The first optimization method denoted OPT1 implemented the Broyden–Fletcher–Goldfarb–Shanno (BFGS) gradient based method which represents a modified version of the quasi-Newton methods as described below [32]. The second optimization method denoted OPT2 is a non-gradient based global optimization algorithm after Jones [33] that balances between global and local search. The optimization process was developed under Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) environment (cf. [34]).

Fig. 5 provides a schematic representation of the optimization process and the optimization/simulation interface. Other optimization methods can also be used to perform the required optimization. We limit our discussion here to these two methods for space limitation. The choice of the two methods was to demonstrate the difference between gradient and non-gradient optimization approaches.

In this process, the vector of design variables \( x = \{x_1, x_2\} \) is passed by the optimization environment (DAKOTA) to the simulation algorithm to compute the maximum tensile and compressive stresses in all the layers. The two objective functions \( f_1 \) and \( f_2 \) (Eqs. (9) and (10)) are computed and then used to compute the combined objective function \( f \) (Eq. (11)) using one set of weights \( w_1 \) and \( w_2 \). Once the optimization process terminates, the \( j \)-th set of weights is used and the process is repeated until all assigned weights are examined. Variation of weights enables forming the Pareto front for multi-objective optimization. As the number of weights increases, a fine Pareto front can be established. However, increasing the number of weights results in increasing the computation time. Our preliminary experiments showed that 0.025 increments in weights are sufficient for obtaining a good Pareto front. Fig. 6 shows the surface of the objective function for three different sets of weights.

The OPT1 method implements the BFGS algorithm. This algorithm is based on updating an initial variable vector \( \alpha_0 \) using an approximate Hessian matrix \( B_0 \). The approximate Hessian matrix can be initiated as the identity matrix similar to the gradient des-
Fig. 6. Surface of the combined weighted objective function $f$ versus CNT content in Layer 2 and 4 represented by the variables $a_1$ and $a_2$ for three sets of weights: (a) $w_1 = 0.1$, $w_2 = 0.9$, (b) $w_1 = 0.5$, $w_2 = 0.5$ and (c) $w_1 = 0.9$, $w_2 = 0.1$. 
cent method. The step size \( s^k \) for the \( k \)th iteration can be computed using the gradient of the objective function \( \nabla f(x^k) \) as

\[
B^k s^k = - \nabla f(x^k)
\]

A maximum step size \( s_{\text{max}} \) is typically used to limit the trust region size. The maximum step size in the case study was set to 1000. The updated solutions \( x^{k+1} \) can be identified as

\[
x^{k+1} = x^k + b^k s^k
\]

where \( b^k \) is the optimal search direction satisfying Wolfe conditions [35]. The approximate Hessian matrix of the \( k + 1 \) iteration is updated by computing the change in gradient \( \Delta \) as

\[
B^{k+1} = B^k + \frac{\Delta A^k \Delta s^k}{\Delta x^2 s^k} - \frac{b^k s^k (B^k s^k)^T}{s^T B^k s^k}
\]

Convergence is checked by observing the change in the objective function gradient norm \( |\nabla f(x^k)| \). A convergence limit was set to \( 1 \times 10^{-4} \) in the case study. Termination of the OPT1 method for each set of weights was achieved by meeting the convergence limit or performing the maximum number of iterations (function evaluations) set to 1000.

The second optimization method denoted OPT2 known as Dividing Rectangles (DIRECT) starts by scaling the feasible region into an \( n \)-dimensional unit hypercube. The search begins at the center point of the hypercube to find the optimal solution for the combined weighted objective function \( f \). Sampling is used to select feasible points that will be the center of the potentially optimal rectangles and these rectangles are further divided into smaller rectangles until the termination criterion is met [36]. One can decide to divide a sub-region or a bigger sub-region by setting a threshold to the ratio of the sub-region of interest to the largest sub-region. Fig. 7 shows the design space partitioning with search method. Termination is based on meeting the maximum number of iterations (function evaluations) or reaching the minimum box size \( b = b_{\text{max}} \). The minimum box size \( b_{\text{min}} \) was set here to \( 1 \times 10^{-8} \) and the maximum number of iterations was set to 1000.

6. Results and discussion

Numerical experiments for the case study were run under Ubuntu 8.04 with 4 GB RAM. Results of the stress to strength ratios at the different composite layers of the original composite (no carbon nanotubes) are presented in Fig. 8. It is obvious that the composite would have failed at the interface Layers 2 and 4, as the stress/strength ratio exceeded unity. The results of the optimization methods are shown in Fig. 9. Two Pareto-optimal curves are

Table 3

<table>
<thead>
<tr>
<th>Solution #</th>
<th>( x_1 %)</th>
<th>( x_2 %)</th>
<th>\text{Tensile stress/strength ratio} (f_1)</th>
<th>\text{Compressive stress/strength ratio} (f_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.64</td>
<td>4.88</td>
<td>0.332</td>
<td>0.411</td>
</tr>
<tr>
<td>2</td>
<td>1.80</td>
<td>4.15</td>
<td>0.297</td>
<td>0.416</td>
</tr>
<tr>
<td>3</td>
<td>2.01</td>
<td>3.97</td>
<td>0.277</td>
<td>0.421</td>
</tr>
<tr>
<td>4</td>
<td>2.74</td>
<td>3.44</td>
<td>0.226</td>
<td>0.437</td>
</tr>
<tr>
<td>5</td>
<td>3.66</td>
<td>4.20</td>
<td>0.218</td>
<td>0.449</td>
</tr>
</tbody>
</table>

Fig. 7. Schematic representation of the search method used for non-gradient optimization OPT2.

Fig. 8. Tensile stress to strength time history for all five layers of the original composite without CNTs showing failure at Layer 4 as the stress to strength ratio exceeds unity.

Fig. 9. Pareto front and results for multi-objective optimization using two optimization methods OPT1 and OPT2.

Fig. 10. Tensile stress to strength time history for all five layers of the composite laminate including CNTs (2% in Layer 2 and 4% in Layer 4).
shown in Fig. 9 using OPT1 and OPT2 optimization techniques. Each point on the Pareto-optimal curve represents a viable solution with a different combination of CNT contents $x_1$ and $x_2$. It can be ob-
served from Fig. 9 that the non-gradient search method (OPT2) was more successful than the gradient based optimization (OPT1) in finding solutions that resulted in a lower stress to strength ratio. The optimal CNTs contents based on OPT2 is presented in Table 3. While all the points on the Pareto front represent possible optimal solutions, we select the solution corresponding to a relatively mini-
mized value of both functions $f_1$ and $f_2$, with weights 0.225 and 0.775, respectively. This means that the addition of 2% and 4% CNTs to the two epoxy interface layers can significantly enhance the blast resistance of the structural composite. Fig. 10 shows the stress to strength time-history in the five layers of the composite laminates due to the blast with the optimal CNT contents. Fig. 11 compares the stress to strength time history of the interface (epoxy) layers with and without CNTs.

It can be observed that the use of CNTs with the polymer inter-
face (here epoxy) can alter the stress wave propagation in structural composites and can significantly enhance the structural composite resistance to blast events. Optimization for OPT1 re-
quired 0.28 s of CPU time whereas optimization for OPT2 required 5.18 s of CPU time. That indicates that OPT2 method will typically need much longer computation time (about 19-folds) compared with OPT1 method. Computation time was not a significant influence on this case study because of its relatively inexpensive simu-
lation. However, this issue might be of interest when computa-
tionally expensive simulation is considered.

Finally, both optimization methods were capable of identifying the Pareto-optimal solution. However, the non-gradient search method OPT2 was capable of identifying better solutions than those found by the modified quasi-Newton method OPT1. By setting the maximum number of iterations to 1000, we gave sufficient tolerance for both methods to converge since the maximum num-
ber of iterations was never reached by either of them. In average, OPT1 required 18 iterations and OPT2 required 819 iterations. Termination of OPT1 was due to the convergence limit and termina-
tion of OPT2 was due to the minimum box size limit. These might be attributed to the existence of a number of local minima in the surface of the combined weighted function $f$ associated with some weight combinations. Such local minima might influence the performance of the gradient based method OPT1 but would not af-
fect the non-gradient search method OPT2. This comparison is lim-
ited to the termination and convergence conditions imposed on each method as described above.

7. Conclusions

A numerical approach for design of composite laminates for en-
hanced blast resistance using carbon nanotubes (CNTs) is pre-
presented. The hypothesis is based on the fact that mixing CNTs with the polymer interface can result in changing the interface mechanical characteristics including strength, stiffness and imped-
ance. A simplified simulation for wave propagation in composite laminates is developed. An optimization approach based on deter-
mining the optimal CNT content in the composite interface is developed. A case study for enhancing the blast resistance of a five-layer composite laminate is presented. Optimal CNT contents of 2% and 4% are identified. Gradient and non-gradient based opti-
mization methods were shown to be capable of establishing the Pareto front. The non-gradient method proved to be more capable of identifying the optimal solutions. Experimental investigations are underway to prove the proposed hypothesis.

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