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Damage Mechanics of Carbon Nanotubes

George Z. Voyiadjis [1,*], Peter I. Kattan [2]

1. Boyd Professor, Department of Civil and Environmental Engineering, Louisiana State University, Baton Rouge, LA 70803, USA; E-Mail: voyiadjis@eng.lsu.edu
2. Visiting Professor, Department of Civil and Environmental Engineering, Louisiana State University, Baton Rouge, LA 70803, USA; E-Mail: pkattan@petrabooks.com

* **Correspondence:** George Z. Voyiadjis; E-Mail(s): voyiadjis@eng.lsu.edu

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Abstract

A robust mathematical method for the characterization of damage in carbon nanotubes is presented the presentation here is limited to elasticity. In this regard, the second and third order elastic stiffnesses are employed. All this is based on damage mechanics. The hypotheses of elastic strain equivalence and elastic energy equivalence are utilized. A new damage variable is proposed that is defined in terms of the surface area. This is in contrast to the classical damage variable which is defined in terms of the cross-sectional area. In the presentation, both the one-dimensional case (scalars) and the three-dimensional case (tensors) are illustrated.

Keywords

Carbon nanotubes; damage mechanics; material modelling; elasticity; elastic energy equivalence; elastic strain equivalence; damage variable

1. Introduction

Carbon nanotubes have been used recently in worldwide applications. Their research is taking off at exponential speeds [1-5]. Recent work has been done also on grapheme [6-10]. The aim of this presentation is to provide a way to characterize damage inc carbon nanotubes. The authors in this respect utilize the principles of continuum damage mechanics. The topic of continuous damage mechanics was first proposed by Kachanov [11] and further developed by Lee et al. [12], Voyaadjis and Kattan [13-16], Sidoroff [17], Krajcinovic [18], and others; and Kattan and Voyadjis [19-21].

In 1958, Kachanov [11] first proposed the concept of effective stress and introduced the theme of continuous damage mechanics. Rabotnov[22] and later others [14-16, 20, 21, 23, 24] followed closely behind. In this framework, a damage variable is introduced that is defined in terms of the cross-sectional area. This damage variable has a zero value for the virgin undamaged material and a value of 1 for the case of complete rupture (total damage).

Research in damage mechanics has progressed very quickly in the past 50 years [12, 13, 17, 19, 25-35]. In addition, there are also some noteworthy researches on the corresponding topics of healing mechanics [24, 36-39]. Some recent research work is considered to be a combined damage/repair model for different types of materials. Basaran has introduced a new way to define damage based on entropy generation [40, 41]. This work consists of two main parts, which deal with the complete theoretical characteristics of carbon nanotube damage within the framework of continuous damage mechanisms. More recent work has been done on damage mechanics especially for rocks [42-48].

One-dimenstional damage in carbon nanotubes is presented in Section 1 in terms of scalars. To illustrate this method, both the hypothesis of elastic strain equivalence and the hypothesis of elastic energy equivalence have been utilized. Especially for nanomaterials like carbon nanotubes, a new damage variable is introduced that is defined based on the surface area as the surface area plays a major role in these types of materials.

Three-dimenstional damage in carbon nanotubes is illustrated in Section 2 in terms of tensor. For this purpose, the two hypotheses of elastic strain equivalence and elastic energy equivalence are utilized. Furthermore, the damage tensor is defined in terms of the surface area. This damage tensor is a generalization of the new damage variable that was introduced in Section1 previously.

2. One-Dimensional Formulation (Scalars)

The elastic stress-strain formula for carbon nanotubes is given by the following formula for the one-dimensional case using scalars (uniaxial tension) [4]:

$$\sigma = E\varepsilon + D\varepsilon^2 \tag{1}$$

where σ and ε are the stress and strain, respectively, while *E* and *D* are the second-order elastic stiffness and third-order elastic stiffness, respectively. The purpose of this work is to show the damage process and the transition of the damage process within the framework of continuous damage mechanics.

In Continuum Damage Mechanics, the effective stress $\bar{\sigma}$ is given by:

$$\bar{\sigma} = \frac{\sigma}{1-\phi} \tag{2}$$

where φ is the classical damage variable. This damage variable is defined in terms of the loss of cross-sectional area due to damage. The effective stress is defined as acting in the virtual undamaged structure, while the actual stress acts in the damaged structure of the material. The value of the damage variable ranges from 0 (undamaged material state) to 1 (completely broken).

The purpose of this work is to show the material constants E and D conversion methods in the damage process, that is, to show the two relations of the following form $\bar{E} = E\, f(\phi)$ and $\bar{D} = D\, g(\phi)$, where f and $g$are unspecified functions. The authors will show the explicit expressions of the scalar functions where $\bar{E}$ and $\bar{D}$ are the second-order effective lossless elastic stiffness and the third-order effective lossless elastic stiffness, respectively. For this purpose, two classical assumptions of elastic strain equivalent and elastic energy equivalent will be used.

2.1 Scalar Formula Using Elastic Strain Equivalence Assumption

The first one starts with the assumption of elastic strain equivalence. In this assumption, it is assumed that the elastic strain is the same in the deformed/damaged configuration and the virtual/undamaged configuration. This assumption can be written as:

$$\bar{\varepsilon} = \varepsilon \tag{3}$$

Write the formula (1) in the effective/undamaged configuration for the barred quantities, as shown below:

$$\bar{\sigma} = \bar{E}\, \bar{\varepsilon} + \bar{D}\, \bar{\varepsilon}^2 \tag{4}$$

Then substitute the strain in equation (3) into equation (4), and substitute the stress in equation (2) into equation (4) to get:

$$\frac{\sigma}{1-\phi} = \bar{E}\, \varepsilon + \bar{D}\, \varepsilon^2 \tag{5}$$

Comparing equations (1) and (5), the following conversion equations for the two elastic stiffnesses of carbon nanotubes can be immediately obtained:

$$E = \bar{E}\, (1-\phi) \tag{6}$$

$$D = \bar{D}\, (1-\phi) \tag{7}$$

It should be noted from equations (6) and (7) that the two elastic stiffness conversions involve the same damage variable. For more elaborate models, two different and independent damage variables should be used-one for each elastic stiffness. This avenue of research will be discussed in Section 1.3.

2.2 Scalar Formula Using Elastic Energy Equivalence Assumption

The sequel discusses how the two elastic stiffnesses can be converted under the assumption of elastic energy equivalent. In this assumption, it is assumed that the elastic energy is the same between the deformed/damaged configuration and the virtual/undamaged configuration. The mathematical formula of this hypothesis is as follows:

$$\bar{U} = U \tag{8}$$

where U is the elastic energy in the deformed/damaged configuration and $\bar{U}$ is the elastic energy in the fictitious/undamaged configuration.

Using equation (1), in the deformed/damaged configuration, the strain energy of carbon nanotubes is obtained as follows:

$$U = \int \sigma \, d\varepsilon = \int (E\,\varepsilon + D\,\varepsilon^2)\, d\varepsilon = \frac{1}{2} E\,\varepsilon^2 + \frac{1}{3} D\,\varepsilon^3 + c_1 \tag{9}$$

where c_1 is a constant of integration to be determined. Similarly one can show that the elastic energy for carbon nanotubes can be written as follows in the fictitious/undamaged configuration:

$$\bar{U} = \frac{1}{2} \bar{E}\,\bar{\varepsilon}^2 + \frac{1}{3} \bar{D}\,\bar{\varepsilon}^3 + c_2 \tag{10}$$

where c_2 is a constant of integration to be determined. Substituting equations (9) and (10) into equation (8), and utilizing the fact that $c_1 = 0$ and $c_2 = 0$ based on the initial conditions in each configuration, one obtains:

$$\frac{1}{2} \bar{E}\,\bar{\varepsilon}^2 + \frac{1}{3} \bar{D}\,\bar{\varepsilon}^3 = \frac{1}{2} E\,\varepsilon^2 + \frac{1}{3} D\,\varepsilon^3 \tag{11}$$

In the next formula, one rewrites equation (4) in the following form:

$$\bar{E} = \frac{\bar{\sigma}}{\bar{\varepsilon}} - \bar{D}\,\bar{\varepsilon} \tag{12}$$

Similarly equation (1) is re-written as follows:

$$E = \frac{\sigma}{\varepsilon} - D\,\varepsilon \tag{13}$$

Substituting equations (12) and (13) into equation (11) and simplifying, we can obtain:

$$\frac{1}{2} \bar{\sigma}\,\bar{\varepsilon} - \frac{1}{6} \bar{D}\,\bar{\varepsilon}^3 = \frac{1}{2} \sigma\,\varepsilon - \frac{1}{6} D\,\varepsilon^3 \tag{14}$$

If the simplified assumptions expressed in the following two equations are not made based on the above equation (14), it cannot be further proceeded:

$$\frac{1}{2} \bar{\sigma}\,\bar{\varepsilon} = \frac{1}{2} \sigma\,\varepsilon \tag{15}$$

$$\frac{1}{6} \bar{D}\,\bar{\varepsilon}^3 = \frac{1}{6} D\,\varepsilon^3 \tag{16}$$

People immediately recognized the expression in equation (15) as a hypothesis of the elastic energy equivalence of linear elastic materials. Next, it is performed by substituting equation (2) into equation (15). After simplifying the obtained equation, the following elastic strain conversion equation is obtained:

$$\bar{\varepsilon} = \varepsilon\,(1-\phi) \tag{17}$$

The next equation substitutes equation (17) into equation (16). After simplifying the obtained equation, the following third-order elastic stiffness conversion equation can be obtained:

$$D = \overline{D}\,(1-\phi)^3 \tag{18}$$

Next, substitute equations (17) and (18) into equation (11). After simplifying the obtained equation, the conversion equation of elastic stiffness can be obtained, as shown below:

$$E = \bar{E}(1-\phi)^2 \tag{19}$$

Therefore, it can be seen from the two conversion equations (18) and (19) that the two elastic stiffnesses of carbon nanotubes are converted in two completely different ways. However, the same single damage variable is still used in both cases. The sequel explores the possibility of using two different and independent damage variables for the two elastic stiffnesses of carbon nanotubes.

2.3 Elastic Stiffness Degradation Damage Variables and Surface Area Damage Variables

In addition, two other scalar damage variables will be studied. The first is the damage variable defined by the degradation of elastic stiffness, and the second is the damage variable defined by the third-order degradation of elastic stiffness [32, 49, 50]. These two damage variables will be compared with the classical damage variables.

One attempts to define two new distinct and independent damage variables ℓ and m defined as follows in terms of elastic stiffness reduction:

$$\ell = \frac{\bar{E}-E}{E} \tag{20}$$

$$m = \frac{\overline{D}-D}{D} \tag{21}$$

From the above two equations, you can immediately get:

$$\bar{E} = E\,(1+\ell) \tag{22}$$

$$\overline{D} = D\,(1+m) \tag{23}$$

From equations (20) and (21) it appears that the maximum values of the two damage variables ℓ and m are infinity. This is because that the values of E and D tend to zero. However, in practical applications, the stiffness does not reduce that much. In addition, if one looks at equation (2) for the effective stress, one notices that when the value of the damage variable Φ is 1, the value of the effective stress explodes to infinity. Thus the damage variable will approach 1 as its maximum value.

Again, it is seen from equation (2) that any value of the damage variable that is beyond 1 is meaningless. The maximum value of Φ is 1. By analogy, the authors limit the maximum values of ℓ and m to 1 also.

First, use the elastic strain equivalent assumption proposed in the transformation equation (6). One substitutes equation (22) into equation (6). After simplifying the obtained equation, we can obtain:

$$(1-\phi)\,(1+\ell)=1 \tag{24}$$

The next equation (23) is substituted into equation (7). After simplifying the obtained equation, we can obtain:

$$(1-\phi)\,(1+m)=1 \tag{25}$$

Comparing equations (24) and (25), one can immediately conclude that for the special case of the elastic strain equivalence assumption, the two independent damage variables are the same. The conclusion is as follows:

$$\ell=m \tag{26}$$

The next step is to explore the nature of the relationship between the two independent damage variables when using the elastic energy equivalent assumption, as shown in the transformation equations (18) and (19). This is a repeat of the previous derivation but for the hypothesis of elastic energy equivalence. For this purpose, equation (22) is substituted into equation (19). After simplifying the obtained equation, we can obtain:

$$(1-\phi)^2\,(1+\ell)=1 \tag{27}$$

Similarly, substituting equation (23) into equation (18) and simplifying the resulting expression, we can obtain:

$$(1-\phi)^3\,(1+m)=1 \tag{28}$$

Comparing the two expressions in equations (27) and (28), some simple algebraic operations can be performed to obtain the following relationship between the two independent damage variables:

$$(1+\ell)^{\frac{1}{2}}=(1+m)^{\frac{1}{3}} \tag{29}$$

Solving equation (29) for ℓ in terms of m, one obtains:

$$\ell=(1+m)^{\frac{2}{3}}-1 \tag{30}$$

It is immediately seen from equation (30) that both damage variables ℓ and m vanish for the virgin/undamaged material. However, when the value of m reaches 1, then the value of ℓ reaches the value 0.587. This means that the maximum damage to the elastic stiffness E is only about half of the maximum damage to the third-order elastic stiffness D. The relationship between these two damage variables of elastic stiffness degradation is illustrated further by plotting the expression of equation (30) as shown in Figure 1.

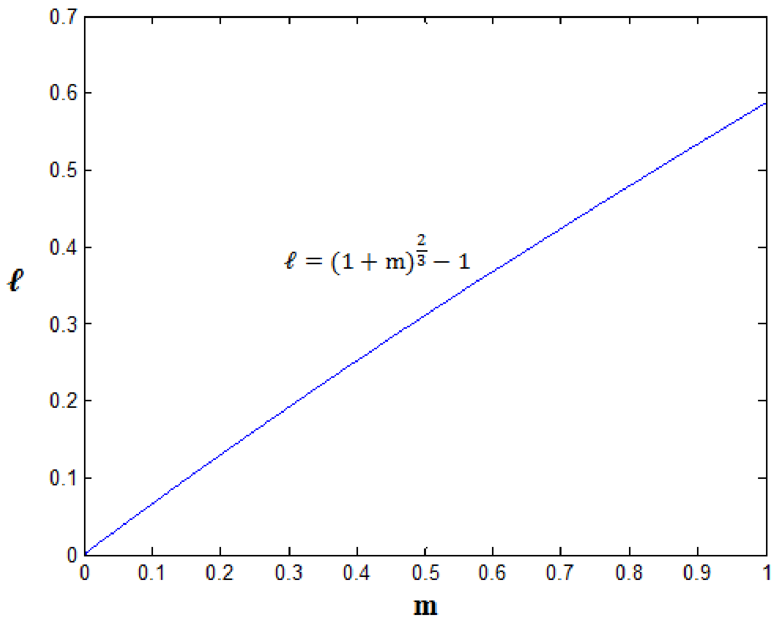

Figure 1 Relationship between the two Damage Variables l and m.

One can get further insight into the relationship between the two damage variables ℓ and m by writing an approximation to equation (30) that is applicable to small values of damage. This can be accomplished easily by writing the Taylor series expansion of the power expression in parenthesis of equation (30). The following Taylor series expansion will be utilized:

$$(1+m)^{\frac{2}{3}} \approx 1 + \frac{2}{3}m - \frac{1}{9}m^2 + \cdots \ldots. \tag{31}$$

Only substituting the first two terms on the right side of equation (31) into equation (30), we can get:

$$\ell \approx \frac{2}{3}m \tag{32}$$

Thus it is seen from equation (32) that for small values of damage, the reduction in the elastic stiffness E is about two-thirds of the reduction in the third-order elastic stiffness D. It is also noted from Figure 1 that for higher values of damage (approaching 1), the reduction in the elastic stiffness E reduces to about one-half of the reduction in the third-order stiffness D. This fact can also be noted from Figure 1 in the relevant applicable range of values.

In nanomaterials, surface area is critical. Therefore, it is important to introduce a new damage variable, which is defined in terms of surface area reduction. To this end, the new damage variable (called the surface area damage variable) is defined as follows:

$$\phi_s = \frac{S - \bar{S}}{S} \tag{33}$$

where S is the surface area in the deformed/damage configuration while $\bar{S}$ is the corresponding surface area in the fictitious/undamaged configuration.

If one looks at equation (2) for the effective stress, one deduces immediately that the value of the cross-sectional area cannot be 1 or more. The effective stress explodes to infinity when Φ is equal to 1. Thus, its maximum value is limited to unity. The same argument holds for the surface area damage variable. Although the equation for the effective stress in terms of the surface area damage variable is not shown in the manuscript, the effective stress also explodes to infinity when the surface area damage variable approaches 1. Thus, its value is limited to unity also.

Next one writes the following geometric relationships that are applicable for Euclidean shapes/solids [51]:

$$S = P \cdot t \tag{34}$$

$$A = \alpha \cdot P^2 \tag{35}$$

where A is the cross-sectional area, S is the surface area, P is the perimeter, t is the thickness, and α is a shape constant (e.g. $\alpha = \frac{1}{16}$ for a square and $\alpha = \frac{1}{4\pi}$ for a circle).

Starting with the definition of the classical cross-sectional area damage variable as follows:

$$\phi = \frac{A - \bar{A}}{A} \tag{36}$$

one substitutes for A from equation (35) into equation (36), and for $\bar{A}$ a similar expression but using barred quantities to obtain:

$$\phi = \frac{\alpha\, P^2 - \alpha\, \bar{P}^2}{\alpha\, P^2} \tag{37}$$

Note from equation (37) that it is assumed that the shape constant is not damaged. This is a reasonable assumption and can simplify the equation well. Formula (37) is simplified as follows:

$$\phi = 1 - \left(\frac{\bar{P}}{P}\right)^2 \tag{38}$$

Equivalently the above equation is re-written as follows:

$$\frac{\bar{P}}{P} = \sqrt{1 - \phi} \tag{39}$$

Next one substitutes equation (34) for S into equation (33), and similar equation for $\bar{S}$ but with barred quantities to obtain:

$$\phi_s = \frac{P \cdot t - \bar{P} \cdot t}{P \cdot t} \tag{40}$$

It is assumed that no damage occurs along the thickness t. In order to draw conclusions and simplify the equation, this is a reasonable and necessary assumption. Therefore, equation (40) is simplified as follows:

$$\frac{\bar{P}}{P} = 1 - \phi_s \tag{41}$$

Finally, compare equations (39) and (41) to arrive at the desired relationship:

$$1 - \phi_s = \sqrt{1 - \phi} \tag{42}$$

The above expression is the relationship between the cross-sectional area damage variable ϕ and the surface area damage variable ϕ_s. This relationship is re-written in its final form as follows based on equation (42):

$$\phi_s = 1 - \sqrt{1 - \phi} \tag{43}$$

It can be seen from equation (43) that for the original/undamaged material, both the cross-sectional damage variable and the surface area damage variable disappear. Similarly, both variables reach the maximum value of 1 at the same time. This can be seen by plotting the relationship of equation (43), as shown in Figure 2.

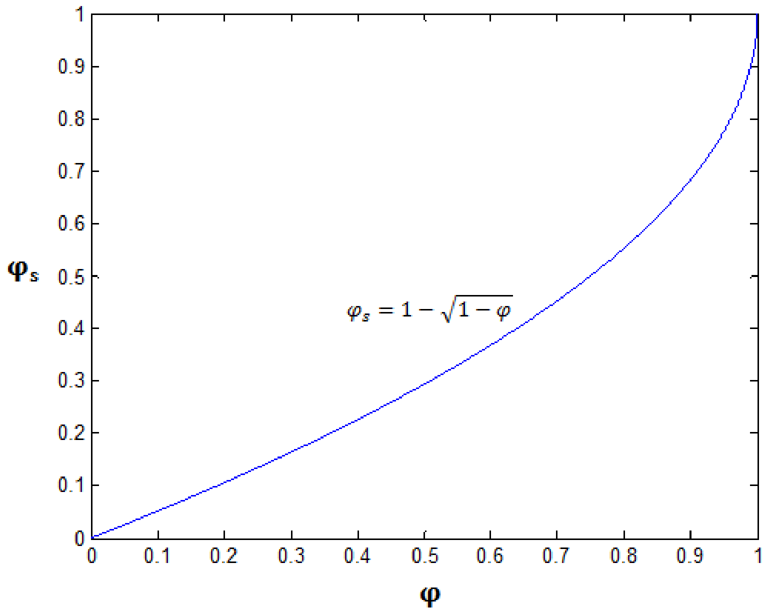

Figure 2 Relationship between the Cross-Sectional Area Damage Variable and the Surface Area Damage Variable.

Indeed, the presentation is mainly theoretical but rigorous. These are two of the main features of this work. The figures are indicative of this issue.

3. Three-Dimensional Formulation (Tensors)

Finally, the whole process is extended to (using tensors) the three-dimensional deformation and damage state of carbon nanotubes. Classic indicial symbols will be used to represent tensors. For this, the following generalization of equation (1) will be used [4].

$$\sigma_{ij} = E_{ijkl}\,\varepsilon_{kl} + \frac{1}{2} D_{ijklmn}\,\varepsilon_{kl}\,\varepsilon_{mn} \tag{44}$$

where σ_{ij} and ε_{kl} are the components of the second-rank stress and second-rank strain tensors, respectively. In equation (44), E_{ijkl} and D_{ijklmn} are the fourth-rank second-order elasticity tensor and the sixth-rank third-order elasticity tensor, respectively. Tensorial generalizations of the transformation equations (6), (7), (18), and (19) will be formulated. Note that by comparing the tensorial equation (44) with the scalar equation (1), one notes that $E \equiv E_{1111}$ and $D = D_{1111}/2$.

Based on equation (44) and using the following derivative derived from the foundation of solid mechanics:

$$\sigma_{ij} = \frac{dU}{d\varepsilon_{ij}} \tag{45}$$

where U is the strain energy in the deformed/damaged configuration, one obtains the stresses. Substituting equation (45) into equation (44) and solving for U (by integrating the relevant expression), one obtains:

$$U = \frac{1}{2} E_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \frac{1}{6} D_{ijklmn}\varepsilon_{ij}\varepsilon_{kl}\varepsilon_{mn} \tag{46}$$

Next one derives the transformation equations for the fourth-rank second-order elasticity tensor E_{ijkl} and the sixth-rank third-order elasticity tensor D_{ijklmn} twice – one time using the hypothesis of elastic strain equivalence and another time using the hypothesis of elastic energy equivalence.

3.1 Tensor Formula Using Elastic Strain Equivalence Assumption

Start with the assumption of elastic strain equivalence. The strain tensor is represented in the following form:

$$\bar{\varepsilon}_{ij} = \varepsilon_{ij} \tag{47}$$

The generalization of the effective stress conversion equation (equation (2)) is usually written in the following form within the framework of continuous damage mechanics [14, 15, 17].

$$\bar{\sigma}_{ij} = M_{ijkl}\sigma_{kl} \tag{48}$$

where $\bar{\sigma}_{ij}$ is the effective stress tensor (defined in the fictitious/undamaged configuration) and M_{ijkl} is the fourth-rank damage effect tensor.

Next, use the barred quantity to write the nonlinear elastic constitutive equation of carbon nanotubes in virtual/lossless configuration (44):

$$\bar{\sigma}_{ij} = \bar{E}_{ijkl}\,\bar{\varepsilon}_{kl} + \frac{1}{2} \bar{D}_{ijklmn}\,\bar{\varepsilon}_{kl}\,\bar{\varepsilon}_{mn} \tag{49}$$

Substituting for the effective stress tensor $\bar{\sigma}_{ij}$ from equation (48) into equation (49), one obtains:

$$M_{ijkl}\sigma_{kl} = \bar{E}_{ijkl}\,\bar{\varepsilon}_{kl} + \frac{1}{2}\bar{D}_{ijklmn}\,\bar{\varepsilon}_{kl}\,\bar{\varepsilon}_{mn} \tag{50}$$

Pre-multiplying equation (50) by M^{-1}_{pqij}, carrying out the relevant multiplications, contractions, and simplifications, one arrives at the following equation:

$$\sigma_{pq} = M^{-1}_{pqij}\bar{E}_{ijkl}\bar{\varepsilon}_{kl} + \frac{1}{2}M^{-1}_{pqij}\bar{D}_{ijklmn}\bar{\varepsilon}_{kl}\bar{\varepsilon}_{mn} \tag{51}$$

Substituting equation (47) into equation (51) (this means replacing the barred strain tensor components with unbarred strain tensor components), one obtains:

$$\sigma_{pq} = M^{-1}_{pqij}\bar{E}_{ijkl}\varepsilon_{kl} + \frac{1}{2}M^{-1}_{pqij}\bar{D}_{ijklmn}\varepsilon_{kl}\varepsilon_{mn} \tag{52}$$

Finally, the stress tensor equations (44) and (52) are compared, and two conversion equations for the fourth and sixth order elastic tensors are obtained:

$$E_{pqkl} = M^{-1}_{pqij}\bar{E}_{ijkl} \tag{53}$$

$$D_{pqklmn} = M^{-1}_{pqij}D_{ijklmn} \tag{54}$$

The above two expressions represent the conversion equations of the fourth and sixth order elastic tensors of carbon nanotubes under the assumption that the elastic strains are equivalent. It can be seen from the above two equations that both elastic tensors are transformed in exactly the same way using the same transformation tensor M^{-1}_{pqij} in the two expressions. This is not the case when using more complex assumptions of elastic energy equivalence, as shown below.

3.2 Tensor Formula Using Elastic Energy Equivalence Assumption

Next, using the assumption of elastic energy equivalence, the conversion equations of the fourth and sixth order elastic tensors of carbon nanotubes are derived. The mathematical formulation of this hypothesis is as follows:

$$\bar{U} = \int \bar{\sigma}_{ij}\; d\bar{\varepsilon}_{ij} = \int \sigma_{ij}\; d\varepsilon_{ij} = U \tag{55}$$

where U is the elastic energy in the deformed/damaged configuration and $\bar{U}$ is the elastic energy in the fictitious/undamaged configuration.

Using equation (44), in the deformed/damaged configuration, the strain energy of carbon nanotubes is obtained as follows:

$$U = \int \sigma_{ij}\, d\varepsilon_{ij} = \int \left(E_{ijkl}\,\varepsilon_{kl} + \frac{1}{2}D_{ijklmn}\,\varepsilon_{kl}\,\varepsilon_{mn}\right)d\varepsilon_{ij} \tag{56}$$

Carrying out the above tensorial integration, and using the relations $d\left(\varepsilon_{ij}\,\varepsilon_{kl}\right) = 2\varepsilon_{kl}\,d\varepsilon_{ij}$ and $d\left(\varepsilon_{ij}\,\varepsilon_{kl}\,\varepsilon_{mn}\right) = 3\varepsilon_{kl}\;\varepsilon_{mn}d\varepsilon_{ij}$, one obtains:

$$U = \frac{1}{2} E_{ijkl}\, \varepsilon_{ij}\, \varepsilon_{kl} + \frac{1}{6} D_{ijklmn}\, \varepsilon_{ij}\, \varepsilon_{kl}\, \varepsilon_{mn} \tag{57}$$

Set the integral constant to zero according to the initial conditions. Similarly, we can prove that the elastic energy of carbon nanotubes can be written as follows in a virtual/undamaged configuration (using the same form of equation (57), but with a barred quantity):

$$\bar{U} = \frac{1}{2} \bar{E}_{ijkl}\, \bar{\varepsilon}_{ij}\, \bar{\varepsilon}_{kl} + \frac{1}{6} \bar{D}_{ijklmn}\, \bar{\varepsilon}_{ij}\, \bar{\varepsilon}_{kl}\, \bar{\varepsilon}_{mn} \tag{58}$$

The next one starts with the expression of the effective stress tensor of equation (49) and rewrites it in the following form:

$$\bar{E}_{ijkl}\, \bar{\varepsilon}_{kl} = \bar{\sigma}_{ij} - \frac{1}{2} \bar{D}_{ijklmn}\, \bar{\varepsilon}_{kl}\, \bar{\varepsilon}_{mn} \tag{59}$$

Post-multiplying equation (59) by $\bar{\varepsilon}_{lp}^{-1}$ and carrying out the needed algebraic manipulations, one arrives at:

$$\bar{E}_{ijpl} = \frac{1}{2} \bar{D}_{ijrsmn}\, \bar{\varepsilon}_{rs}\, \bar{\varepsilon}_{mn}\, \bar{\varepsilon}_{lp}^{-1} - \bar{\sigma}_{ij}\, \bar{\varepsilon}_{lp}^{-1} \tag{60}$$

Equation (60) can be written in the deformed/damaged configuration using unbarred quantities as follows:

$$E_{ijpl} = \frac{1}{2} D_{ijrsmn}\, \varepsilon_{rs}\, \varepsilon_{mn}\, \varepsilon_{lp}^{-1} - \sigma_{ij}\, \varepsilon_{lp}^{-1} \tag{61}$$

Substituting equations (60) and (61) together with equations (57) and (58) into the elastic energy equivalence hypothesis (550), and performing the required algebraic operations, we can get:

$$\begin{gathered} \frac{1}{4} \bar{D}_{ijrsmn}\, \bar{\varepsilon}_{rs}\, \bar{\varepsilon}_{mn}\, \bar{\varepsilon}_{ij}\, I_{ll} - \frac{1}{2} \bar{\sigma}_{ij}\, \bar{\varepsilon}_{ij} I_{ll} + \frac{1}{6} \bar{D}_{ijklmn}\, \bar{\varepsilon}_{ij}\, \bar{\varepsilon}_{kl}\, \bar{\varepsilon}_{mn} \\ = \frac{1}{4} D_{ijrsmn}\, \varepsilon_{rs}\, \varepsilon_{mn}\, \varepsilon_{ij}\, I_{ll} - \frac{1}{2} \sigma_{ij}\, \varepsilon_{ij} I_{ll} + \frac{1}{6} D_{ijklmn}\, \varepsilon_{ij}\, \varepsilon_{kl}\, \varepsilon_{mn} \end{gathered} \tag{62}$$

where I_{ll} is related to the second-rank identity tensor $I_{ij} \equiv \delta_{ij}$.

In order to proceed further and simplify the equation, it is necessary to assume that equation (62) can be decomposed into the following two equivalent equations:

$$\frac{1}{2} \bar{\sigma}_{ij}\, \bar{\varepsilon}_{ij}\, I_{ll} = \frac{1}{2} \sigma_{ij}\, \varepsilon_{ij}\, I_{ll} \tag{63}$$

$$\frac{5}{12} \bar{D}_{ijrsmn}\, \bar{\varepsilon}_{rs} \bar{\varepsilon}_{mn} \bar{\varepsilon}_{ij} = \frac{5}{12} D_{ijrsmn}\, \varepsilon_{rs} \varepsilon_{mn} \varepsilon_{ij} \tag{64}$$

where $I_{ll} = 3$ is used to obtain equation (64) above.

The expression represented by equation (63) is immediately regarded as the form of the elastic energy equivalence hypothesis for linear elastic materials. Substituting formula (48) into formula (63), we can obtain:

$$M_{ijkl}\,\sigma_{kl}\,\bar{\varepsilon}_{ij} = \sigma_{ij}\,\varepsilon_{ij} \tag{65}$$

Pre-multiplying equation (65) by σ_{pq}^{-1} and simplifying, one obtains:

$$M_{ijpq}\,\bar{\varepsilon}_{ij} = \varepsilon_{pq} \tag{66}$$

Solving the effective strain tensor equation (66), the transformation equation of the strain tensor can be obtained, as shown below:

$$\bar{\varepsilon}_{ij} = M_{ijpq}^{-1}\,\varepsilon_{pq} \tag{67}$$

Next, continue to derive the transformation equations of the two elastic tensors. Substituting the effective elastic strain tensor of equation (67) into equation (64), we can obtain:

$$\bar{D}_{ijrsmn}\,M_{rspq}^{-1}\,\varepsilon_{pq}\,M_{mnkl}^{-1}\,\varepsilon_{kl}\,M_{ijab}^{-1}\,\varepsilon_{ab} = D_{ijrsmn}\,\varepsilon_{rs}\,\varepsilon_{mn}\,\varepsilon_{ij} \tag{68}$$

By performing the required tensor manipulation and contraction to solve equation (68), the conversion equation of the sixth-level third-order elastic tensor will be obtained:

$$D_{abpqkl} = \bar{D}_{ijrsmn}\,M_{rspq}^{-1}\,M_{mnkl}^{-1}\,M_{ijab}^{-1} \tag{69}$$

All that remains now is to find the transformation equation for the fourth-level elasticity tensor. To this end, formula (48) can be rewritten as:

$$M_{ijmn}^{-1}\,\bar{\sigma}_{ij} = \sigma_{mn} \tag{70}$$

Next, substituting equations (69) and (70) into equation (44), we get:

$$M_{cdji}^{-1}\,\bar{\sigma}_{cd} = E_{ijkl}\,\varepsilon_{kl} + \frac{1}{2}\bar{D}_{abpqrs}\,M_{abij}^{-1}\,M_{pqkl}^{-1}\,M_{rsmn}^{-1}\,\varepsilon_{kl}\,\varepsilon_{mn} \tag{71}$$

Pre-multiplying equation (71) by M_{efij} and solving for the effective stress tensor, one obtains:

$$\bar{\sigma}_{ef} = M_{efij}\,E_{ijkl}\,\varepsilon_{kl} + \frac{1}{2}\bar{D}_{abpqrs}\,I_{efab}\,M_{pqkl}^{-1}\,M_{rsmn}^{-1}\,\varepsilon_{kl}\,\varepsilon_{mn} \tag{72}$$

where I_{efab} represents the fourth-rank identity tensor. Next, rewrite equation (67) in the following form:

$$\varepsilon_{rs} = M_{rsij}\,\bar{\varepsilon}_{ij} \tag{73}$$

Substituting equation (73) into equation (72) and simplifying the resulting expression after some tensor manipulation, we get:

$$\bar{\sigma}_{ef} = M_{efij}\,E_{ijkl}\,M_{klpq}\,\bar{\varepsilon}_{pq} + \frac{1}{2}\bar{D}_{efabcd}\,\bar{\varepsilon}_{ab}\,\bar{\varepsilon}_{cd} \tag{74}$$

Comparing the equation (74) of the effective stress tensor with the original equation (49) of the effective stress tensor, the required conversion equation of the four-level elastic tensor can be immediately obtained, as shown below:

$$\bar{E}_{efab} = E_{ijkl}\, M_{efij}\, M_{klab} \tag{75}$$

3.3 Surface Area Damage Effect Tensor

Next one attempts to generalize equation (43) for the surface area damage variable using tensors. Let m_{ijkl} represent the new surface area damage effect tensor (which is a fourth-rank tensor) that corresponds to the scalar surface area damage variable ϕ_s. Then the scalar relation in equation (43) can be written as follows using tensors with indicial notation:

$$M_{ijkl} = m_{ijmn} m_{mnkl} \tag{76}$$

Now the effective stress tensor equation (48) can be generalized as follows:

$$\bar{\sigma}_{ij} = m_{ijmn} m_{nmkl} \sigma_{kl} \tag{77}$$

4. Conclusion and Discussion

The nonlinear elastic constitutive equation of carbon nanotubes is used to establish a damage mechanics model to characterize the damage of carbon nanotubes. To this end, several issues were discussed. The formula is executed twice-using scalars and tensors. The two parts containing the scalar formula and the tensor formula are kept separate. In these two parts, the transformation relationship between linear elastic variable/tensor and third-order elastic variable/tensor is derived.

New damage variables are also derived based on the surface area. This damage variable is very useful for studying the damage of nanomaterials such as carbon nanotubes, because surface area is critical in these types of materials. The surface area damage variable is compared with the classical damage variable based on the cross-sectional area. In addition, a tensor summary of the fourth-level surface area damage effect tensor is also proposed.

This a theoretical model based on the surface area damage effect tensor or scalar. This damage variable is very useful for studying the damage of nanomaterials such as carbon nanotubes, because surface area is critical in these types of materials. The surface area damage variable is compared with the classical damage variable based on the cross-sectional area. The theoretical formulation is rigorous, however, experimental data on damage are not available at this time to calibrate the model for specific materials.

The model is valid for any configuration as this formulation is fundamental for the nonlinear elastic constitutive equation of carbon nanotubes and is used to establish a damage mechanics model to characterize the damage in carbon nanotubes. All configurations are valid for using this formulation for carbon nanotubes (CNTs) or multiwalled carbon nanotubes (MWCNTs).

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Competing Interests

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