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A Continuum Model For Stone-wales Defected Carbon Nanotubes

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ABSTRACT

In this paper, a continuum model is proposed so that a Stone-Wales (SW) defected carbon nanotube (CNT) is replaced by an initial circumferential crack in a continuum cylindrical shell. For this purpose, the critical energy release rate and then the fracture toughness of a defected CNT are calculated using the results of an existing atomistic-based continuum finite element simulation. Finally, the equivalent crack length is obtained from the fracture toughness. The proposed model can be applicable tovarious kinds of continuum-based simulations of nano-structures like nano-composites and nano-probes where the fracture resistance studies become important. It is concluded for a case study that the armchair (12, 12) CNT containing a SW defect could be replaced with a continuum cylindrical shell with a circumferential crack length of 0.83 nm. Furthermore, the damage variable is discussed to achieve a method for estimating the effective Young's modulus of defected nanotubes with numerous defects subjected to the progressive damage. This estimation method is evaluated by the atomistic based FE simulation of a double defected CNT.

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1. INTRODUCTION

Carbon nanotubes (CNTs) have extraordinary mechanical, chemical, thermal and electronic properties. These novel characteristics have the combination of light weight, high strength and stiffness. Thus, these carbon particles made a great interest in the areas of nano researches and nano devices. During the last decade the potential of using CNTs for multiple usages such as high precision sensors and novel classes of advanced composites has been expanding [1-4] To study the mechanical properties of nanostructures the theoretical and numerical simulations are more prevalent than experimental methods which encounter many technological challenges [5]. Thus, many researchers are trying to develop new methodologies for the analysis of physical properties of such new materials. The ab initio [6-8], tight binding [9-10], molecular dynamic (MD) [11-12], equivalent continuum modeling [13-15] and molecular structural mechanics methods (MSM) [16-18] are the most popular computational methods to model nano-structures.

Experimental observations have shown that a carbon nanostructure is not defect-free and it contains many kinds of topological defects, such as the Stone–Wales and vacancy defects. These defects are mostly the result of the manufacturing process and they can appearwith mechanical loading [19-20] and electron irradiation [21]. The defects influence mechanical, physical and chemical properties of a nano-structure. Many researchers have simulated the carbon nano-structures to predict the effect of defects on Young's modulus, ultimate strength and other important mechanical properties. Zhang and et al. [22] developed an atomistic-based continuum theory. In their model interatomic potential is directly incorporated into the continuum analysis. Using this continuum model the fracture nucleation in CNTs is studied. Jiang and et al. [23] proposed a hybrid continuum/atomistic model to predict the critical strain of carbon nanotubes with the Stone–Wales (SW) defects. Tserpes and et al. [17, 24] took into account the initial topological and vacancy defects and used the molecular structural mechanics method based on the nonlinear finite element to simulate the progressive fracture of defected single-walled zigzag,

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armchair and chiral nanotubes subjected to axial tension. Xiao and et al. [25] used similar method to investigate the effects of the SW defect on the Young's moduli, fracture and progressive failure of CNTs. They also studied the variation of ultimate stress, strain at failure, and Young's modulus values of carbon nanotubes and graphene sheets as a function of the distance between two defects aligned in the axial and hoop directions [26]. They found that CNTs exhibit brittle behavior at fracture and the fracture nucleation is occurred near the defects.

According to the mentioned researches, we found that each defect in a nanotube potentially could be replaced with a crack in a continuum shell. Thus, in this paper the concept of critical energy release rate is used to obtain the fracture toughness of a SW-defected carbon nanotube. Then, the equivalent crack length is obtained from the fracture toughness. This model could be appropriate to simulate the large CNTs, where using the atomistic models encounters many computational limitations. This model could also be made by finite element method for further studies. Furthermore, using the concept of damage variable, a method is suggested to estimate the effective Young's modulus of damaged CNTs with numerous defects.

2. CRITICAL ENERGY RELEASE RATE

Consider an infinite cracked body of thickness B with a central crack of length a, which is subjected to a uniaxial tensile loading of P (Figure 1). The energy release rate G, is a measure of the energy available per unit crack surface area for infinitesimal crack extension and is calculated from the following equation [27]:

$$G = \frac{1}{B}\frac{\partial}{\partial a}(W - U) \quad (1)$$

where W is the work performed by the external forces applied to the body and U the elastic energy contained in the body.

At the onset of fracture, $G=G_C$, which is a measure of crack driving force or fracture toughness and is called critical energy release rate. Accordingly, at the fracture initiation, the critical energy release rate can be expressed as:

$$G_C = \frac{1}{B}\frac{\partial}{\partial a}(W - U) \quad (2)$$

The global concepts of strain energy release rate hasbeen connected to an easier-to-use crack-tip parameter, stress intensity factor K by Irwin [28]. K is usually a function of the stress applied at far end, the crack length and the geometry of the specimen. At fracture initiation, $K=K_C$. For mode I fracture (opening crack),

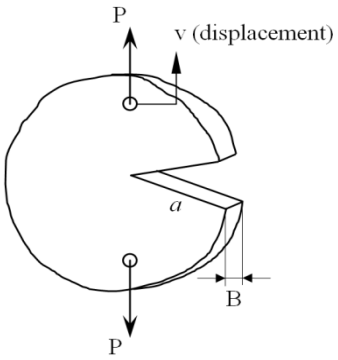


Figure 1. A cracked body under uniaxial tensile loading

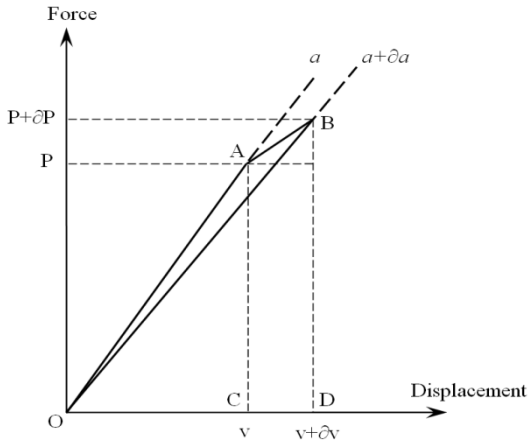


Figure 2. Load-displacement diagram

$$G = K_I^2 / E' \quad (3)$$

where $E' = E$ for plane stress and $E' = E/(1-\nu^2)$ for plane strain (E stands for Young's modulus, and ν stands for Poisson's ratio).

The load-displacement response of the body of Figure 1 with a linear elastic behavior and an initial crack of length a is represented in Figure 2 by the straight line OA. During loading up to point A elastic strain energy represented by the area OAC (SOAC) is stored in the body. This energy is released when the load is removed from the body. Assume that at point A the crack starts to grow to a new length $a+\partial a$. The straight line OB represents the load-displacement behaviour of the body with a longer crack of length $a+\partial a$. Line OB should lie below line OA since the stiffness of the body drops when the crack length increases from point A to B. The elastic strain energy saved in the body at point B is represented by the area OBD (SOBD). If the applied load is removed at point B the unloading path will be the line BO.

In order to calculate the critical strain energy release rate using Equation (3), two terms of ∂W and ∂U are

required. U1 as the elastic energycontained in the bodywith the crack a is equal to the area OAC. Also, U2 is the elastic energy contained in the body with the crack length $a+\partial a$ is equal to the area OBD. On the other hand, the change in the work performed by the external forces, ∂W is the area CABD. Therefore, $\partial(W-U)$ is represented by the area OAB (SOAB), and employing Equation (3) the critical strain energy release rate of the body will be given.

3. EQUIVALENT CONTINUUM CRACKED NANOTUBE FOR SW-DEFECTED CNTs

In some researches [17, 24, 25] the force-displacement or stress-strain curves of various types of carbon nanotubes (CNTs) including armchair, zigzag and chiral types with/without defects have been computed by Molecular Dynamics (MD) or atomistic-based Finite Element (FE) simulations.

Various types of defects have been introduced for the CNTs [17] like rehybridization defects, incomplete bonding, impurity attachments, substitutions, vacancies and topological defects such as the SW transformation [29]. The Stone–Wales defect is formed by the 90 degrees rotation of a sp2 bond of carbon atoms. It is composed of two pentagon-heptagon pairs as shown in Figure 3. The stress-strain curve of an armchair (12, 12) CNT containing a SW defect has been predicted by atomistic-based FE simulations in Ref. [17] and is shown in Figure 4. Using the curve, the critical energy release rate of the CNT and then the fracture toughness can be calculated;this is done in the following. Based on the FE simulations, fracture has been initiated from the longitudinal bond connecting the two pentagons at the strain level of 9% (Figure 5) [17]. In view of Figure 4,

$$u_1 = \frac{U_1}{V_{CNT}} = S_{OAC} = 3.82 \ \ GPa \tag{4}$$

In fact, the stress-strain response of the armchair (12, 12) CNT has a non-linear behaviour as shown in Figure 4, but in calculating u_1 it is approximated by the straight line OA. also,

$$u_2 = \frac{U_2}{V_{CNT}} = S_{OBD} = \frac{1}{2}\times 0.1148 \times 97.04 = 5.57 \ \ GPa \tag{5}$$

Therefore,

$$\partial u = u_2 - u_1 = 1.75 \ GPa \tag{6}$$

On the other hand,

$$\partial w = \frac{\partial W}{V_{CNT}} = S_{CABD} = 2.27 \ \ GPa \tag{7}$$

and then,

$$\partial(W-U) = V_{CNT}(\partial w - \partial u) = 0.525 V_{CNT} \ \ GPa \tag{8}$$

V_{CNT} is the nanotube volume given by $\pi d.t.L$, where d is the diameter and t the thickness of the nanotube. For the nanotube thickness, the value of 0.34 nm, which corresponds to the interlayer spacing of graphene is chosen [18]. The nanotube length L, has been taken as 4.18 nm in the FE simulation [17]. The diameter of the nanotube can be calculated as [30]:

$$d = \frac{\alpha}{\pi}\sqrt{3(n_1^2 + n_2^2 + n_1 n_2)} \tag{9}$$

where α = 0.142 nm is the C–C bond length [26], and the pair of integers (n_1, n_2) are indices to represent its helicity such as armchair ($n_1 = n_2$) and zigzag ($n_2 = 0$) nanotubes. At the fracture initiation in which the longitudinal bond fails, the defect increment of the CNT can be considered as $\partial a = 2.43\alpha = 0.345 \ nm$according to Figures 5 and 3. Thus, G_c can be found from Equation (2) as

$$G_C = \pi d.L\frac{(\partial w - \partial u)}{\partial a} = \pi(1.63\times10^{-9})(4.18\times10^{-9})\times \frac{0.525\times10^{9}}{3.45\times10^{-10}} = 32.50 \ \ J/m^2 \tag{10}$$

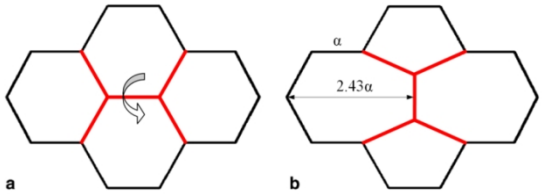


Figure 3. Atomic configuration of the SW defect in the armchair nanotube.

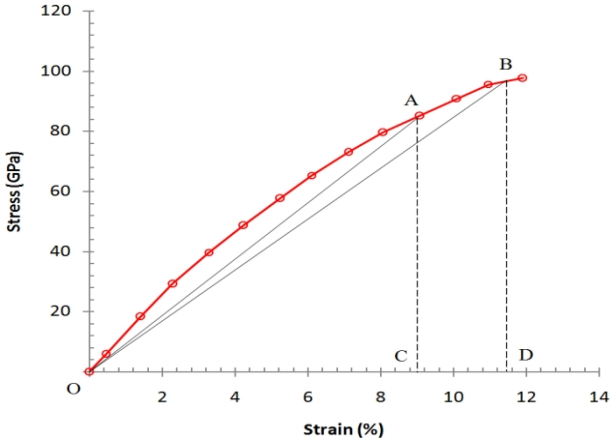
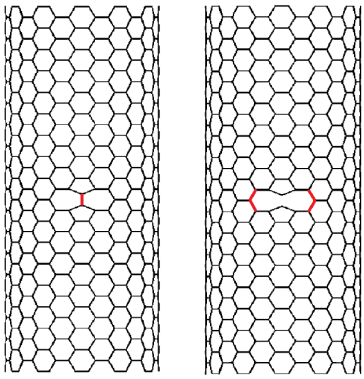


Figure 4. Predicted stress–strain curve of the defective armchair (12, 12) SWCNT



9% strain 11.48% strain

Figure 5. Fracture evolution of the armchair (12, 12) CNT containing a SW defect [17]

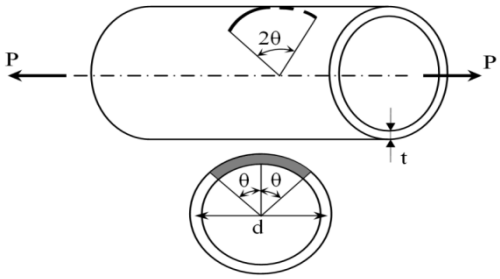


Figure 6. A circumferential crack in a cylindrical shell under tensile loading

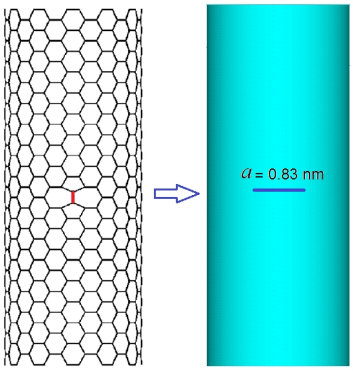


Figure 7. Stone-Wales defect in (a) atomistic and (b) continuum model

On the other hand, the elasticity modulus of the armchair nanotube is obtained as $E = 0.56\ TPa$ from the stress-strain curve of Figure 4 at the fracture initiation strain ($\varepsilon = 9\%$). Then, the calculated G_c and the elasticity modulus result in the fracture toughness of $K_{IC} = 4.27\ MPa\sqrt{m}$ using Equation (3) for plane stress state.A cylindrical shell under tensile loading with a circumferential crack of 2θ shown in Figure 6 can represent the CNT containing a SW defect as a defective continuum nanotube. For the cracked shell the stress intensity factor of fracture mode I (opening mode) is [31]:

$$K_I = \sigma\sqrt{\pi \frac{d.\theta}{2}} F(\theta) \tag{11}$$

where

$$F(\theta) = 1 + 7.5\left(\frac{\theta}{\pi}\right)^{3/2} - 15.0\left(\frac{\theta}{\pi}\right)^{5/2} + 33.0\left(\frac{\theta}{\pi}\right)^{7/2} \tag{12}$$

Consequently, by the given stress at the fracture initiation which is 84.94 GPa for the considered defective CNT (from Figure 4) and the calculatedfracture toughness, the angle of equivalent crack is obtained from Equation (11). Thus, it can be concluded that the armchair (12, 12) CNT containing a SW defect is equivalent to a continuum cylindrical shell with a circumferential crack length of 0.83 nm (Figure 7).

The mechanical properites of carbon nano tubes are depend on their diameters and chirality including zigzag and armchair, so the superseded crack length changes for each Stone-Wales defect. Therefor,havingcomplete information about each CNT, one can follow the mentioned procedure to obtain this crack length.

4. EFFECTIVE YOUNG'S MODULUS OF DAMAGED CNT

Elastic deformation happens by applying the tensile stress to a CNT like an elastic continuum material, and after unloading process the stress-strain curvature doesnot change, However, the fracture of C-C bond changes the behavior of the CNT, and unloading process could not repair it. This phenomenon similarly occurs for the continuum materials when microcracks grow and damage the material. Some of the elastic parameters like Young's modulus and Poisson's ratio decrease because of this damage growth. In continuum mechanics, the damage variable is defined as [32]:

$$D = \frac{S - \tilde{S}}{S} \tag{13}$$

where S is the cross section area of the element before loading and $\tilde{S}$ the effective area after degradation caused by the presence of micro-cracks and cavities due to loading. The effective Young's modulus ($\tilde{E}$) in the direction of tensile stress can be obtained from Equation (14):

$$\tilde{E} = E(1 - D)^2 \tag{14}$$

If we consider a CNT as a cylindrical continuum material, it is not easy to estimate the effective section area ($\tilde{S}$) directly.

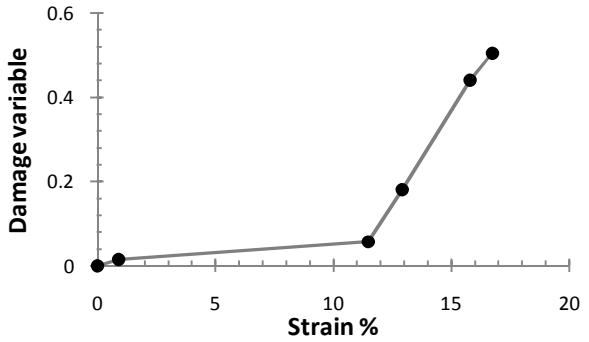


Figure 8. Damage variable versus the strain of a CNT in armchair direction

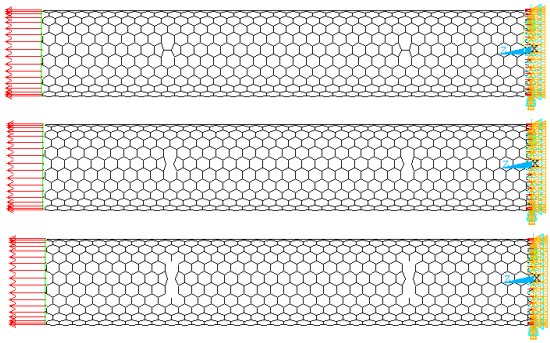


Figure 9. The FE model of double defected CNT

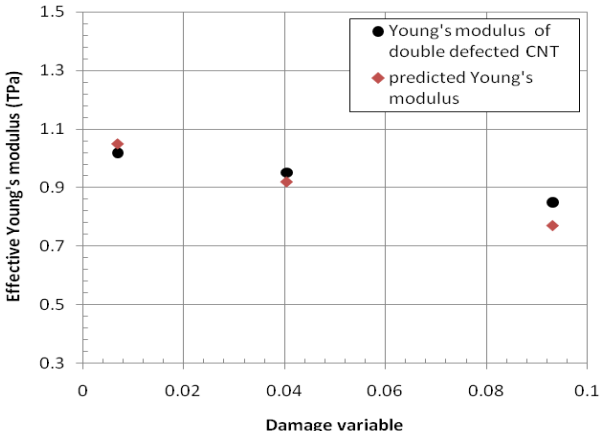


Figure 10. The effective Young's modulus of a double defected CNT versus damage variable

Thus, according to the results of an atomistic simulation [17], the effective Young's modulus is directly calculated for each step of progressive fracture and damage variable is obtained from Equation (15).

$$D = 1 - \sqrt{\frac{\tilde{E}}{E}} \tag{15}$$

The damage variable versus strain is shownin Figure 8,. This curve reveals that the damage variable increases dramatically after the second step of the bond fracture.

Xiao et al. [26] have shown that for the cases with two SW defects located at the same axial location, the bond fracture occurs concurrently for both of them. They have also shown that there is no defect interaction when the separation distance is greater than 2 nm. Thus, we can predict that the second SW defect reduces the effective area as same as the first defect reduction. Thus, according to Equation (13), it is concluded that the damage variable can be estimated by multiplying the damage variable of one defect by the number of damages. Therefore, the effective Young's modulus of damaged CNT after the unloading process can be calculated from the following equation:

$$\tilde{E} = E(1 - n.D)^2 \tag{16}$$

where n is the number of SW defect and D the damage variable for the case with only one defect. In Figure 10, the Young's modulus of a double-defected CNT (Figure 9) predicted using Equation (16) is compared with those obtained directly from the molecular structural mechanics model. In this FE simulation, the C-C bonds are replased by 3D beam elements during the numerical solution. The details of this atomistic method are discussed in[33]and are not presented here.As it is shown in Figure 10, the effective Young's modulus decreases be increasing the damages. In continuum mechanics, damages are made of the micro crack growth, but in this scale it is considered to be the breakage of C-C bonds. However, the precision of this estimation decreases by increasing the damage; the presented simple equation could predict the effective Young's modulus of a multi-defected CNT with good accuracy.

5. CONCLUSION

In the present paper, a continuum model for the defected CNTs is proposed in which a Stone-Wales defect is replaced by a crack with a definite length in a cylindrical continuum shell. In order to obtain the equivalent crack length, the critical energy release rate and then the fracture toughness of a CNT are calculated using the results of an atomistic-based continuum work previously done. Furthermore, the damage variable versus the strain is calculated for a SW-defected armchair CNT and also a simple relation is proposed to predict the effective Young's modulus of a CNT with the multiple defects.

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Damage

چکیده

در این مقاله یک مدل محیط پیوسته برای شبیه سازی نانولوله‌ی حاوی خرابی از نوع استونوالس ارائه می‌شود. بدین منظور نانولوله‌ی تک جداره با یک استوانه‌یجدارنازک حاوی یک ترک با طول مشخص جایگزین می‌شود. از همین رو نرخ انرژی رهایی بحرانی و چقرمگی شکست یک نانولوله‌ی حاوی خرابی استون‌والس بر اساس یکی از مطالعات قبلی با استفاده از روش مکانیک ساختارمولکولی محاسبه شده و براساس آن طول ترکی محاسبه می‌شود که می‌تواند جایگزین این خرابی در یک استوانه‌ی معادل توخالی شود. این مدل می‌تواند در بسیاری از شبیه‌سازی‌های نانولوله که از روش محیط پیوسته استفاده می‌کنند و در آنها در نظر گرفتن خرابی استون‌والس دارای اهمیت است (مانند شبیه سازی نانوکامپوزیت‌ها و نانوحس‌گرها) مورد استفاده قرار گیرد. این مطالعه به طور موردی برای یک نانولوله‌ی (۱۲و۱۲) انجام پذیرفت و مشخص شد طول ترکی که می-تواند جایگزین خرابی استون‌والس شود باید دارای طول ۰/۸۳ نانومتر باشد. علاوه بر این، در این مقاله پارامتر خرابی مورد بررسی قرار گرفت و روشی برای تخمین مدولیانگنانولوله‌ی حاوی چندین خرابی به دست آمد. ارزیابی این روش با نتایج حاصل از مطالعات مکانیک ساختار مولکولی حکایت از دقت مناسب این روش دارد.

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