INFLUENCE OF HEALING RATE ON STRENGTH OF HIERARCHICAL FIBER BUNDLE MATERIALS

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ABSTRACT

Self-healing is one of the fascinating properties for bio-materials such as bone and tendon. Hierarchy is the basic feature of bio-materials. For example, up to seven levels of hierarchy for bone and six levels for tendon have been observed. In this paper, the effect of self-healing rate on the strength of hierarchical fiber bundle materials is theoretically studied. By considering the healing rate, the strength is first derived in the mean sense by using the Weibull distribution and the Daniels' theory. On this basis, the strength is then evaluated for carbon nanotubes with various hierarchical structures, and influence of the healing rate on the strength is finally discussed. The results show that the strength increases rapidly for fiber bundle materials with more hierarchical level when the healing rate is greater than a critical value, inverting the common notion. For different hierarchical modes with the same level, the strength is greater for the mode with fewer fibers on the lower level.

1. INTRODUCTION

One of attractive characteristics of biological materials such as bone and tendon is the ability of self-healing after an instantaneous "trigger" or damaging event. The long term goal of material science is to fabricate bio-material mimicking bio-materials [1, 2]. The original self-healing polymer was developed in 2001 by White et al. [3] who embedded microcapsules containing a healing agent in a polymer composite, the cracking of which caused the healing agent to spread out, then react with catalysis, and polymerize in the composite to extend the life. Owing to the drawback of self-healing mechanism of microcapsules system that only allows one-time healing at a specific position, a variety of healing mechanisms were developed. The vascular-based self-healing system [4] allows a certain number of self-healing cycles. The molecular-based self-healing system [5] can theoretically heal countless times, but usually requires an external trigger such as light or heat. As another approach, the covalent bond was introduced into the polymer matrix to obtain the self-healing characteristic, for example, based on the Diels-Alder reaction [6] and acylhydrazones [7]. In particular, the self-healing mechanism has been found in carbon nanotubes [8] and graphene sheets [9] as a result of metal catalyst at the atomic level for realizing bioinspired nanocomposites. A comprehensive review of self-healing mechanism in artificial materials can be found in literature [10].

In order to reveal the effect of the hierarchical structure on the mechanical properties of bio-materials, a variety of hierarchical models have been developed. Based on fracture mechanics theory, Gao et al [18, 19] viewed the bone like materials as a tension-shear chain model at one level scale, and, with the self-similar hierarchical assumption, the mechanical properties and crack-like flaw tolerances were studied for bone-like material, which were successfully utilized to mimic the gecko attachment system [12]. By using top-down approach, Carpinteri et al. [20] proposed a hierarchical method to analyze the relations of the hardness and toughness of composite materials with the numbers of hierarchical levels. In addition, the effects of hierarchical levels on strength and toughness were also studied by using the hierarchical bell model [21] and the hierarchical lattices model [22].

To comprehensively understand the mechanical property of collagen fiber bio-material, the hierarchical fiber bundle model [23-25] was proposed to treat bioinspired nanostructured materials. This model is the collection of a set of parallel fibers, and the bundle is loaded parallel to the fiber direction, and suits for bone and tendon which are constituted by collagen fibers. Based on this model, Mishnaevsky [26] numerically simulated the damage process of fiber bundle materials (FBMs) while Bosia et al analytically studied the effect of hierarchical level [27] and the fiber healing [28] on the strength.

In this paper, the strength of self-healing hierarchical FBMs is systematically studied. In Section 2, the Weibull distribution is introduced to statistically predict the strength of fibers. In Section 3, by using Weibull distribution and Daniels theory, hierarchical FBMs are studied with recursive evolution of the scale parameter and the shape parameter. In Section 4, the self-healing effect is studied for self-healing FBMs and evolution of the scale parameter with healing rate is derived. In Section 5, the strength is evaluated and discussed for different hierarchical modes of 64 carbon nanotube (CNT) fibers at different healing rate. The concluding remarks are made in Section 6.

2. WEIBULL DISTRIBUTION BASED SINGLE FIBER

The Weibull distribution assumes that the material comprises link units, on the weakest of which the material strength σ depends.

The Weibull distribution [28] is expressed by

$$W(\sigma) = 1 - \mathrm{e}^{-(\sigma/\sigma_0)^{m_0}}, \quad \sigma \in (0, +\infty) \tag{1}$$

where σ_0 is the scale parameter and m_0 is the shape parameter.

If the Weibull density function is denoted by $w(\sigma)$, then we have

$$W(\sigma) = \int_0^{\sigma} w(\sigma) d\sigma \tag{2}$$

According to Eq. (1), Eq. (2) yields

$$w(\sigma) = \frac{m_0}{\sigma_0}\left(\frac{\sigma}{\sigma_0}\right)^{m_0 - 1} e^{-(\sigma/\sigma_0)^{m_0}} \tag{3}$$

Thus, through the first-order moment of Weibull density function $w(\sigma)$, the mean strength of fiber is obtained by

$$\langle \sigma_W \rangle = \int_0^{\infty} \sigma w(\sigma) d\sigma \tag{4}$$

Through the second-order central moment of Weibull density function $w(\sigma)$, the standard deviation is obtained by

$$\theta_W = \int_0^{\infty} \left(\sigma - \langle \sigma_W \rangle \right)^2 w(\sigma) d\sigma \tag{5}$$

Upon substituting Eq. (3), after manipulation, Eq. (4) yields

$$\langle \sigma_W \rangle = \sigma_0 \Gamma(1 + 1/m_0) \tag{6}$$

where $\Gamma(t)$ is the Gamma function as

$$\Gamma(t) = \int_0^{+\infty} x^{t-1} e^{-x} dx, \quad t \in [0, +\infty) \tag{7}$$

Likewise, Eq. (5) yields

$$\theta_W = \langle \sigma_W \rangle \sqrt{\frac{\Gamma(1 + 2/m_0)}{\Gamma^2(1 + 1/m_0)} - 1} \tag{8}$$

3. STRENGTH ANALYSIS FOR HIERARCHICAL FBMS

3.1 THE DANIELS THEORY

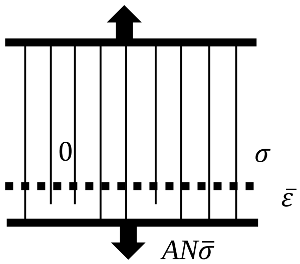


Fig. 1 The FBM composed of N fibers with cross-section A where the top surface is fixed and the bottom surface moves to produce the strain $\bar{\varepsilon}$.

As shown in Fig. 1, a bundle with N elastic fibers stretches under the strain $\bar{\varepsilon}$. The fibers in the bundle are assumed to have identical elastic constants with the strength obeying the Weibull distribution. In the Daniels' fiber bundle theory [23], it is supposed that, a fiber comes to failure when its stress exceeds the threshold, and the load is then equally shared by the remaining intact fibers. Thus, given $\bar{\varepsilon}$, if denoting the strength of fiber by σ, according to the Daniel' theory, the stress of intact fibers in the bundle is also σ.

With the scale parameter σ_0 and the shape parameter m_0 for the Weibull distribution of fibers, from the Daniels theory, the mean strength of bundle is obtained as [27]

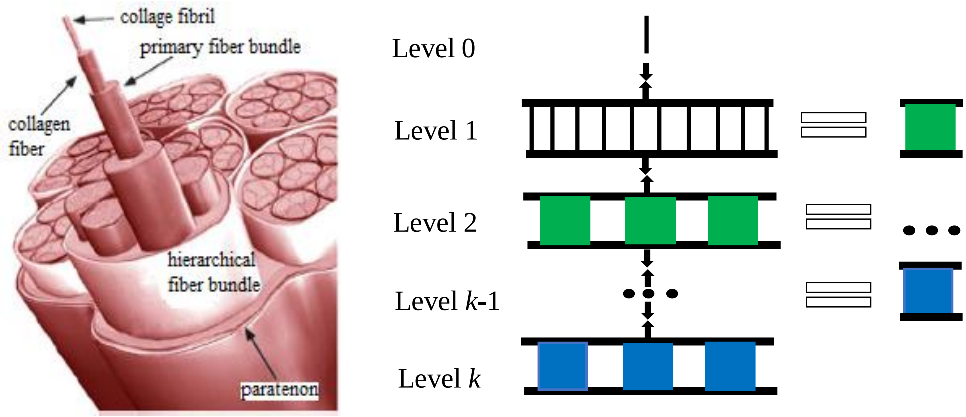
$$\langle \sigma_D \rangle = \sigma_0 (m_0 e)^{-1/m_0} \tag{9}$$

with corresponding standard deviation being [27]

$$\theta_D = \sqrt{\langle \sigma_D \rangle^2 \frac{1-e^{-1/m_0}}{Ne^{-1/m_0}}} \tag{10}$$

3.2 STRENGTH ANALYSIS

Almost all biological collagen fibrous materials can be viewed as a hierarchical structure. For example, tendon is a hierarchical FBM shown in Fig 2a with the hierarchical mode shown in Fig 2b. Each level of fiber bundle is composed of the lower lever fiber bundles, and thus, the level-0 bundle has only a single fiber with the strength obeying the Weibull distribution, the level-1 bundle has N^0 level-0 bundles (i.e. fibers), the level-2 bundle has N^1 level-1 bundles, and so on.



(a) (b)

Fig. 2 Schematic diagram of structure (a) and the hierarchical mode (b) of tendon [29]

Thus, on one hand, the N^{k+1} level-(k+1) bundles can be regarded as the constituent of the level-(k+2) bundle which obey the Weibull distribution so that Eqs. (6) and (8) are followed like a fiber. On the other hand, the level-(k+1) bundles can be regarded as the one composed of N^k level-k bundle which obey the Daniels bundle theory so that Eqs. (9) and (10) are followed.

Hence, it is reasonable to have

$$\begin{cases} \langle \sigma_W^{k+1} \rangle = \langle \sigma_D^k \rangle \\ \theta_W^{k+1} = \theta_D^k \end{cases} \tag{11}$$

where $\langle \sigma_W^{k+1} \rangle$ and θ_W^{k+1} are those of Eqs. (6) and (8) pertaining to the level-(k+1) FBM whereas $\langle \sigma_D^k \rangle$ and θ_D^k are those of Eqs. (9) and (10) pertaining to the level-k FBM.

Making use of Eqs. (6) and (8) and Eqs. (9) and (10), Eq. (11) yields

$$\sigma_0^{k+1}\Gamma(1+1/m_0^{k+1}) = \sigma_0^k \left(m_0^k e\right)^{-1/m_0^k} \tag{12}$$

and

$$\frac{\Gamma\left(1+2/m_0^{k+1}\right)}{\Gamma^2\left(1+1/m_0^{k+1}\right)}=\frac{1-e^{-1/m_0^k}}{N^k e^{-1/m_0^k}}+1 \tag{13}$$

where σ_0^k and m_0^k are the scale parameter and the shape parameter of level-k bundle, respectively.

From Eqs. (12) and (13), the scale parameter and shape parameter of level-(k+1) bundle can be recursively obtained from those of level-k by using the two-step procedure:

Step 1: with known m_0^k and N^k, m_0^{k+1} is obtained from Eq. (13);

Step 2: with known m_0^k, m_0^{k+1} and σ_0^k, σ_0^{k+1} is obtained from Eq. (12).

Eq. (12) and Eq. (13) indicate that the hierarchy effect is equivalent to evolution of the scale parameter and the shape parameter in a recursive form with hierarchical level.

4. STRENGTH ANALYSIS FOR SELF-HEALING HIERARCHICAL FBMS

From Eq. (1), for a sufficient number of fibers N, the number of intact fibers N_i can be obtained by

$$N_i = Ne^{-(\sigma/\sigma_0)^{m_0}} \tag{14}$$

Next, the self-healing FBM is studied. To this end, we define the fiber failure rate ϕ_i^* as [28]

$$\phi_i^* = -\int_N^{N_i}\frac{dN}{N} = -\ln\frac{N_i}{N} \tag{15}$$

where N is the number of fiber in the bundle and N_i is the intact number thereof. Hence, after self-healing to some extent, the number of intact fibers will be N_{ih}, and the fiber failure rate ϕ_h^* as

$$\phi_h^* = -\int_N^{N_{ih}}\frac{dN}{N} = -\ln\frac{N_{ih}}{N} \tag{16}$$

In this context, the self-healing rate η is defined as the rate of the failure rate after healing effect to the total failure rate without healing. That is, we have

$$\eta = 1-\frac{\phi_h^*}{\phi_i^*} \tag{17}$$

Considering Eqs. (15) and (16), we eventually obtain

$$\eta = 1-\ln\frac{N_h}{N}\Big/\ln\frac{N_s}{N} \tag{18}$$

Thus, with the self-healing effect, from Eq. (14), the number of intact fibers N_h is obtained as

$$N_h = Ne^{-\left(\sigma/\left[(1-\eta)^{-1/m_0}\sigma_0\right]\right)^{m_0}} \tag{19}$$

Comparing Eq. (19) with Eq. (1), when taking the self-healing effect into account, the Weibull strength distribution function $W(\sigma)$ becomes

$$W(\sigma) = 1 - e^{-(\sigma/\tilde{\sigma}_0)^{m_0}} \tag{20}$$

where

$$\tilde{\sigma}_0 = \sigma_0 (1-\eta)^{-1/m_0} \tag{21}$$

According to Eqs. (20) and (21), the self-healing effect on the fiber bundle is equivalent to evolution of the scale parameter with the healing rate in the Weibull distribution.

It is reasonable to believe that, replacing σ_0^k with $\tilde{\sigma}_0^k$, the self-healing effect can also be taken into account for hierarchical FBMs. Thus, the strength of hierarchical FBMs with healing rate η is derived as

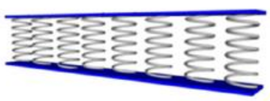
$$\langle \sigma_D \rangle = \tilde{\sigma}_0^k \left(m_0^k e\right)^{-1/m_0^k} \cdot f\left(m_0^k, N^k\right) \tag{22}$$

where $\tilde{\sigma}_0^k$ and m_0^k are respectively the scale parameter and the shape parameter at level k, and $f\left(m_0^k, N^k\right)$ is the correction factor for limited N^K fibers of bundle at level k and takes the form of [27]

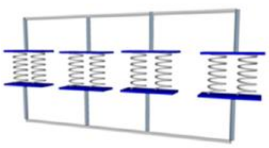
$$f\left(m_0^k, N^k\right) = 1 + \left(\frac{\Gamma\left(1+1/m_0^k\right)}{\left(m_0^k e\right)^{-1/m_0^k}}\right)\left(N^k\right)^{-2/3} \tag{23}$$

5. INFLUENCE OF HEALING RATE ON STRENGTH OF HIERARCHICAL CNT-FBMS

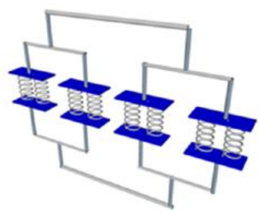
5.1 HIERARCHICAL MODES



(a)The nonhierarchical (one-level hierarchical) mode: (8)



(b)The two-level hierarchical mode: (2, 4)



(c)The three-level hierarchical mode: (2, 2, 2)

Fig. 3 The three consecutively hierarchical modes of 8 fibers

For illustration reason, total 8 fibers are used to study the consecutively hierarchical modes, as schematically shown in Fig. 3. That is, in Fig 3a, 8 fibers (i.e. N^0=8) are totally arranged in parallel to form a nonhierarchical (one-level hierarchical) mode which is denoted by (N^0) = (8). In Fig. 3b, every 2 fibers (i.e. N^0=2) are first arranged in parallel to form a level-1 bundle, and 4 level-1 bundles (i.e. N^1=4) are finally arranged in parallel to form the two-level hierarchical mode which is denoted by (N^0, N^1) = (2, 4). In Fig. 3c, every 2 fibers (i.e. N^0=2) are first arranged in parallel to form a level-1 bundle, every 2 level-1 bundles (i.e. N^1=2) are then arranged in parallel to form a level-2 bundle, and 2 level-1 bundles (i.e. N^2=2) are finally arranged to form the three-level hierarchical mode which is denoted by (N^0, N^1, N^2) = (2, 2, 2).

For the CNT material, the Weibull distribution parameters are obtained as σ_0=34Gpa and

m_0=2.0 [27], and the material is assumed to have 64 fibers. In this case, the FBM be assigned as one level fiber bundle denoted by (64), two levels by (32, 2), three levels by (16, 2, 2) or four levels by (8, 2, 2, 2).

5.2 INFLUENCE OF HEALING RATE ON STRENGTH OF CNT-FBM

In this subsection, influence of the healing rate on the strength is studied in detail.

5.2.1 DEPENDENCE OF STRENGTH ON THE HEALING RATE

Firstly, we examine dependence of the strength on the healing rate. To this end, the FBM with (8, 2, 2, 2) mode is taken as an example. Variation of the strength with the healing rate is shown in Fig. 4. It is seen that, the strength increases with the healing rate, and the greater healing rate the more increase in strength.

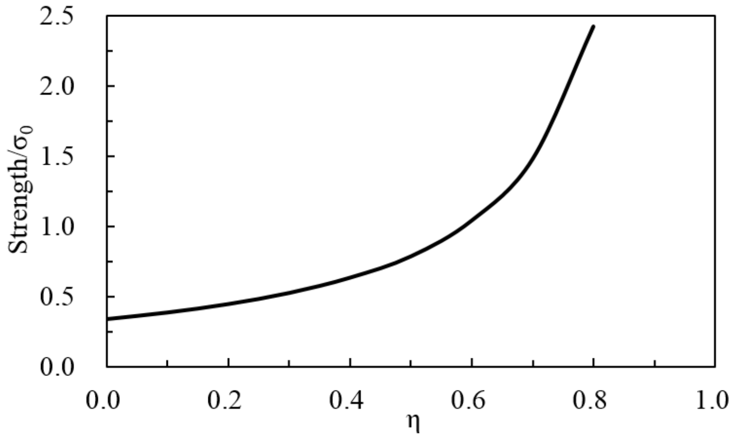


Fig. 4 Variation of strength with the healing rate

5.2.2 STRENGTH FOR DIFFERENT HIERARCHICAL LEVELS

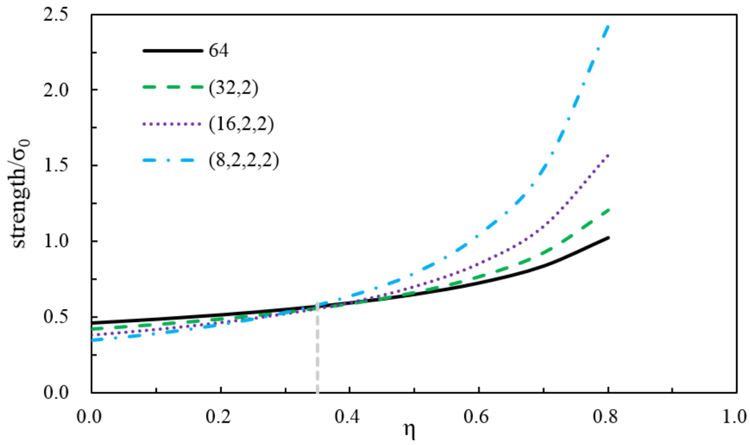


Fig. 5 Variation of strength with healing rate for different hierarchical levels

Secondly, we examine the strength of different hierarchical levels. To this end, the FBM with four consecutively hierarchical modes, i.e. mode (8, 2, 2, 2), (16, 2, 2), (32, 2) and (64), are considered. Variation of the strength with the healing rate is shown in Fig. 5 for the four modes. It is seen that, when the healing rate is greater than a critical value of $\eta = 0.35$, the FBM with more levels has the bigger strength, and therefore the four-level structure of (8,2,2,2) has the highest strength.

5.2.3 STRENGTH FOR THE SAME HIERARCHICAL LEVEL WITH DIFFERENT MODES

Next, we examine the FBM with the same hierarchical level but different modes.

5.2.3.1 FOR THE TWO-LEVEL STRUCTURE

For two-level structures, there are five consecutively different modes such as mode (32, 2), (16, 4), (8, 8), (4, 16) and (2, 32). The results are shown in Fig. 6. It is seen that the strength gains an apparent increase when the lowest level (i.e. the first level in this case) has 2 fibers (i.e. mode (4,16)) or 2 fiber (i.e. mode (2,32)). Consequently, the FBM with mode (2, 32) has the highest strength. It is interesting that the strengths for mode (32,2) and (16,4) are very close during the whole healing process.

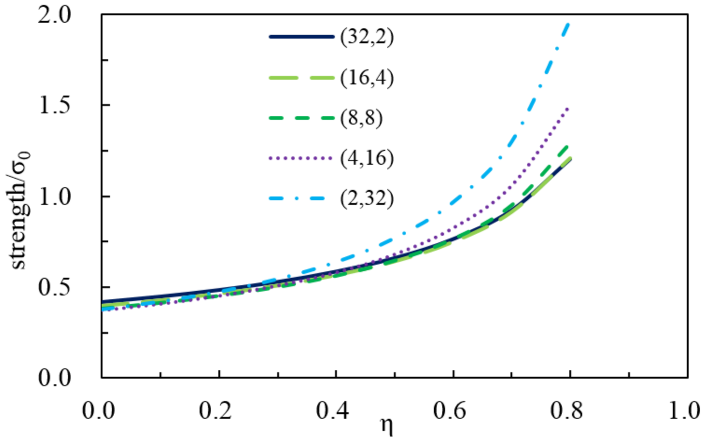


Fig. 6 Variation of strength with the healing rate for five consecutive two-level modes

5.2.3.2 FOR THE THREE-LEVEL STRUCTURE

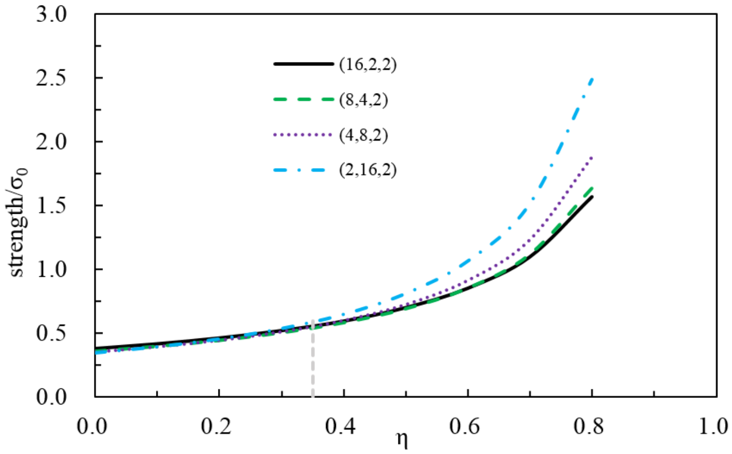
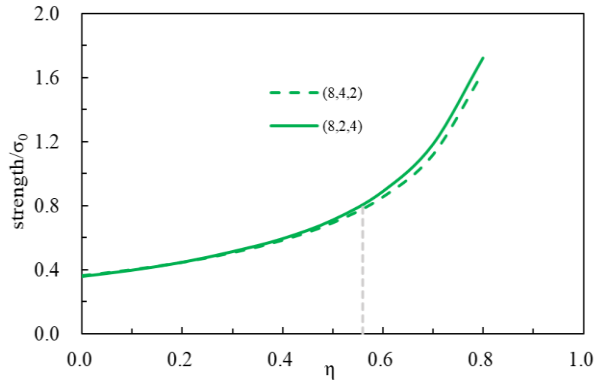
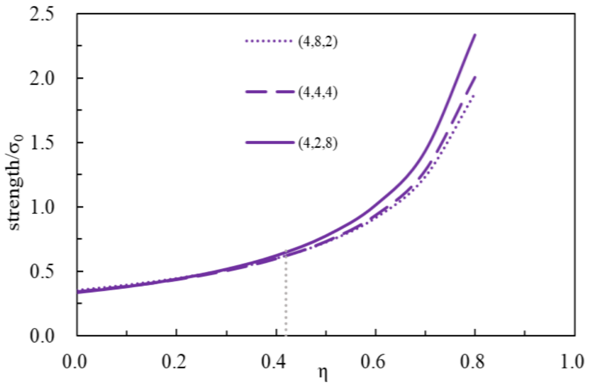


Fig. 7 Variation of strength with the healing rate for four consecutive three-level modes

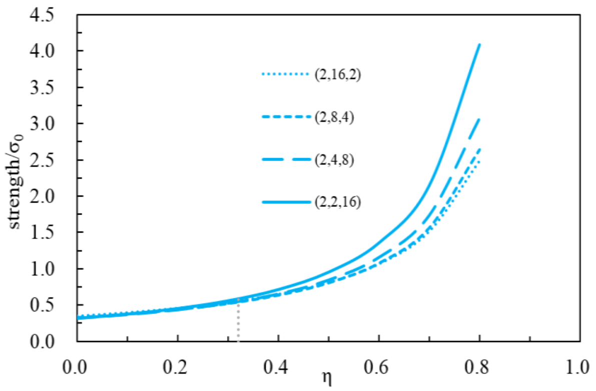
For three-level structures, the four consecutively hierarchical modes (i.e. (16,2,2),(8,4,2), (4,8,2) and (2,16,2)) are first studied, and variation of strength with the healing rate is shown in Fig. 7. It is seen that, when the healing rate is less than η=0.35, the difference is trivial for all the modes. Only mode (4,8,2) or (2,16,2) can produce an apparent increase in strength when the healing rate is greater than η=0.35. As a consequence, the FBM with mode (2,16,2) has the highest strength.



(a)



(b)



(c)

Fig. 8 Variation of strength: (a) for mode (8,*,*); (b) for mode (4,*,*) and (c) for mode (2,*,*)

For the three-level structure of 64 fibers, given the number of the first level, there may be some other hierarchical modes. If the first level has 8 fibers, we can have two different modes, i.e. mode (8,4,2) and (8,2,4), and the strengths are shown in Fig. 8a. Likewise, we can have three different modes, i.e. mode (4,8,2), (4,4,4) and (4,2,8) as shown in Fig. 8b, if the first level has 4 fibers, while we have four different modes such as mode (2,16,2), (2,8,4), (2,4,8) and (2,2,16) as shown in Fig. 8c if the first level has 2 fibers. It is seen that, there are some respective critical values which are become smaller (e.g. from η=0.56, 0.41 and then to η=0.32 for around 0.9 GPa absolute error) for the modes with fewer fibers on the first level. In addition, before the critical values, the difference in strength is trivial. However, after the critical values, the strength gains a more apparent increase for the mode with the fewest fibers on the lower level.

5.2.3.3 FOR FOUR-LEVEL STRUCTURES

The study can also be carried out for the four level structure. For the case of consecutive four-level modes, i.e. mode (8, 2, 2, 2), (4, 4, 2, 2) and (2, 8, 2, 2), variation of strength is similar to that of the three-level structure. Hence, the FBM with mode (2, 8, 2, 2) increases rapidly after relative critical value η=0.38 for 5% relative error in strength and eventually has the highest strength.

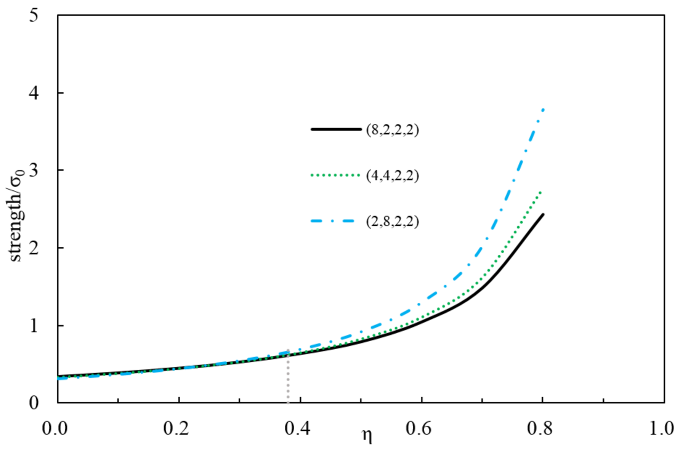
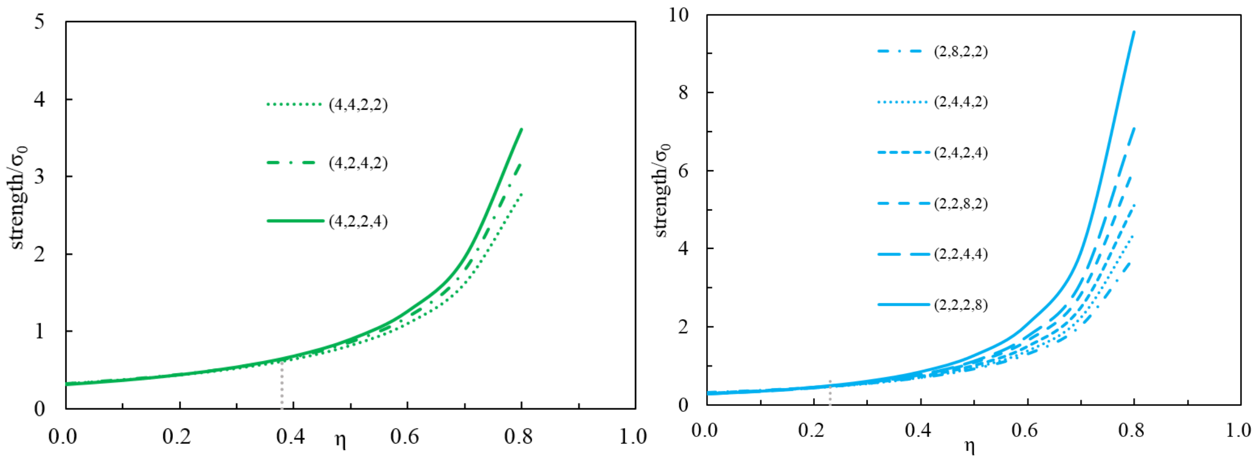


Fig. 9 Variation of strength for consecutive four-level structures with healing rate



(a) (b)

Fig. 10 Variation of strength: (a) for mode (4,*,*,*); (b) for mode (2,*,*,*)

For the four-level structure, given the fiber number on the first level, there are quite a number of different modes. As examples, mode (4,*,*,*) shown in Fig. 10a and mode (2,*,*,*) shown in Fig. 10b are examined. It is not difficult to find similar dependence of strength on modes and the healing rate, and hence, mode (4, 2, 2, 4) in Fig. 10a and mode (2, 2, 2, 8) in Fig. 10b increase rapidly after relative critical value η=0.39 and η=0.25 for 5% relative error in strength, respectively, and eventually has the highest strength in the respective case.

6 CONCLUSIONS

In this paper, the strength of self-healing hierarchical FBMs was first derived by using the Weibull distribution and the Daniels theory, and then evaluated for 64 CNT fibers. The results show that, when the healing rate is greater than a critical value, the common notion is inverted that the weaker strength the more hierarchical levels [25-27]. For the modes with the same hierarchical level, the strengths increase rapidly for the modes with fewer fibers on the lower levels when the healing rate is greater than some critical values. On this basis, the mechanism why natural bio-materials are of hierarchical structure may probably be explained to some extent, and is therefore exploited for the design of artificial self-healing materials.

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