MODELING THE SELF-HEALING OF BIOLOGICAL OR BIO-INSPIRED NANOMATERIALS

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Abstract: *Self-healing materials are a class of solids that have the capability to repair damage autonomically, as often observed in living materials. Here, a first model is presented that incorporates self repairing fibers to determine the expected mechanical behavior of a self-healing bundle.*

1. Introduction

Biological systems have the ability to sense, react, regulate, grow, regenerate, and heal. Recent advances in materials chemistry and micro- and nanoscale fabrication techniques have enabled biologically inspired materials systems that mimic many of these remarkable functions. Self-healing materials are motivated by biological systems in which damage triggers a site-specific, autonomic healing response. Self-healing has been achieved using several different approaches for storing and triggering healing functionality in polymers. There are different models for the prediction of the fatigue behavior of self-healing polymers [1-3].

Other classes of synthetic materials can undergo healing processes, which in mechanics are basically the mechanisms leading to the recovery of strength and stiffness after damage. However, most synthetic materials require outside intervention such as the application of heat or pressure to initiate and sustain the healing process. For example, Ando et al. [4-7] have shown the healing capability of sintered ceramics while exposed to high temperatures (1000 °C).

In addition, supramolecular materials naturally feature so-called «reversible» (non-permanent) intermolecular bonds, in contrast with polymers derived from traditional chemistry, which are based on so-called «irreversible» (permanent) bonds. This reversibility feature imparts a natural capacity to self-heal: cracks or breaks occurring in supramolecular materials can be repaired simply by putting the fractured surfaces back together and applying light pressure; the material nearly recovers its initial strength without the need for bonding or heating.

Too model in general self-healing materials, fiber bundle models can be used. A large number of non-healing models exist for fiber bundles [e.g. 8-11]. In contrast, according to the authors knowledge, there is no model for the prediction of the tensile behavior of self-healing fiber bundles.

This model is the aim of the present letter.

2. Engineering self healing parameter

For a large number, N_0, of fibers in a bundle, the number of surviving fibers N_{s0}, under an applied strain ε, is given by [2]:

$$N_{s0} = N_0 \exp[-(\frac{\varepsilon}{\varepsilon_0})^m] \quad (1)$$

where ε_0 and m are the scale and shape parameters of the Weibull flaw distribution.

The fraction of broken fibers is given by:

$$N_{s0} = N_0 \exp[-(\frac{\varepsilon}{\varepsilon_0})^m] \quad (2)$$

and in case of self-healing:

$$\alpha_h = \frac{N_{bh}}{N_0} = \frac{N_0 - N_{sh}}{N_0} \quad (3)$$

where N_{sh} is the actual number of surviving fibers in the presence of self-healing.

Note that eqs. (2) and (3) resemble the definition of an engineering strain ($\varepsilon = \frac{l - l_0}{l_0}$).

We introduce the parameter λ, as the ratio between the number of broken fibers with self-healing, N_{bh}, and the number of broken fibers without healing N_{b0}:

$$\lambda = \frac{\alpha_h}{\alpha_0} = \frac{N_{bh}}{N_{b0}} = \frac{N_0 - N_{sh}}{N_0 - N_{s0}} \quad (4)$$

Finally, we introduce the healing parameter η, as:

$$\eta = 1 - \lambda = \frac{N_{sh} - N_0}{N_0 - N_{s0}} \quad (5)$$

Note that when η=1 we have N_{sh}=N_0, whereas for η=0, N_{sh} =N_{s0}.

3. True self healing parameter

We now introduced the true parameter α_h^* as:

$$\alpha_h^* = \int_{N_0}^{N_{sh}} \frac{\mathrm{d}N}{N} = \ln N_{sh} - \ln N_0 = \ln \frac{N_{sh}}{N_0} \tag{6}$$

in analogy with the true strain ($\varepsilon = \int_{l_0}^{l} \frac{\mathrm{d}l}{l} = \ln \frac{l}{l_0}$).

In absence of healing it becomes:

$$\alpha_0^* = \ln \frac{N_{s0}}{N_0} \tag{7}$$

From equations (4) and (5), the true self-healing parameter is given by:

$$\eta = 1 - \lambda = 1 - \frac{\alpha_{sh}^*}{\alpha_0^*} = 1 - \frac{\ln \frac{N_{sh}}{N_0}}{\ln \frac{N_s}{N_0}} \tag{8}$$

The introduction of the true self-healing parameter of eq. (8) is needed in order to take into account the variation of the total number of fibers induced by the self-healing (similarly to the true strain that is accounting for the length variation).

From equation (1) we immediately derive:

$$\ln \frac{N_s}{N_0} = (-(\frac{\varepsilon}{\varepsilon_0})^m) \tag{9}$$

By substituting equation (9) into equation (8) we find:

$$\ln \frac{N_{sh}}{N_0} = ((\eta - 1)(\frac{\varepsilon}{\varepsilon_0})^m) \tag{10}$$

and thus:

$$N_{sh} = N_0 \exp[(\eta - 1)(\frac{\varepsilon}{\varepsilon_0})^m] \tag{11}$$

The introduction of the self-healing into eq. (11) generalizes the classical Weibull approach [12], eq. (1).

The last expression is related to the applied tensile load, *P*, by:

$$P(\varepsilon) = AE\ \varepsilon[N_0 \exp[(\eta - 1)(\frac{\varepsilon}{\varepsilon_0})^m]] \quad (12)$$

where *A* is the cross sectional area of the single fiber and *E* is its Young's modulus. Then, if *A, L, E,* N_0, *m* and ε_0 are known, the curve stress vs. strain can be obtained:

$$\sigma(\varepsilon) = \frac{P(\varepsilon)}{AN_0} = E\ \varepsilon[\exp[(\eta - 1)(\frac{\varepsilon}{\varepsilon_0})^m] = E_{\text{eq}}(\varepsilon, \eta)\varepsilon \quad (13)$$

4. Results and discussion

As an example we apply our calculation to carbon nanotube (CNT) bundle with strength randomly assigned, $\varepsilon_0 = 0.04$ and $m_0 \approx 2.7$, based on the nanoscale Weibull distribution [13].

Fig.1 shows the mechanism of the self-healing of a carbon nanotube. Self-healing of CNTs may accelerate the development of the CNT apace-elevator mega cable [15-17].

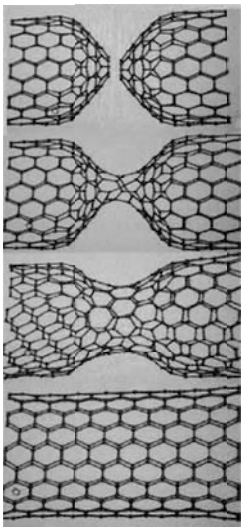

Fig. 1 Carbon nanotube self-healing mechanism [14].

In Fig. 2, the stress–strain response is predicted for a bundle with different values of the healing parameter, η, from 0 to 1, while all the other parameters in equation (13) are kept constant. When increasing the self-healing parameter, both the maximum stress, see Fig. 2, and the strain at which the maximum stress is reached, increase. (This can also be seen in Fig. 7, where the ratio between the maximum stress with healing and maximum stress without healing is increasing in a monotonic way with an increase in the healing parameter.) For a self-healing parameter equal to 1 the bundle becomes unbreakable.

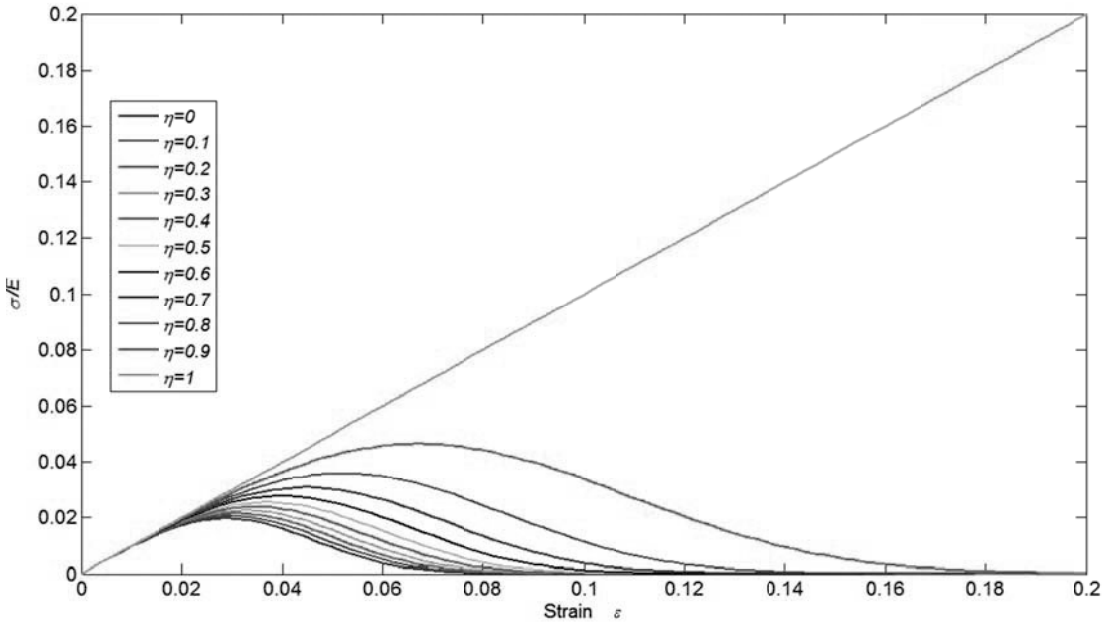

Fig. 2 Stress-strain response by varying the self-healing parameter.

Fig. 3 shows the variation of the number of survival fibers as a function of the applied strain, with different values of the healing parameter.

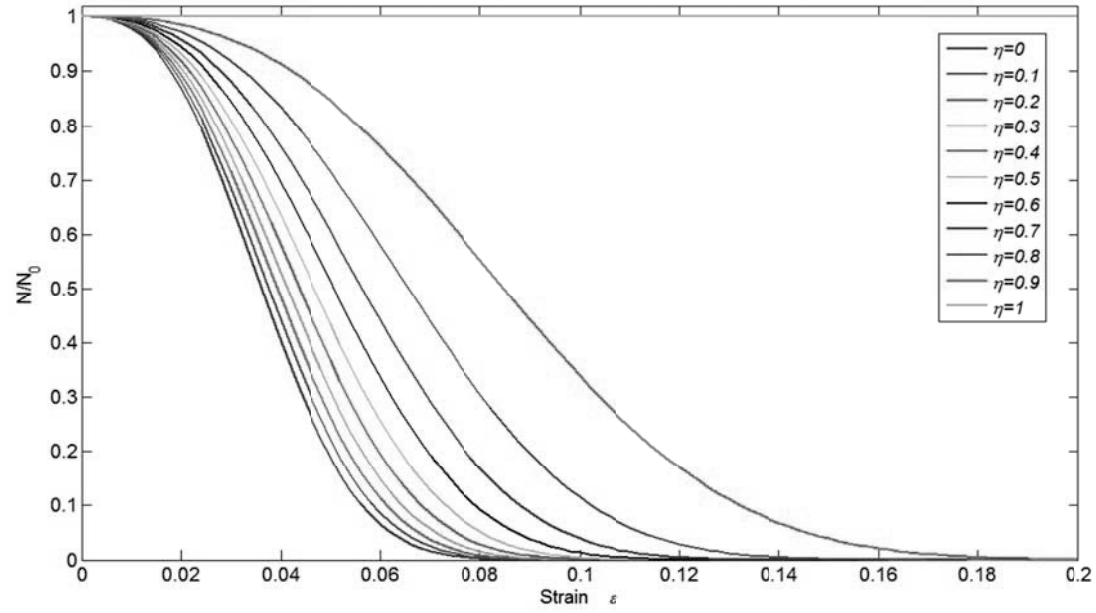

Fig. 3 Survival fibers, $N_{sh} \equiv N$ vs. strain, by varying the healing parameter.

Fig. 4 shows two different type of curves. The upper curves represent the stress-strain curves of Fig. 2 and the lower curves are the rates of variation of the number of survival fibers in the bundle, by varying the applied strain and for different self-healing. The maxima of the lower curves represent the points at maximal failure rate of the bundle. From Fig. 4 we can see that the strains at which the maximum stress is reached, ε_{σ}^{*}, are lower than the strains at the maximal failure rate, ε_{n}^{*}, as specifically reported in Fig. 5.

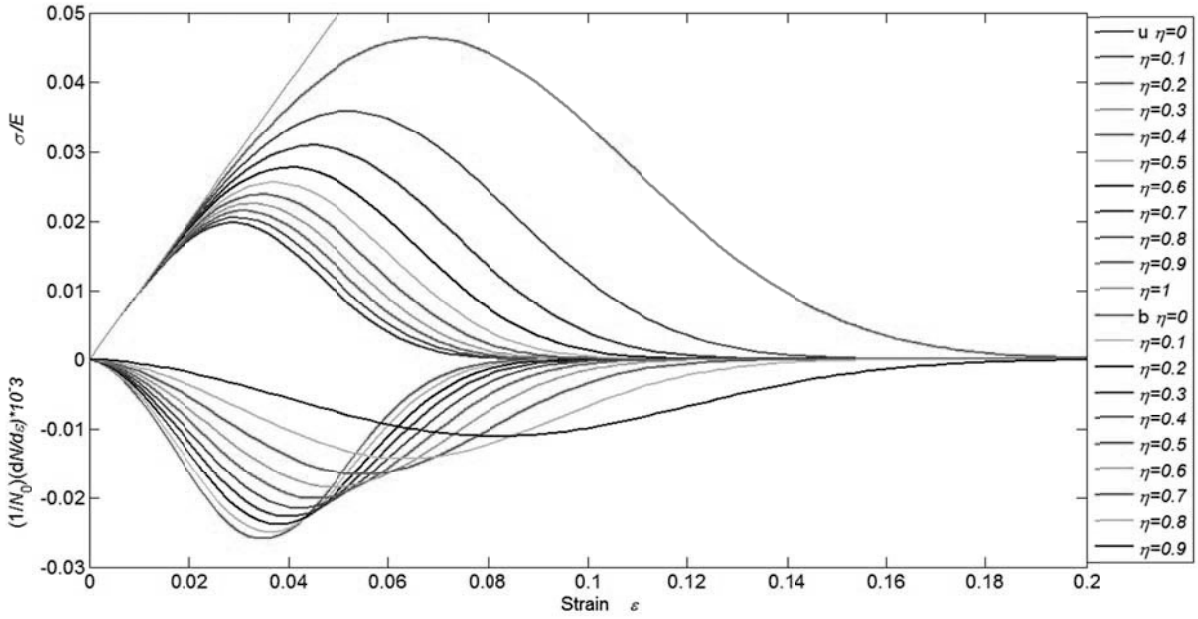

Fig. 4 Stress or rate of survival fibers vs. strain by varying the healing parameter.

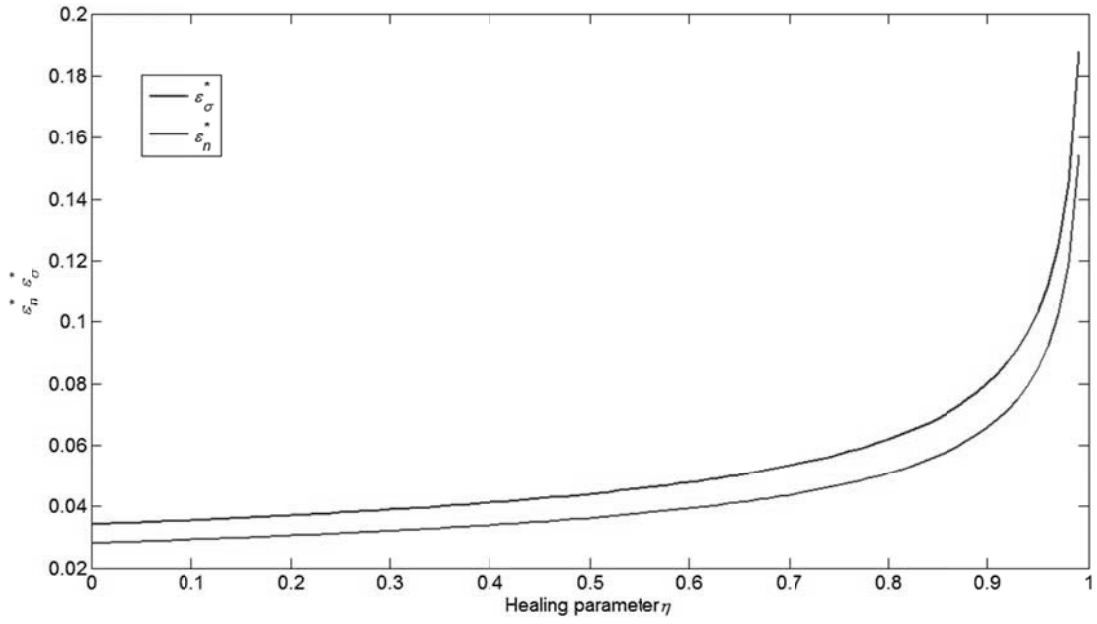

Fig. 5 Strains corresponding to maximum stress or failure rate vs. healing parameter.

The area under the stress-strain curve is the total dissipated energy density (in our calculations we assumed that the bundle is fractured when the stress is 1% of its maximum). In Fig. 6 the ratio between the dissipated energy density with and without healing is reported and clearly increases with increasing the self-healing parameter.

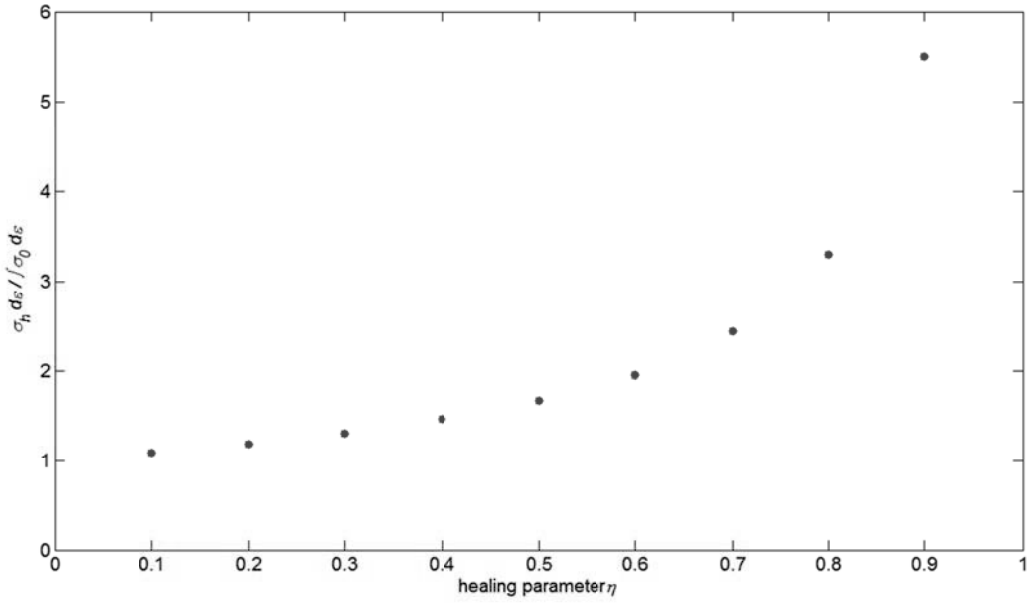

Fig. 6 Dissipated energy density with self-healing normalized to the non healing case vs. healing parameter.

The ratio between the strains corresponding to the maximum stresses with and without healing $\varepsilon_{max,h}$ and $\varepsilon_{max,0}$ respectively and the ratio between the related maximum stresses $\sigma_{max,h}$ and $\sigma_{max,0}$ respectively are reported in Fig. 7: both these ratios increase by increasing the healing parameter.

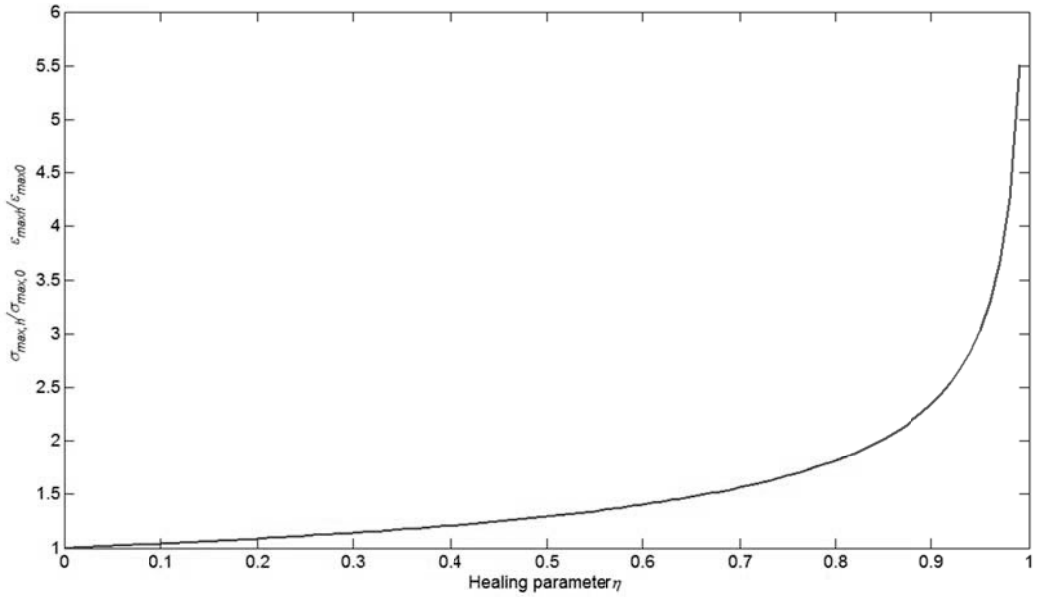

Fig. 7 Dimensionless maximum stress and related strain vs. healing parameter.

5. Conclusions

The presented simple self-healing fiber bundle model is able to quantify the increments of the mechanical performances induced by the self-healing. Applications to design a new class of bio-inspired nanomaterials are envisioned.

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