Toughness and damage tolerance of fractal hierarchical metamaterials

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We present a theory for the toughness, damage tolerance, and tensile strength of a class of hierarchical, fractal, metamaterials. We show that the even though the absolute toughness and damage tolerance decrease with increasing number of hierarchical scales, the specific toughness (toughness per-unit density) grows with increasing number of hierarchical scales in the material, while the specific tensile strength and damage tolerance remain constant.

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Three-dimensional (3D) metamaterials — materials with designed structural features spanning several orders of magnitude in length scales — exhibit remarkable optical [1-3], thermal [4, 5], and mechanical [6-11] properties. It has been demonstrated that such materials can have large tensile strain (∼ 20%), elastic recovery, and can avoid the catastrophic failure mode usually associated with brittle materials. This is particularly intriguing since the nanoscale building blocks of these structures are often brittle. While considerable amount of work has been done towards understanding the modulus and compressive behavior of such materials [9-11], the theoretical underpinnings of their fracture and flaw tolerance properties remain poorly understood. Further, toughness of such materials has never been investigated. In this Letter we present a theoretical framework for understanding the fracture toughness, tensile strength, and flaw tolerance of a simple fuse network based model of such fractal, hierarchical materials.

Materials with structure at several length scales are, of course, not new. The biological world is full of such structural metamaterials [12, 13], including bone, nacre, tooth, antler, wood etc. In fact, one would be hard pressed to find even one example of a biological material which is monolithic in its structure across length scales. Most man-made materials are, by contrast, bland. For instance, metallic alloys have no intrinsic structural features beyond the grain size, and most composites do not have features much below the 10-100μm range. Further, even when traditional artificial materials have structural features, they are limited to one or two length scales, and lack the hierarchy of length scales observed in their biological counterparts. However, recent technological developments in high-resolution large area additive manufacturing techniques have led to the development of samples with macroscopic dimensions approaching tens of centimeters, and a hierarchical structure spanning seven orders of magnitude with the finest structural features at the tens of nanometer scale [9].

Materials manufactured in this manner often have a fractal character [7,8] and do not admit a continuous stress field at all length scales. On the other hand, since continuum elasticity has no inherent length scales, continuous fields are bound to emerge at a length scale comparable to the largest length scale in the hierarchical structure. In other words, since averaging is possible at the largest length scale of the structure, thus continuum fields must emerge at this length scale. However, damage must initiate at the smallest length scale and propagate to the macroscopic scale upwards through the hierarchy. Thus, it is important to understand how the continuum stress transfer and use it to develop scaling relations for toughness and strength of one simple model of a hierarchical metamaterial.

Figure 1 shows a schematic representation of our model material. The overall geometric dimension of the sample is L, while it has several hierarchical structural length scales, l i such that l 0 ≪ l 1 ≪ … ≪ l n ≪ L. Each length scale is related to the next scale by a magnification factor m i defined as m i = l i / l i-1. The fundamental structural unit of the model is the element at the smallest length scale l 0. This unit, and its interaction with the units connected to it, can be modeled in many ways. For instance, the units could be modeled as trusses, and the connections as pin joints, or the units could be modeled as beams, and the connections as rigid beam connectors. An even more realistic simulation would perhaps model the units as hollow thin-walled tubes. However, simulating such realistic models would be computationally taxing. Even a small two dimensional system with n = 2, m = 8, and L = 64 l 2 would contain over 10 7 units, thus making the simulation extremely challenging. We make several simplifications in order to enable meaningful simulations with modest computational resources. First, we study a two dimensional system. Second, we model the units as fuses, thus making a scalar approximation of tensorial elasticity [14]. This approximation is known as the fuse network model. While this seems to be a drastic over-simplification, the fuse network model has been used widely to study brittle fracture [14,21]. This model is formally equivalent to the anti-plane shear idealization of elasticity. Finally, we restrict our simulations to mod-
els with just one order of hierarchy, i.e., $n = 1$.

The basic fuse network model has been described in detail in several references \[19, 20\]. Briefly, in this model the current density is the analog of stress, the electric field that of strain, and the conductivity that of Young’s modulus. Each fuse models a chunk of a brittle material that has a linear stress-strain (current density - electric field) characteristic up to a threshold stress, after which it breaks irreversibly. A fracture simulation is carried out by quasi-statically ramping the voltage across the network and removing fuses as their stress (current density) thresholds are reached. The voltage (displacements) at the nodes needs to be recalculated after each fuse rupture event. The network is said to be fractured when its conductivity drops to zero.

We begin by considering the transfer of stress across the hierarchical length scales. In a network with $n$ hierarchical scales, the continuum stress, $\sigma_c$, emerges at a length scale comparable to the largest hierarchical scale $l_{n}$. If we imagine the next lowest length scale, $l_{n-1}$, as being monolithic (i.e., devoid of any further internal structure), then the stress at this scale can be related to the continuum stress at scale $l_n$ by a simple argument. The ratio of the area covered by the units at length scale $l_{n-1}$ and $l_n$ is given by $a_{n-1}/a_n = (6m_n - 9)/m_{n}^2$, where $m_n$ is the magnification factor introduced earlier. Thus, we get $\sigma_c = \sigma_c^h = \sigma_c^{-1}(6m_n - 9)/m_{n}^2$, where $\sigma_c^h$ is the effective hierarchical stress at the level $i$. A similar idea for stress transfer via area-ratios is used in damage mechanics \[22, 23\], however, in damage mechanics one does not usually consider a hierarchy of length scales. Continuing this argument, we can obtain the relation between the continuum stress and the hierarchical stress at any level as

$$\sigma_c^i = \sigma_c \prod_{k=1}^{n-i} \frac{m_{i+k}^2}{6m_{i+k} - 9}. \quad (1)$$

The exact form of the above relation depends on the geometrical details, but the asymptotic relation $\sigma_c^h \sim \sigma_c m_{i+1} \ldots m_n$ is generic. If the magnification factors are constant, then in a structure with $n$ levels of hierarchy, the stress at the lowest level is given by $\sigma_c^h \sim \sigma_c m^n$.

Consider now a system with a notch as shown in figure \[2\]. In order to propagate, the crack tip must cause damage at a distance $L$, where $L$ is the largest hierarchical length scale. The continuum stress a distance $L$ away from a crack tip is given by $\sigma_c \sim K/\sqrt{L}$, where $K$ is the stress intensity factor, $T$ is the first correction to the asymptotic stress (also known as the T-stress), and $f(\theta)$ is a function of the orientation. Ignoring
the T-stress at short distances, the corresponding hierarchical stress at the smallest length scale is then given by $\sigma^*_n \sim K m_1 \ldots m_n / \sqrt{\ell_{0}}$ (Eq. 1). Fracture propagates when the stress at the lowest length scale reaches a critical value $\sigma^*$. This critical value is the strength of the smallest building blocks of the structure. Using this, and the fact the largest hierarchical length scale is given by $l_n = l_0 m_1 \ldots m_n$, we get the scaling of the critical stress intensity factor as

$$K^{cr} \sim \sigma^* l_0^{1/2} \prod_{k=1}^{n} \frac{6m_k - 9}{m_k^{3/2}}. \quad (2)$$

As before, the exact details above depend on the geometry of the structure, but the asymptotic relation $K^{cr} \sim \sigma^* (l_0/m_1 \ldots m_n)^{1/2}$ is generic, and in particular if the magnification factors are constant, then one obtains $K^{cr} \sim \sigma^* (l_0/m_n)^{1/2}$. Thus, the toughness of the material degrades as more hierarchical are added ($n$ is increased) or as the magnification factor is made larger ($m$ is increased). While this sounds discouraging, we must keep in mind that both of these changes lead to a reduction in the density of the material. Thus, perhaps a more meaningful property is the toughness per-unit density, or $K^{cr}/\rho$, where $\rho$ is the density of the material. It can be shown that the density of our model hierarchical material is given by

$$\rho = \frac{2 \sqrt{3} \lambda}{l_0} \prod_{k=1}^{n} \frac{6m_k - 9}{m_k^{2}}. \quad (3)$$

where $\lambda$ is the linear mass density of the elements at scale $l_0$. Thus, the toughness per-unit density is expected to scale as $K^{cr}/\rho \sim \sigma^* (l_0/m_n)^{1/2}$. Thus while the toughness of material decreases with increasing number of hierarchical levels and magnification factors, the specific toughness shows the opposite trend.

We next focus on the damage tolerance and strength of the material. We consider a system that has some pre-existing damage. This is to say that any fuse at the smallest length scale $l_0$ can be missing with a small probability $p$. This random damage introduces a measure of disorder in the system. The strength of a given realization of this disordered structure is defined as the maximum continuum current density that it can support before fracturing and becoming non-conductive. Our objective is to establish a relationship between the mean strength and parameters such as the damage threshold $p$, number of hierarchical levels $n$, and the magnification factors $m_i$. We restrict ourselves to small values of $p$. The variation of mean strength with $p$ has the interpretation of quantifying the tolerance of the structure to microscopic damage and flaws.

The effect of microscopic damage on the strength of fuse networks (and brittle materials in general) is a well studied problem [14, 16, 20, 24, 25]. However, the structures studied previously were monolithic. By contrast, the fractal nature of our model material gives rise to new phenomenology. Figure 2a shows a snapshot of a simulation of fracture in a network with one order of hierarchy ($n = 1$, $m = 8$), and figure 2b shows the corresponding evolution of stress. Monolithic (non-hierarchical) fuse networks are known to be extremely brittle with a monotonically decreasing stress curve. However, due to the hierarchical nature, the stress curve shown in figure 2a is not monotonically decreasing. A non-monotonic stress curve suggests that the material can sustain some damage before failure, and does not fail catastrophically. This is due to the fact that the effective continuum stress decreases as one moves up the levels of hierarchy, thus progressively higher stress is needed to propagate the damage through the material.

Like any brittle material, the hierarchical fuse network fractures via crack nucleation at a rare large crack-like flaw. This ‘rare large crack-like flaw’ is in turn created by statistical fluctuations that lead to several neighboring fuses being damaged. If such a crack-like flaw has a length $l_c$, then the continuum stress at which it starts propagating is given by $\sigma^*_c \sim K^{cr}/\sqrt{\ell_{0}}$. Since we have demonstrated that the specific toughness, $K^{cr}$, decays as $(m_1 \ldots m_n)^{-1/2}$, one might assume that the mean strength will follow a similar trend. However, we will show that this intuition is incorrect, and the mean strength decays much faster as $(m_1 \ldots m_n)^{-1}$. As we shall show, this is due to the fact that as the number of hierarchical levels or the value of the magnification factor grows, it takes lesser and lesser amount of damage to produce cracks of the same fixed length.

We begin by estimating the probability of having a crack of the length $l_c = rl_0$ in the material. We estimate this probability in a bottom up manner. At the shortest length scale the probability of creating a crack of length $l_0$ is simply given by $p$. One scale up, one has to remove
at least 5 fuses to create a crack of length $l_1$, however, this can be done at any of $m_1$ positions. Thus, the probability of creating a crack of length $l_1$ is of the order of $p^5m_1$. Another scale up, 5 cracks of length $l_1$ need to be created in order to create a crack of length $l_2$, and this can be done at any one of $m_2$ lattice sites. Thus, the probability of creating a crack of length $l_2$ scales as $(p^5m_1)^5/m_2$. Proceeding in this manner, the probability of creating a crack of length $l_n$, at the longest hierarchical scale is of the order of $P_c(l_n) \sim p^n m_1^{c_1} m_2^{c_2} \ldots m_n$. Thus, the probability of creating a crack of length $r_l$ scales as $P_c(r_l) \sim P_c(l_n)^r$.

We next estimate the mean length of the longest crack in the system \[16, 20\]. Let the length of such a crack be $r_l$. Since such a crack appears once per lattice, and the lattice has $(L/l_n)^2$ nucleation spots, thus we get $(L/l_n)^2 P_c(r_l) \sim 1$. This is to say that the expected number of such cracks in the system is 1. Upon simplification, we find the following expression for the mean length of the longest crack in the lattice

$$\langle l_c \rangle \sim \frac{-2 n \log(L/l_n)}{5^n \log p + 5^{n-1} \log m_1 + \ldots + \log m_n}. \quad (4)$$

Combining equations 2, 4, and using $\langle \sigma^c \rangle \sim Kc^*/\sqrt{c}$, we get the following expression for the scaling of the mean strength with the various parameters of interest

$$\langle \sigma^c \rangle \sim \frac{\sigma^*}{m_1 \ldots m_n} \times \left(\frac{-5^n \log p - 5^{n-1} \log m_1 \ldots - \log m_n}{2 \log(L/l_n)}\right)^{1/2}. \quad (5)$$

Specializing equation 5 for the case $n = 1$, and holding $L/l_n$ constant gives $\langle \sigma^c \rangle \sim \sigma^*(-5 \log p - \log m)^{1/2}/m$. We test this prediction by fitting the numerical observed mean strength to the functional form $\langle \sigma^c \rangle = c_1(-c_2 \log p - \log m)^{1/2}/m$, where we introduce the fitting parameter $c_2$ to account the fact that equation 5 is an approximation, and the geometric factors like 5 are not expected to be accurate. Statistical sampling is done by averaging over 100 realizations of the disorder at each value of $m$ and $p$. The fit shown in figure 3 yields a value $c_2 = 2.66$: one standard deviation error bars are indicated. Proceeding similarly one can show that the specific strength scales as $\langle \sigma^c \rangle / \rho \sim (c_3 + c_4/m)(-c_5 \log p - \log m)^{1/2}$, and figure 3 shows a fit of this form to the numerical data. Thus, the specific strength asymptotically approaches a constant, and has a very slow decay with the damage probability $p$.

In summary, we have developed a theory for understanding the scaling properties of the strength, damage tolerance, and toughness of hierarchical, fractal, brittle metamaterials. Our theory is able to provide satisfactory explanation to the results of our simulations, and provides a principled way to relate the continuum scale properties, such as toughness and strength, to the hierarchical structure of the material. However, much work remains to be done in this nascent field. Our model ignores the bending and buckling of the elemental building blocks even though these modes of deformation can be important. We have also ignored plastic deformation in the elements, which is another potentially important effect, particularly if the elements are metallic and have thickness $\gtrsim 100$nm. These limitations notwithstanding, we hope that our results will lead to a better understanding of fracture in this fascinating class of materials.

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