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Towards the Artsutanov's dream of the space elevator: The ultimate design of a 35 GPa strong tether thanks to graphene

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ABSTRACT

In this paper, we have evaluated the strength of a graphene/nanotube bundle considering the two possible failure mechanisms, i.e. intrinsic fracture or sliding. We have accordingly proposed smart strengthening strategies, such as a flaw tolerant design and the nanotube self-collapse. The flaw tolerant design reduces the required strength whereas the self-collapse can increase the achievable strength. Only by coupling these complementary, and possibly other e.g. self-healing, smart strategies, the Artsutanov's dream of the space elevator could be realized. The ultimate design of a 35 GPa strong tether is thus proposed for the first time in this paper, thanks to graphene bundles and the numerous previous investigations performed by the author. Graphene bundles and composites, in which sliding is the current weakest link, are demonstrated to be two times stronger than their nanotube counterparts.

1. Introduction

An explosion of interest in the scaling-up of buckypapers, nanotube bundles and graphene sheets is taking place in contemporary material science. In particular, nanostructures can be assembled (or well dispersed in a matrix) in order to produce new strong materials and structures. Recently, macroscopic buckypapers [1–5], nanotube bundles [5–12] and graphene sheets [13–16] have been realized. In spite of these fascinating achievements of the contemporary material science and chemistry we are evidently far from an optimal result. The reported mechanical strength of buckypapers and graphene sheets, for example, is comparable to that of a classical sheet of paper and macroscopic nanotube bundles have a strength still comparable to that of steel.

This paper aims to couple the previous calculations performed by the same author, on the strength of graphene/nanotubes [1,17–20] or their bundles [21–23] assuming intrinsic fracture (i) or sliding (ii). This suggests the design of a flaw tolerant and (self-collapsed) superstrong (nanotube) graphene bundle, corresponding to a maximum cable strength of ~33 GPa, comparable to the thermodynamic limit assuming intrinsic graphene/nanotube fracture of a km-long cable (see [23], highlighted by Nature 450, (2007) 6). Our results also suggest that graphene bundles are expected to be superior in strength with respect to self-collapsed nanotube bundles and that both of them are stronger than classical nanotube bundles. Note that the collapse under pressure, and even under atmospheric pressure, i.e. the self-collapse of nanotubes in bundle [1], was firstly investigated by atomistic simulations in Ref. [24]. Moreover, the self-collapse of nanotubes in a bundle has been recently experimentally observed [25].

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Fig. 1. The authors of this paper (right), Prof. B. Yakobson and the Nobel Laureate R. Smalley, designed the cover of American Scientist considering a realistic, thus defective, cable (left, see the red arrows), whereas the final cover presented a more appealing but also unrealistic defect-free space elevator cable (right). People do not like defects, in both materials and human relationships, and try to ignore them: a current big mistake in both material science and marriages. The winning strategy is the present flaw tolerant design. (For interpretation of the reference to color in this figure legend, the reader is referred to the web version of this article).

Such flaw tolerant and self-collapsed nanotube or graphene super-strong bundles are thus ideal for space elevators, where high specific strength is needed to prevent cable failure. Defects cannot be further ignored (Fig. 1). Only by coupling these complementary, and possibly other e.g. self-healing, smart strategies, the Artsutanov's dream of the space elevator could be realized.

2. Fracture strength

Local theories have to be rejected in order to properly compute the strength of a structure, since these are unable to predict size-effects, as a consequence of the lack of a characteristic internal length. For example, computing with a maximum stress local approach the tensile failure of a linear elastic infinite plate containing a hole would always result in one third of the defect-free strength, as a consequence of the impossibility for the local theory to distinguish between a "small" or a "large" (with respect to what?) hole. On the contrary, Quantized Fracture Mechanics (QFM), invented by the author [17–19], has been derived from classical Linear Elastic Fracture Mechanics (LEFM) by simply removing the hypothesis of the continuous crack growth and thus naturally introducing an internal characteristic length, namely the fracture quantum. Such a discrete crack advancement is a material/structural property and is expected to increase by increasing the size scale. However, atomistic simulations demonstrate that in atomic structures the fracture quantum is close to the distance between two broken adjacent chemical bonds. QFM can treat in a simple analytical way different defect sizes and shapes and not just the "long" sharp cracks of LEFM.

By considering QFM, the ratio of the failure stress σ_N of a defective graphene/nanotube to its defect-free strength $\sigma_N^{(theo)}$ (i.e., the theoretical strength, e.g. as virtually computed stretching pristine graphene/nanotubes using *ab-initio* quantum mechanical simulations based on density functional theory) can be calculated by equating the mean value along fracture quantum of the energy release rate with fracture energy per unit area of carbon; for a graphene/nanotube having a fracture quantum q (the "atomic size") and containing an elliptical hole of half-axes a, perpendicular to the applied load, and b, we accordingly find

$$\frac{\sigma_N(a,b)}{\sigma_N^{(theo)}}=\sqrt{\frac{1+2a/q(1+2a/b)^{-2}}{1+2a/q}} \tag{1}$$

For transversal cracks having length m, in unit of fracture quanta, $\sigma_N(m)/\sigma_N^{(theo)}\approx(1+m)^{-1/2}$ ($b\approx 0$, $m\approx 2a/q$).

Imposing the force equilibrium for a cable composed of defective graphene/nanotubes allows one to derive the cable strength σ_C (if defect-free denoted by $\sigma_C^{(theo)}$) as a function of those of the graphene/nanotubes:

$$\frac{\sigma_C}{\sigma_C^{(theo)}}=\sum\nolimits_{a,b} f_{ab}\frac{\sigma_N(a,b)}{\sigma_N^{(theo)}} \tag{2}$$

The summation is extended to all the different holes; f_{ab} is the numerical fraction of graphene/nanotubes containing an elliptical hole of half-axes a and b (the numerical fraction f_{00} is defect-free and $\sum_{a,b} f_{ab}=1$). If all the defective graphene/nanotubes in the bundle contain identical holes $f_{ab}=f=1-f_{00}$, and the following simple relation between the strength reductions holds: $1-\sigma_C/\sigma_C^{(theo)}=f(1-\sigma_N/\sigma_N^{(theo)})$.

Defects are thermodynamically unavoidable, especially at the megascale [23]. At the thermal equilibrium the vacancy fraction $f=n/N\ll 1$ (n is the number of vacancies and N is the total number of atoms) is estimated as

$$f\approx e^{-E_1/(k_B T_a)} \tag{3}$$

where $E_1\approx 7$ eV is the energy required to remove one carbon atom and T_a is the absolute temperature at which the carbon is assembled, typically in the range between 2000 and 4000 K. Thus, $f\approx 2.4\times 10^{-18}$–$1.6\times 10^{-9}$. For

the megacable having a carbon mass of $\sim$5000 kg, the total number of atoms is $N \approx 2.5 \times 10^{29}$; thus a huge number of equilibrium defects, in the range $n \approx 0.6 \times 10^{12}$–$3.9 \times 10^{20}$ are expected, in agreement with a recent discussion and observations [23].

The strength of the cable will be dictated by the largest transversal crack on it, according to the weakest link concept. The probability of finding a nanocrack of size m in a bundle with vacancy fraction f is $P(m)=(1-f)f^m$, and thus the number M of such nanocracks in a bundle composed of N atoms is $M(m)=P(m)N$. The size of the largest nanocrack, which typically occurs once, is found from the solution to the equation $M(m) \approx 1$, which implies [23]

$$m \approx -\ln[(1-f)N]/\ln f \approx -\ln N/\ln f \tag{4}$$

Accordingly, we deduce a size $m \approx 2$–4 for the largest thermodynamically unavoidable defect in the megacable. Inserting Eqs. (3) and (4) in Eq. (1) evaluated for the worst case of a transversal crack ($b \approx 0$ and $m \approx 2a/q$), we deduce the statistical counterpart of Eq. (1):

$$\frac{\sigma_N(N)}{\sigma_N^{(theo)}} \leq \frac{\sigma_N^{(max)}(N)}{\sigma_N^{(theo)}} = \frac{1}{\sqrt{1+(k_B T_a/E_1)\ln N}} \tag{5}$$

The corresponding maximum achievable fracture strength is thus predicted to be

$$\sigma_C^{(fracture)} \approx 35\,\text{GPa} \tag{6}$$

3. Sliding strength

On the other hand, assuming sliding failure, the energy balance during a longitudinal delamination (here "delamination" has the meaning of Mode II crack propagation at the interface between adjacent graphene/nanotubes) dz under the applied force F is

$$d\Phi - F\,du - 2\gamma(P_C + P_{vdW})dz = 0 \tag{7}$$

where $d\Phi$ and du are the strain energy and elastic displacement variation, respectively, due to the infinitesimal increment in the compliance caused by the delamination dz; P_{vdw} describes the still existing van der Waals attraction (e.g. attractive part of the Lennard-Jones potential) for vanishing nominal contact area and γ is the surface energy. Elasticity poses $d\Phi/dz = -F^2/(2ES)$, where S is the cross-sectional surface area of the graphene/nanotube, whereas according to Clapeyron's theorem $F\,du = 2d\Phi$. Thus, the following simple expression for the bundle strength ($\sigma_C = F_C/S$, effective stress and cross-sectional surface area are here considered; F_C is the force at fracture) is predicted:

$$\sigma_C^{(theo)} = 2\sqrt{E\gamma\frac{P}{S}} \tag{8}$$

in which the ratio of the effective perimeter ($P=P_C+P_{vdW}$) to the cross-sectional surface area of the graphene/nanotubes in contact appears.

Assuming a non-perfect alignment of the graphene/nanotubes in the bundle, described by a non-zero angle β, the longitudinal force carried by the graphene/nanotubes will be $F/\cos\beta$; thus the equivalent Young's modulus of the bundle will be $E\cos^2\beta$, as can be evinced by the corresponding modification of the energy balance during delamination; accordingly

$$\sigma_C = 2\cos\beta\sqrt{E\gamma\frac{P}{S}} \tag{9}$$

For nanotubes, the maximal achievable bundle strength is predicted for collapsed (see condition of Eq. (12)) perfectly aligned (sufficiently overlapped) nanotubes, i.e. $P/S \approx 1/(t)$, where t is the graphene thickness, $\beta=0$:

$$\sigma_C^{(theo,N)} = 2\sqrt{\frac{E\gamma}{Nt}} \tag{10}$$

Taking $E=1$ TPa (Young's modulus of graphene), $\gamma=0.2$ N/m (surface energy of graphene; however note that in reality γ could be also larger as a consequence of additional dissipative mechanisms, e.g. fracture and friction in addition to adhesion expected at larger size scales and in composites; smaller values of the equivalent surface energy are expected at the nanoscale in case of pure sliding, i.e. without surface area formation but due to friction), the predicted maximum sliding strength for a single walled nanotube ($N=1$) cable is

$$\sigma_C^{(sliding)} = \sigma_C^{(theo,1)} \approx 37\,\text{GPa} \tag{11a}$$

For graphene the contact perimeter is doubled with repsect to a self-collapsed nanotube, i.e. $P/S=1/t$, and thus for a graphene bundle we predict:

$$\sigma_C^{(sliding)} = \sqrt{2}\sigma_C^{(theo,1)} \approx 52\,\text{GPa} \tag{11b}$$

4. The flaw tolerant design

The buckling pressure of a nanotube in a bundle can be calculated with the classical elastic buckling formula but including the "Laplace-like" surface adhesion pressure term [1] $p_C=(3N^\alpha D/R^3)-(\gamma/R)$, where D is the graphene bending rigidity, N is the nanotube wall number, R is the nanotube external radius and γ is the surface energy. The first term, for $\alpha=3$, is that governing the buckling of a perfectly elastic cylindrical long thin shell, whereas $\alpha=1$ would describe fully independent walls. Thus, we derive the following condition for the self-collapse, i.e. collapse under zero pressure, of a nanotube in a bundle [1]:

$$R \geq R_C^{(N)} = \sqrt{\frac{3N^\alpha D}{\gamma}} = \sqrt{6}R_0^{(N)} \tag{12}$$

Taking $D=0.1$ nN $\times$ nm and $\gamma=0.18$ N/m we find $2R_C^{(1)} \approx 2.7$ nm. Considering an intermediate coupling between the walls ($\alpha \approx 2$), the critical diameters for double and triple walled nanotubes are $2R_C^{(2)} \approx 5.4$ nm and $2R_C^{(3)} \approx 8.1$ nm. This condition has to be verified to reach the strength reported in Eq. (11), otherwise we expect a weakening of about 30% [1].

Finally, a taper-ratio λ larger than its theoretical value would consequently be required for the megacable to be flaw-tolerant [2] at the stress-level predicted by Eq. (6) (and thus (11)); we find the corresponding flaw-tolerant taper-ratio to be

$$\lambda_{\substack{flaw \\ tolerant}} = \lambda^{(theo)(\sigma_C^{(theo)}/\sigma_C)} \approx 5 \tag{13}$$

Fig. 2. Artsutanov's dream is artistically represented in this figure, including the additional dream of a "cable city" located where the acceleration of gravity is $-g$ (Studio ATA).

5. Conclusions

The calculations reported in Eqs. (7) and (11) suggest a maximal achievable strength of about 35 GPa, thus compatible with the feasibility of the space elevator, if the flaw tolerant design reported in Eq. (13) is considered. The Artsutanov's dream, artistically represented in Fig. 2, could thus become real especially thanks to graphene bundles. Graphene bundles and composites, in which sliding is the current weakest link, are demonstrated to be two times stronger than their nanotube counterparts.

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