THE EFFECT OF COLLAPSED NANOTUBES ON NANOTUBE BUNDLE STRENGTH

Nicola M. Pugno
1) Laboratory of Bio-Inspired & Graphene Nanomechanics, Department of Civil, Environmental and Mechanical Engineering, Università di Trento, via Mesiano, 77, I-38123 Trento, Italy,
2) Center for Materials and Microsystems, Fondazione Bruno Kessler,
Via Sommarive 18, I-38123 Povo (Trento), Italy.
nicola.pugno@unitn.it

Abstract: In this paper, we have evaluated the strength of a nanotube bundle, with or without collapsed nanotubes. The self-collapse can increase the strength up to a value of about 30%, suggesting a design towards Artsutanov's dream of the space elevator, thanks to the design of a 30MYuri strong tether. Graphene bundles are expected to be even stronger.

Keywords: nanotubes, bundles, self-collapse, space elevator, Artsutanov, 30MYuri.

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, are comparable to that of a classical sheet of paper and macroscopic nanotube bundles have a strength still comparable to that of steel.

This paper, following [1], aims to extend the previous calculations performed by the same author, on the strength of nanotubes [17-20] or nanotube bundles [21-23] and assuming the intrinsic fracture of the composing nanotubes (i), for nanotube sliding (ii). For such a case, we have for the first time analytically calculated that single walled nanotubes with diameters larger than ~3nm will self-collapse in the bundle as a consequence of the van der Waals adhesion forces and that the self-collapse can enlarge the cable strength up to ~30%. This suggests the design of self-collapsed super-strong nanotube bundles, corresponding to a maximum cable strength of ~48GPa, comparable to the thermodynamic limit assuming intrinsic nanotube fracture of km-long cable (see [23], highlighted by Nature 450, 6, 2007). This results suggests that nanotube bundles are stronger than classical nanotube bundles. Such self-collapsed nanotube super-strong bundles are thus ideal for space elevator missions, where high strength is needed to prevent cable and mission failure. Note that the collapse under pressure, and even under atmospheric pressure, i.e. the self-collpase of nanotubes in bundle, was firstly investigated by atomistic simulations in [24]. Moreover, the self-collapse of nanotubes in a bundle has been recently experimentally observed [25]. Thus such super-strong bundles are becoming feasible. Graphene bundles are expected to be even stronger [26].

Self-buckling

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]:

$$p_C = \frac{3N^{\alpha}D}{R^3} - \frac{\gamma}{R} \tag{1}$$

where D is the graphene bending rigidity, N is the nanotube wall numbers, R is the nanotube external radius and γ is the surface energy. The first term in eq. (1), for $\alpha = 3$ is that governing the buckling of a perfectly elastic cylindrical long thin shell, whereas $\alpha = 1$ would describe fully independent walls.

From eq. (1) we derive the following condition for the self-collapse, i.e. collapse under zero pressure, of a nanotube in a bundle:

$$R \geq R_C^{(N)} = \sqrt{\frac{3N^{\alpha}D}{\gamma}} = \sqrt{6}R_0^{(N)} \tag{2}$$

Taking $D = 0.11\text{nN}\cdot\text{nm}$ and $\gamma = 0.18\,\text{N/m}$ we find $2R_C^{(1)} \approx 2.7\text{nm}$. Considering an intermediate coupling between the walls ($\alpha \approx 2$), the critical diameters for double and triple walled nanotubes are $2R_C^{(2)} \approx 5.4\text{nm}$ and $2R_C^{(3)} \approx 8.1\text{nm}$.

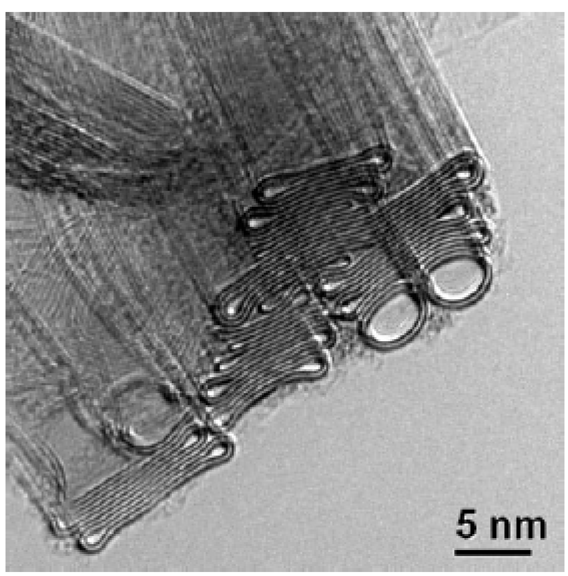

Figure 1: Self-collapsed nanotubes in a bundle [25].

In [25], 17 experimental observations on the self-collapse of nanotubes in a bundle have been reported, see Figure 1 and related Table 1. A number of 5 single walled nanotubes with diameters in the range 4.6-5.7nm were all observed as collapsed; moreover, while the 3 double walled nanotubes observed with internal diameters in the range 4.2-4.7nm (the effective diameters are larger by a factor of ~0.34/2nm) had not collapsed, the observed 8 double walled nanotubes with internal diameters in the range 6.2-8.4nm had collapsed. Finally, a triple walled nanotube of 14nm internal diameter (the effective diameter is ~14.34m) was observed as collapsed too. All these 17 observations are in agreement with our theoretical predictions of eq. (2), supporting our conjecture of liquid-like nanotube bundles [1].

Nanotube number	Number N of walls	Diameter of the internal wall [nm]	Collapsed (Y/N) Exp. & Theo.
1	1	4.6	Y
2	1	4.7	Y
3	1	4.8	Y
4	1	5.2	Y
5	1	5.7	Y
6	2	4.2	N
7	2	4.6	N
8	2	4.7	N
9	2	6.2	Y
10	2	6.5	Y
11	2	6.8	Y
12	2	6.8	Y
13	2	7.9	Y
14	2	8.3	Y
15	2	8.3	Y
16	2	8.4	Y
17	3	14.0	Y

Table 1: Self-collapse of nanotubes in a bundle: our theory exactly fits the experimental observations [1].

Sliding strength

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 nanotubes) dz under the applied force F, is:

$$\mathrm{d}\Phi - F\mathrm{d}u - 2\gamma\left(P_C + P_{vdW}\right)\mathrm{d}z = 0 \tag{3}$$

where $\mathrm{d}\Phi$ and $\mathrm{d}u$ are the strain energy and elastic displacement variation due to the infinitesimal increment in the compliance caused by the delamination $\mathrm{d}z$; P_{vdw} describes the still existing van der Waals attraction (e.g. attractive part of the Lennard-Jones potential) for vanishing nominal contact nanotube perimeter $P_C = 6a$ (the shear force between two graphite single layers becomes zero for nominally negative contact area); 6a is the contact length due to polygonization of nanotubes in the bundle, caused by their surface energy γ. Elasticity poses $\frac{\mathrm{d}\Phi}{\mathrm{d}z} = -\frac{F^2}{2ES}$, where S is the cross-sectional surface area of the nanotube, whereas according to Clapeyron's theorem $Fdu = 2d\Phi$. 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:

$$\sigma_C^{(theo)} = 2\sqrt{E\gamma \frac{P}{S}} \tag{4}$$

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

Assuming a non perfect alignment of the nanotubes in the bundle, described by a non zero angle β, the longitudinal force carried by the nanotubes will be $F/\cos\beta$, thus the equivalent Young' 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:

$$\sigma_C = 2\cos\beta\sqrt{E\gamma \frac{P}{S}} \tag{5}$$

The maximal achievable strength is predicted for collapsed perfectly aligned (sufficiently overlapped) nanotubes, i.e. $\frac{P}{S} \approx \frac{1}{Nt}$, where t is the graphene thickness, $\beta = 0$:

$$\sigma_C^{(theo,N)} = 2\sqrt{\frac{E\gamma}{Nt}} \tag{6}$$

Taking $E = 1\mathrm{TPa}$ (Young's modulus of graphene), $\gamma = 0.2\,\mathrm{N/m}$ (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), the predicted maximum strength for single walled nanotubes (*N*=1) is:

$$\sigma_C^{(\max)} = \sigma_C^{(theo,1)} = 48.5\mathrm{GPa} \tag{7}$$

whereas for double or triple walled nanotubes $\sigma_C^{(theo,2)} = 34.3\mathrm{GPa}$ or $\sigma_C^{(theo,3)} = 28.0\mathrm{GPa}$. Eq. (7) suggests the feasibility of 30MYuri strong tethers.

Self-buckling and sliding strength coupling

According to the previous analysis, the ratio between the bundle strength $\sigma_C^{(0)}$, in the presence of self-collapse, and $\sigma_C^{(\mathrm{O})}$, in the absence of self-collapse, is predicted to be:

$$\frac{\sigma_C^{(0)}}{\sigma_C^{(\mathrm{O})}} = \sqrt{\frac{2\pi R + P_{vdW}}{2\pi R\left(1 - \frac{1}{R}\sqrt{\frac{N^{\alpha} D}{2\gamma}}\right) + P_{vdW}}}, \quad \text{for} \quad R \geq R_C^{(N)} = \sqrt{\frac{3N^{\alpha} D}{\gamma}} \tag{8}$$

The maximal strength increment induced by the self-collapse is thus:

$$\left.\frac{\sigma_C^{(0)}}{\sigma_C^{(\mathrm{O})}}\right|_{\max} = \sqrt{\frac{1}{1 - \frac{1}{\sqrt{6}}}} \approx 1.30 \tag{9}$$

Eq. (9) shows that the self-collapse could enhance the nanotube bundle strength up to ~30%. The reason is obviously the incremented surface area of the interfaces between the nanotubes.

Conclusions

The calculation in eq. (7) suggests a maximal achievable strength larger than 30MYuri, thus compatible with the Artsutanov's dream of the space elevator. Strong adhesion energy, high stiffness, low fiber dimension (thus aggregation must be avoided) and high alignment are all key factors for a practical realization of the single walled nanotube super strong bundle. Graphene bundles are expected to be even stronger [26].

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