Buckling of ZnS-Filled Single-Walled Carbon Nanotubes

Andre O. Monteiro,[1,2] **Pedro M. F. J. Costa**,[1,3,4] Paulo B. Cachim,[2,5] David Holec[6]

[1]CICECO, University of Aveiro, 3810-193 Aveiro, Portugal

[2]Department of Civil Engineering, University of Aveiro, 3810-193 Aveiro, Portugal

[3]Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal

[4]Physical Sciences and Engineering Division, KAUST, 23955-6900 Thuwal, Kingdom of Saudi Arabia

[5]LABEST, University of Aveiro, 3810-193 Aveiro, Portugal

[6]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Austria

pedro.dacosta@kaust.edu.sa

Abstract

Filling the cavities of carbon nanotubes generates new hybrid materials, an approach that can lead to the customization and/or improvement of physical properties of either the host nanotube or the guest encapsulated substance. The first record describing these host-guest systems dates back to 1993 [1], when the encapsulation of lead/lead oxide within multi-walled carbon nanotubes (MWCNT) was performed using the so-called “capillary method”. To present, hundreds of these systems have been produced with the prospect for applications touted to be wide-ranging and spanning from drug delivery to storage of sensitive materials and nanopipetting.

Recently, we have been studying a relatively complex system which is composed of a ternary alloy guest, Ga-doped ZnS, confined in turbostratic MWCNTs. Besides characterizing its structure and chemistry, we have also analyzed the reactivity [2], thermal stability [3, 4], nanodelivery [5, 6] and mechanical behavior [7-10].

Here, we will show how molecular dynamics computational simulations were used to study the mechanical response of single-walled carbon nanotubes (SWCNT) filled with crystalline zinc sulphide (ZnS) nanowires under uniaxial compression (Figure 1). These simulations allowed us to analyze the behavior of SWCNT, with and without ZnS filling, in terms of Young’s modulus, buckling force and buckling strain. Force versus strain curves have been computed for hollow and filled systems, where it was noticeable an improvement of the mechanical behavior given by the ZnS nanowire. The same experiments were performed for a large range of dimensions in order to evaluate the influence of the aspect ratio in the mechanical response of the tubes.

References

[1] Ajayan, P.M. and S. lijima, Nature, **361** (1993) 333.
[2] Costa, P.M.F.J., et al., Chemistry – A European Journal, **16** (2010) 11809.
[3] Costa, P.M.F.J., et al., Microscopy and Microanalysis, **18** (2012) 77.
[4] Costa, P.M.F.J., et al., Nature Commun, **2** (2011) 421.
[5] Costa, P.M.F.J., et al., Carbon, **49** (2011) 3747.
[6] Costa, P.M.F.J., et al., Carbon, **49** (2011) 342.
[7] Costa, P.M.F.J., et al., Nanotechnology, **20** (2009) 405706.
[8] Costa, P.M.F.J., et al., Nanotechnology, **20** (2009) 405707.
[9] Costa, P.M.F.J., et al., Carbon, **47** (2008) 541.
[10] Monteiro, A.O., P.M.F.J. Costa and P.B. Cachim, Journal of Materials Science, 49 (2014) 648.

Figures

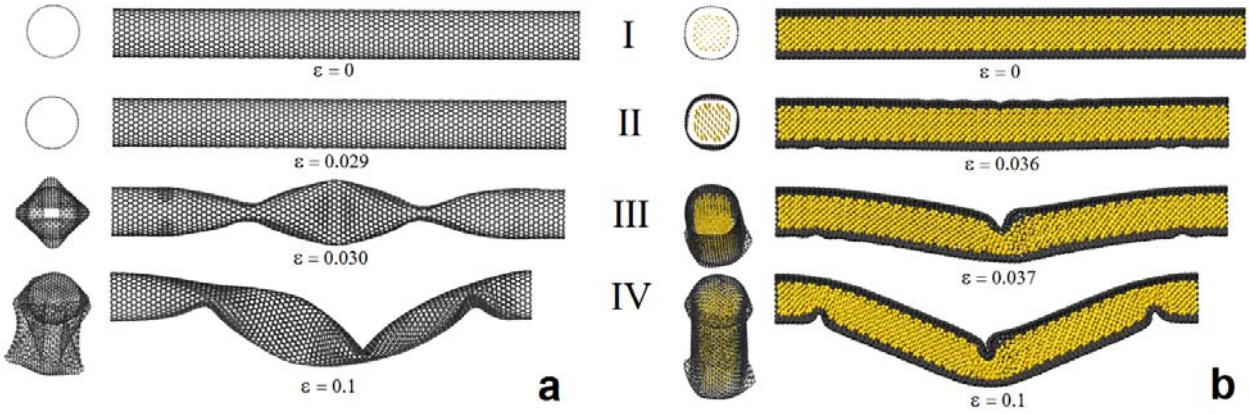

Figure 1. Snapshots of the deformation process of a 20 nm long (26,0) SWCNT in the (a) empty and (b) filled states. The yellow domains in (b) represent the confined ZnS nanowire.