Phys. Status Solidi B **250,** No. 8, 1492–1495 (2013) / **DOI** 10.1002/pssb.201200977

physica status solidi b
www.pss-b.com
basic solid state physics

In silico tensile tests and design of hierarchical graphene fibres and composites

Federico Bosia[*,1] **and Nicola M. Pugno**[**,2,3]

[1] Department of Physics and "Nanostructured Interfaces and Surfaces" Centre of Excellence, University of Torino, Via P. Giuria 1, 10125 Torino, Italy
[2] Laboratory of Bio-Inspired & Graphene Nanomechanics, Department of Civil, Environmental and Mechanical Engineering, University of Trento, via Mesiano 77, 38123 Trento, Italy
[3] Center for Materials and Microsystems, Fondazione Bruno Kessler, Via Sommarive 18, 38123 Povo (Trento), Italy

Received 14 December 2012, revised 19 June 2013, accepted 21 June 2013
Published online 24 July 2013

Keywords graphene, hierarchy, mechanical properties, simulations

* federico.bosia@unito.it, Phone: +39 011 6707889, Fax: +39 011 6707020
** Corresponding author: nicola.pugno@unitn.it, Phone: +39 0461 282525, Fax: +39 0461 282599

In this contribution, we apply a hierarchical fibre bundle model (HFBM), previously developed to estimate the mechanical properties of multiscale carbon nanotube (CNT)-based structures, to the case of graphene macroscopic cables. The nonlinear elastic properties of graphene and its exceptional intrinsic strength, with mean Young's modulus of 1 TPa, third-order elastic stiffness of −2.0 TPa and intrinsic strength of 130 GPa, are drawn from recent experimental studies. The model allows to derive macroscopic characteristics like strength, stiffness, toughness as a function of hierarchical structure, starting from statistically distributed properties at the nanoscale and without the introduction of additional *ad hoc* parameters. The influence of the presence of defects in the graphene bundles is evaluated. We also analyse the properties of graphene-reinforced composites, including the influence of the volume fraction of a ductile polymeric matrix. We show that the composite properties can be engineered to optimize strength and/or stiffness, and that the present model can be a useful tool to help pursue this objective

1 Introduction In recent years, much effort has gone into investigating graphene for its exceptional electronic, thermal, optical and mechanical properties. Various different graphene nano/micro-structures have by now been synthesized and characterized, including graphene paper [1], graphene nanoribbons [2] and also macroscopic assembled graphene fibres [3]. In addition, large area growth techniques have been increasingly developed thanks to specific research in this direction [4, 5]. Another important field is that of graphene-based composites, which could provide the means to harness graphene's exceptional properties for applications [6].

From a mechanical point of view, graphene can be considered 'the strongest material ever measured', ever since Lee et al. managed to measure the elastic properties and intrinsic breaking strength of free-standing monolayer graphene membranes by nanoindentation in an atomic force microscope [7]. In this study, graphene was found to display a nonlinear elastic behaviour of the type

$$\sigma = E\varepsilon + D\varepsilon^2, \tag{1}$$

where σ is the stress, ε the strain, $E = (1.0 \pm 0.1)$ TPa and $D = (-2.0 \pm 0.4)$ TPa. Moreover, its measured intrinsic strength was $\sigma_f = (130 \pm 10)$ GPa, which is the highest value found for any material in nature [7]. However, it is unclear what the effect of defects, grain boundaries, etc. could have on these values. In carbon nanotubes (CNTs), a low-dimensional material like graphene, the introduction of a single vacancy can determine a drop in strength of up to 20% [8]. CNT-based composites have been widely studied in past years [9]. Although graphene can be considered as a two-dimensional system, as opposed to CNTs that are usually considered one-dimensional, both share high aspect ratios and exceptional mechanical properties, which can be exploited in composites. Thus, another question is: in graphene composites, how can we optimize mechanical performance (stiffness, strength, toughness…) by varying constituent material properties, mixing ratio, hierarchical structure or other parameters? Clearly, experimental investigations to reply to these questions would entail very cumbersome studies, therefore it is convenient to develop numerical