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FOREWORD

# Nanoscale fracture

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"Nanoscale Fracture" is the selected topic of this Special Section of the current Issue of International Journal of Fracture. Even if fracture takes place intrinsically at the atomic size scale, it is usually treated according to the famous Griffith's continuum theory of Linear Elastic Fracture Mechanics. As a matter of fact, scientists are today resolving the atomistic details arising at the crack tip even in nanoscale, including biological, systems. Quantized Fracture Mechanics theories (QFM, that we have developed, see Pugno 2002; Pugno and Ruoff 2004; Pugno 2006a,b; note that QFM appears in the literature with different names, e.g. some authors later refer to it as Finite Fracture Mechanics) and Atomistic Simulations (including *ab initio* calculations) have greatly helped in understanding the fracture of nanosystems, such as nanotubes and graphene, as well as the details of the crack propagation arising at the atomic scale, such as bond rearrangements and reconstructions. In spite of this, understanding fracture at the nanoscale remains a challenge for the current fracture mechanics community and has motivated the organization of this Special Section. Moreover, during the last International Conference on Fracture (12th ICF, July 2009, Ottawa, Canada) we have organized a Symposium on the same hot topic, that is thus connected by a *fil rouge* to this Section. Here, after a rigorous peer review process (including paper rejection), we present five key novel contributions in the field, presented at that Conference.

In particular, in the paper "Effect of vacancy diffusion on crack initiation and propagation in the Lennard-Jones crystal subjected to tension" by Vinogradov, the effect of vacancy diffusion on crack initiation and propagation in 2D LJ crystals is investigated numerically using a molecular statics approach. A crystal is represented by a basal plane of a hexagonal closed-packed lattice and the seed vacancy is created by removing one atom. The crystal is subjected to tension by displacing one of its boundaries. The vacancy is allowed to diffuse within some rectangle so that its migration to the crystal surface is prevented. It is assumed that the event of an exchange between the vacancy and the neighboring atom will take place between two sequential loading steps and that there is no preferred direction for a jump, which leads to the vacancy's random walk. It is shown that the migrating vacancy not only results in dislocation formation but also

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leads to the formation of nanovoids and nanocracks. Since the vacancy migration is random, the patterns of structural changes leading to nanovoids, nanocracks and fracture are different for each numerical test.

Atomistic simulations, in addition to a Griffith's approach for the study of adhesion, have also been considered in the paper "Constitutive behavior of pressurized carbon nanoscrolls" by Shi et al., where graphene nanoscrolls are investigated. Carbon nanoscrolls (CNSs) are a class of graphene-based nanoscale materials with great potential for applications in nanotechnology and bioengineering. Fundamental description, understanding and regulation of these materials may ultimately lead to a new generation of integrated systems that utilize their unique properties. A particularly interesting property of a CNS is that there exists a stable equilibrium core size which can be uniquely determined from the basal graphene length, the interlayer spacing, the interaction energy between layers, the bending stiffness of graphene, as well as the difference between the pressure inside the core of the CNS and that on its outer surface. Here the authors investigate the strongly nonlinear constitutive behaviour of a CNS under pressure, focusing on its deformation, stability and biaxial modulus in response to its inner and external pressures. Their study suggests pressure sensitive applications of CNSs such as nanopumps and nanofilters.

Adhesion has been also investigated in the paper "Numerical simulations demonstrate that the double tapering of the spatualae of lizards and insects maximize both attachment resistance and stability" by Pantano et al. The authors observed that many biological attachment devices of insects, spiders and geckos consist of arrays of hairs (setae), which are terminated by contact elements of different shapes. The most frequently observed shape is a thin plate-like spatula. In spite of a rather wide range of sizes and thicknesses, most spatulae are not uniform, but rather possess a gradient in thickness and width. In this paper the authors show that the spatulae of insects and geckos become gradually thinner and wider approaching the end. This geometrical effect is explained in this paper, by using a numerical approach for the modeling of the van der Waals adhesion and friction between the contact elements and the substrate. The approach suggests that the observed negative thickness gradient contributes to the improvement of the adhesion resistance, whereas the positive width gradient increases the stability of the detachment, probably a key factor in controlling the animal walking.

In the paper "Dislocation plasticity and phase transformations in Si–SiC core-shell nanotowers" by Beaber et al. Si nanotowers have been experimentally characterized. Vapor-liquid-solid (VLS) Si nanotowers were coated with nanocrystalline SiC to form a Si-SiC core-shell composite. Due to a mismatch in the coefficients of thermal expansion (CTE), the Si core was under a compressive stress following the deposition. The composite tower was then cross-sectioned using focused ion beam milling, exposing the Si core. Indentation into the Si showed an increased toughness as a function of diameter compared to similar sized Si nanotowers and nanospheres. This result is explained through enhanced dislocation and phase transformation plasticity in the Si core from the CTE compressive stresses.

Finally, in the paper "The theory of multiple peeling" by Pugno, we have derived the theory of multiple peeling, extending the pioneering energy-based single peeling theory of Kendall, including large deformations and pre-stretching. We can thus treat a complex system of films, adhering over a substrate and having a common hinge where the pulling force is applied. Two case studies are investigated: the asymmetric V-shape double peeling and the symmetric cone-shape configuration with $N$ peeling tapes, both requiring the solution of six nonlinear coupled equations (instead of the one needed in the simpler single peeling problem). Remarkable implications emerge: (i) for moderate deformations, the critical strain of a tape is identical to that of the single peeling; (ii) an optimal peeling angle, at which adhesion is maximal, is discovered; (iii) an additional optimization, even for hierarchical structures, is introduced by imposing the delamination force equal to the intrinsic fracture of the tape. Also, the length of the peeling process zone is calculated, suggesting different optimal values for flaw-tolerant peeling at different angles. Applications to gecko adhesion, for which the flaw-tolerant peeling is demonstrated, and spider silk anchors, which we are going to discuss in detail in subsequent papers, are envisioned (including a new pre-stretching mechanism for adhesion control) and suggested by the evidence of a smart mechanism capable of maximizing adhesion simply by increasing the applied tension.

Thus, this Special Section has the aim of ultimately increasing our knowledge of "Nanoscale Fracture", and

accelerating the advent of a new age of flaw tolerant bio-inspired nanomaterials.

## References

Pugno N (2002) A quantized Griffith's criterion, Fracture Nanomechanics, Meeting of the Italian Group of Fracture. Vigevano, Italy, 25–26 Sept

Pugno N, Ruoff R (2004) Quantized fracture mechanics. Philos Mag 84(27):2829–2845

Pugno N (2006a) Dynamic quantized fracture mechanics. Int J Fract 140:159–168

Pugno N (2006b) New quantized failure criteria: application to nanotubes and nanowires. Int J Fract 141:311–323