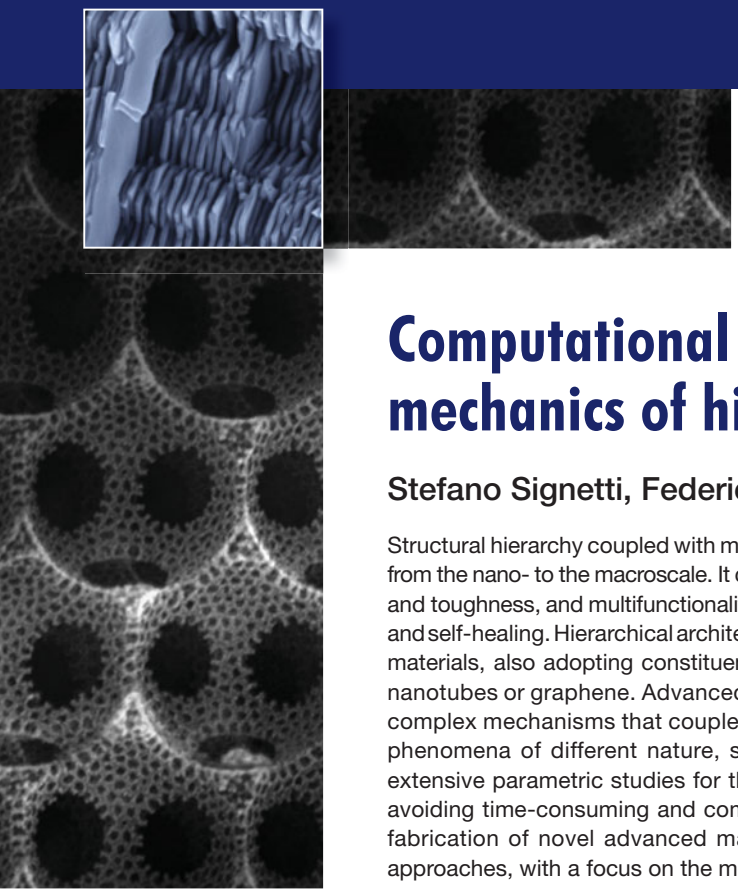

Computational modeling of the mechanics of hierarchical materials

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Structural hierarchy coupled with material heterogeneity is often identified in natural materials, from the nano- to the macroscale. It combines disparate mechanical properties, such as strength and toughness, and multifunctionality, such as smart adhesion, water repellence, self-cleaning, and self-healing. Hierarchical architectures can be employed in synthetic bioinspired structured materials, also adopting constituents with superior mechanical properties, such as carbon nanotubes or graphene. Advanced computational modeling is essential to understand the complex mechanisms that couple material, structural, and topological hierarchy, merging phenomena of different nature, size, and time scales. Numerical modeling also allows extensive parametric studies for the optimization of material properties and arrangement, avoiding time-consuming and complex experimental trials, and providing guidance in the fabrication of novel advanced materials. Here, we review some of the most promising approaches, with a focus on the methods developed by our group.

Introduction

For centuries, nature has provided inspiration for man in the design and manufacture of structural materials. Many natural materials display fascinating physical and mechanical properties that, until recently, have been hard to replicate in artificial materials and structures. These include high stiffness and low density,[1] strong adhesion and easy detachment,[2] self-sharpening,[3] self-healing, growth, and adaptive tissue organization, water-repellence, self-cleaning, and superhydrophobic or superhydrophilic behaviors.[4,5] All of these properties are usually related to complex multiscale structural arrangements of different constituents, from the nano- to the macroscale, involving material mixing and grading, interaction between constituents, and, most importantly, hierarchy, intended as the property whereby a material exhibits structure on more than one length scale.[6–8]

In the study of bioinspired materials, the focus is on the link between material properties and the emergence of specific functions across all relevant scales. The main lesson from nature is that complex behavior and functionality derives from structure, hierarchy, and optimal organization of simple basic components. This is in stark contrast to many engineered materials that exploit the properties of exotic metals or polymers, with associated high production and environmental costs. Nature has successfully done more with less, in terms of material design and production. This paradigm could, in principle, also apply to synthetic materials, and can be transposed to many fields in engineering, with the potential to do even better than nature, in the absence of limiting biological constraints.

Experimental tests and measurements on hierarchical materials can be difficult to rationalize due to high uncertainties and statistical dispersion at the nanoscale, difficulties in sample manipulation and characterization, problematic reproducibility of boundary conditions and, in some cases, the impossibility of direct experimental verification at all the different size scales. Thus, due to the complexity and cross-scale interaction of the physical phenomena involved, further progress requires comprehensive numerical modeling. The challenge is to integrate multiple length scales and physical phenomena within the same simulation framework, since in hierarchical structures, a piecewise understanding of individual parts cannot simply be assembled or superimposed: the whole is greater than the sum of the individual parts.[9,10]

Numerical modeling of biological and bioinspired material properties

Computational methods to model the mechanics of hierarchical materials need to span the various size and time scales of the problems involved. These can be divided schematically

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