



Computational analysis of graphene mechanics: deposition, adhesion and fracture

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Abstract

In this lecture, I report on results of molecular dynamics simulations of the mechanical properties of graphene focusing on three examples with experimental relevance. I will first discuss the deposition of graphene on a nanoparticle-decorated substrate, where I focus on the formation of wrinkles and their interaction. I will then consider the issue of partial delamination of the sheet due to the presence of regions with nigh nanoparticle density. I will then discuss a second problem in which graphene is deposited over a trench and study the effect of stresses and thermal fluctuations. Finally, I will conclude by discussing the behaviour of defected graphene under tensile loading. I will discuss the role of strain rate and temperature on fracture size effects and propose a theory to interpret the results.

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Stefano Zapperi is currently professor of theoretical condensed matter physics at the University of Milano and coordinator of the Center for Complexity and Biosystems. He graduated in physics at the University of Rome "La Sapienza" and received his Ph. D. in physics from Boston University. After a postdoctoral position at ESPCI in Paris, he became tenured researcher at INFM at the University Rome and then at the University Modena and Reggio Emilia. He became then senior researcher at CNR-IENI in Milano. He has been invited as visiting scientist or visiting professor in many institutions worldwide, including LMU Munich, FAU Erlangen-Nuremberg, Cornell University, Aalto University, ENS, Boston College, Rice University and the Weizmann Institute of Science. Prof. Zapperi in an expert in the statistical physics of complex systems and has fostered computational and data driven approaches to materials science and biophysics. His most notable contributions include the theory of the Barkhausen noise in magnets, the statistical physics of plasticity and fracture, and recent work on the physics of cancer and protein aggregation. He published more than 200 scientific papers in the top scientific journals. Prof. Zapperi is the recipient of numerous awards including the Marie Curie Excellence Award, the Humboldt Research Award and an Advanced Grant from the European Research Council. He was elected fellow of the American Physical Society and named Finland Distinguished Professor by the Academy of Finland. He is member of the editorial boards of JSTAT and Physical Biology. He organized several international workshops, summer schools and symposia on a variety of interdisciplinary research topics, ranging from the "Physics of Cancer" to Statistical Physics of Materials and Complex Systems. He has been elected member of the council and the executive committee of the Complex Systems Society and acted as chair of the steering committee of the Conference on Complex Systems. In the area of technology transfer, he received a Proof of concept grant from the European Research Council on the automatic design of metamaterials and he recently co-founded the spinoff company Complexdata.

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