Multi-scale Modeling for MEMS: from physical principles to engineering applications

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Micro- and nano-electro-mechanical systems (MEMS, NEMS) provide a challenging platform to realize micro-nanomechanics and microfluidics experiments at the smallest scales, with an unprecedented control on the experimental parameters. The impact of such technologies, for example in biology and medicine, is increasing at a fast pace. Our theory group at IEMN has developed several collaborations with the LIMMS-Cnrs Laboratory and the IIS, both in the University of Tokyo and world-leading experts in MEMS technologies. I will present here the results of our multiscale approach, combining atomic-scale molecular dynamics, mesoscale Monte Carlo simulations, macroscopic PDE and statistical mechanics models, for two relevant examples.

In a first case, the extreme plasticity observed in MEMS experiments on silicon nanowires [2] is explained in terms of a two-phase theoretical model,[2,3] describing the evolution of a nanocrystalline structure connected by a thin layer of amorphous material. Liquid-like flow in the amorphous is identified as the responsible for the exceptional elongation of the Si nanowires, in excess of 2000%. The continuum model is based on microscopic observations obtained from atomic-scale molecular dynamics simulations, of the tensile deformation of a model Si nanowire. Numerical solutions of stress-strain curves from the analytical model show a multi-stage deformation behavior, in excellent agreement with the experiments.

In a second example, we studied the response of both single DNA molecules and large DNA bundles, stretched by MEMS "nanotweezers". The objective is to understand the failure of DNA fibers exposed to gamma-ray irradiation, to improve the specificity of cancer radiotherapy.[4] We developed combined Monte-Carlo simulations and statistical-mechanics modeling to describe the microscopic kinematics of the damage process. Analysis of the finite-size elasticity of a two-state model of single DNA molecules stretched at large applied forces,[5] demonstrate that the experimental force-extension curves can be described by a unique universal model, despite the differences in polymer size, structure, chemistry and rate-dependence of transition forces. Next, DNA bundle degradation induced by ionizing radiation is modeled by an assembly of parallel fibers, progressively damaged by a random population of breaks.[6] Fibers interact by means of a lateral viscoelastic coupling, thus retaining structural integrity even after substantial damage. Monte Carlo simulations of the Young's modulus degradation for increasing DNA damage density demonstrate a remarkable scaling shift between an exponential and a power-law regime. Analytical solutions of the model confirm this behavior, and provide a thorough understanding of the underlying physics.

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Fields of Research

Statistical mechanics of nanostructured and disordered materials; Biophysics and Nano-Bio interfaces; Multi-scale computer simulation of atomic and molecular systems

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