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COMBINED ATOMISTIC AND CONTINUUM MODELLING OF NONLINEAR ELASTICITY IN NANOSTRUCTURED MATERIALS

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ABSTRACT

Nonlinear elasticity is a dominat feature in complex systems for a large variety of mechanical behaviors, including, e.g., the overall elastic response of composite materials, the hyperelasticity of materials undergoing dynamic fracture [1,2], the propagation of shock waves in elastic media [3].

This work is addressed to the investigation of nonlinear elasticity in nanostructured silicon, a composite material of ramarkable technological relevance in nano- and opto-electronics. The present theoretical effort is sustained by hierarchically combining continuum and atomistic schemes.

It has been widely recognized that different methodologies must be concurrently integrated in order to properly modelling complex materials. This idea leads to the multiscale approach: a paradigm effectively coupling different methods and providing a unique theoretical device able to pass physical information across length scales. In this work we adopt such a paradigm and we work out a multiscale hyerarchical combination of (i) *nonlinear continuum mechanics* and (ii) *molecular dynamics simulations* to investigate the interplay between nonlinear elastic features and nanostructure in silicon.

As for continuum modelling, we develop a thorough description of a dispersion of nonlinear spherical inhomogeneities, embedded into a linear solid matrix. This model system represents in fact the continuum counterpart of nanocrystalline silicon (nc-Si), as indeed grown for advanced applications in optoelectronics and photonics [4]: in nc-Si crystalline nanograins are indeed dispersed into an otherwise amorphous silicon matrix. Our model is worked out within the Eshelby theory for elastic inclusions, as recently applied to multifractured solids [5,6] and further extended to the present case of a composite system [7].

As for atomistic modelling, large-scale molecular dynamics (MD) simulations are used to generate trustworthy samples of nc-Si with different crystallinity [8]. A careful account for nanograins differing in shape, size, and orientation is obtained. The computer-generated samples are used as input to perform a full set of simulated loading experiments (both in traction and shear conditions), aimed at measuring nonlinear elastic moduli.

The results here presented are either valuable and diverse.

First of all, we provide full analytical expressions of the effective nonlinear elastic moduli of the composite system (i.e. the overall nc-Si system). We also prove that it exists a universal scheme of dependence between such moduli and their counterparts within the nonlinear inclusions (i.e. crystalline nanograis), as well as intriguing nonlinearity enhancement effects depending upon nanograin density.

Then, we provide a thorough quantitative estimation of nonlinear moduli by means of atomistic simulations. We also provide a validation of continuum results down to the nanoscale. Finally, we consider as well the limiting case of a purely amorphous silicon matrix (corresponding to a vanishing average grain size), which indeed represents an interesting physical systems worthy of investigation as for its nonlinear elastic behavior.

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