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Material Substructures in Complex Bodies

From Atomic Level to Continuum

Edited by: Gianfranco Capriz and Paolo Maria Mariano

MATERIAL SUBSTRUCTURES IN COMPLEX BODIES: FROM ATOMIC LEVEL TO CONTINUUM

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PREFACE

Stringent industrial requirement of sophisticated performances and of circumstantial control for micro-devices and other types of machinery at multiple scales can be satisfied often only by resort to or allowance for complex materials. The adjective "complex" beckons to the fact that the substructure influences gross mechanical behaviour in a prominent way. Interactions due to substructural changes are represented directly. Examples, just to list a few, are liquid crystals, quasi-periodic alloys, polymeric bodies, spin glasses, magnetostrictive materials and ferroelectrics, suspensions, in particular liquids with gas bubbles, polarizable fluids, etc. Hopefully, substructures can be exploited, even invented anew, to reach predetermined goals. To help in the process, theories must be developed so that severe challenging theoretical problems arise; often of fundamental nature. A precise grasp of the physical meaning of mathematical entities is critical for the correct, adequate proposal of models of behaviour and even of consequent computational analyses. A basic problem is of bridging scales even from atomic to macroscopic level, translating through continuum limit the prominent aspects of the subtle discrete substructural features. Their number and nature may be also enriched by specific circumstances. The collection of chapters composing this book aims to underline some aspects of these questions, proposing also new matter of discussion together with specific solutions.

In Chapter 1, *Pierre Degond* derives hydrodynamic models of plasmas and disparate mass binary mixtures by evaluating the continuum limit of kinetic "small-scale" events represented by means of Fokker-Planck or Boltzmann equations. Macroscopic diffusion equations for density of particles and energy follow, coupled with a Euler-type equation for ions or heavy species. Inconsistencies in existing models are evidenced.

In Chapter 2, *Carlo Cercignani* continues the discussion on how kinetic schemes based on Boltzmann equation may offer microscopic foundations of continuous dynamical models. He examines how old and new techniques in the kinetic theories of dense gases may be useful for describing the fast flow of granular materials.

Substructural kinetic effects may be not as prominent in some circumstances as quantum phenomena. In Chapter 3, *Jan Jerzy Slawianowski* develops a quantization scheme for affine bodies, a special class of complex bodies where the natural morphological descriptor is a second-order tensor: in other words, each material element is considered as a system which may (microscopically) deform independently of the neighbouring fellows.

Once reasonable models have been established, computational techniques are essential in finding explicit solutions in special cases. When phenomena at various scales are involved, non-trivial computational problems arise and may be tackled with different methods, depending on circumstances. In their Chapter 4, *Sukky Jun* and *Wing Kam Liu* discuss computational methods appropriate to analyse the formation of electronic band structures in periodic atomic lattices. The approach makes use of periodic meshless shape functions based on the moving least-square approximation. Wave equations are analysed in the reciprocal space determined by the standard Fourier basis. The analyses of semiconductors, photonic and phononic crystals are natural applications. Complex bodies are produced in non-simple industrial processes so that the process of formation of substructures deserves to be described *per se*.

Amid possible industrial processes, in Chapter 5, *Antonio Fasano, Krishna Kannan, Alberto Mancini* and *Kumbakonam R. Rajagopal* propose a new model for the Ziegler-Natta polymerization in a high-pressure reactor by considering, after fragmentation, a single agglomerate of catalytic particles, then analyzing the mechanics of growing nano-spheres. A non-linear hyperbolic system of governing equations arises.

Other aspects of the mechanics of polymers are further discussed by *Krishna Kannan* and *Kumbakonam R. Rajagopal* in their Chapter 7. The attention is focused on the solidification process of molten polymers where there is competition between the effects of substructural quenching and deformation of the melt: The former effect is an obstacle to the crystallization while the latter enhances it in a way in which memory effects have to be accounted for. Deformation and the corresponding macroscopic stress influence also the formation of nanostructures in semiconductors during their fabrication and the collective mechanical behaviour in applications. The modelling of these effects include atomistic, continuum and multiscale features. These topics are discussed in Chapter 8 by *Harley T. Johnson*.

Finally, our personal contributions are in Chapters 6 and 9. Basic foundations of the mechanics of bodies in which substructural phenomena have kinetic nature are discussed in Chapter 6 (by G.C.) without resorting to the use of some version of Boltzmann equation. The interaction between gross deformation and spin structures are discussed in Chapter 9 (by P.M.M.) paying attention on the evolution of disclination lines and point defects. The covariance of the relevant evolution equations is proven.

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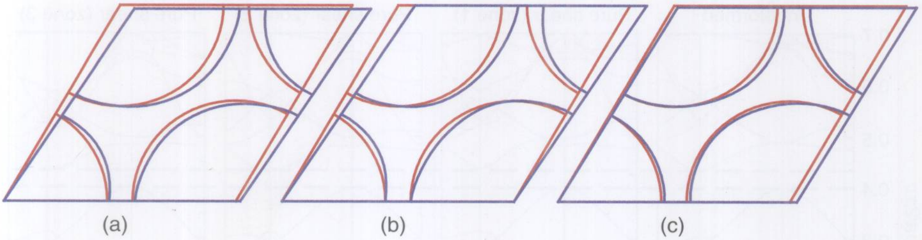

Plate 1 Undeformed (red) and deformed (blue) unit cells of 2D triangular photonic crystal with cylindrical air rods: (a) pure shear, (b) simple shear and (c) uniaxial tension. In each mode, corresponding shear or tensile strain of 3% is applied.

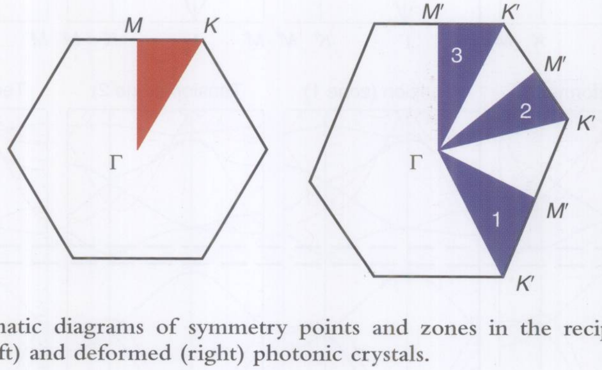

Plate 2 Schematic diagrams of symmetry points and zones in the reciprocal lattice of undeformed (left) and deformed (right) photonic crystals.

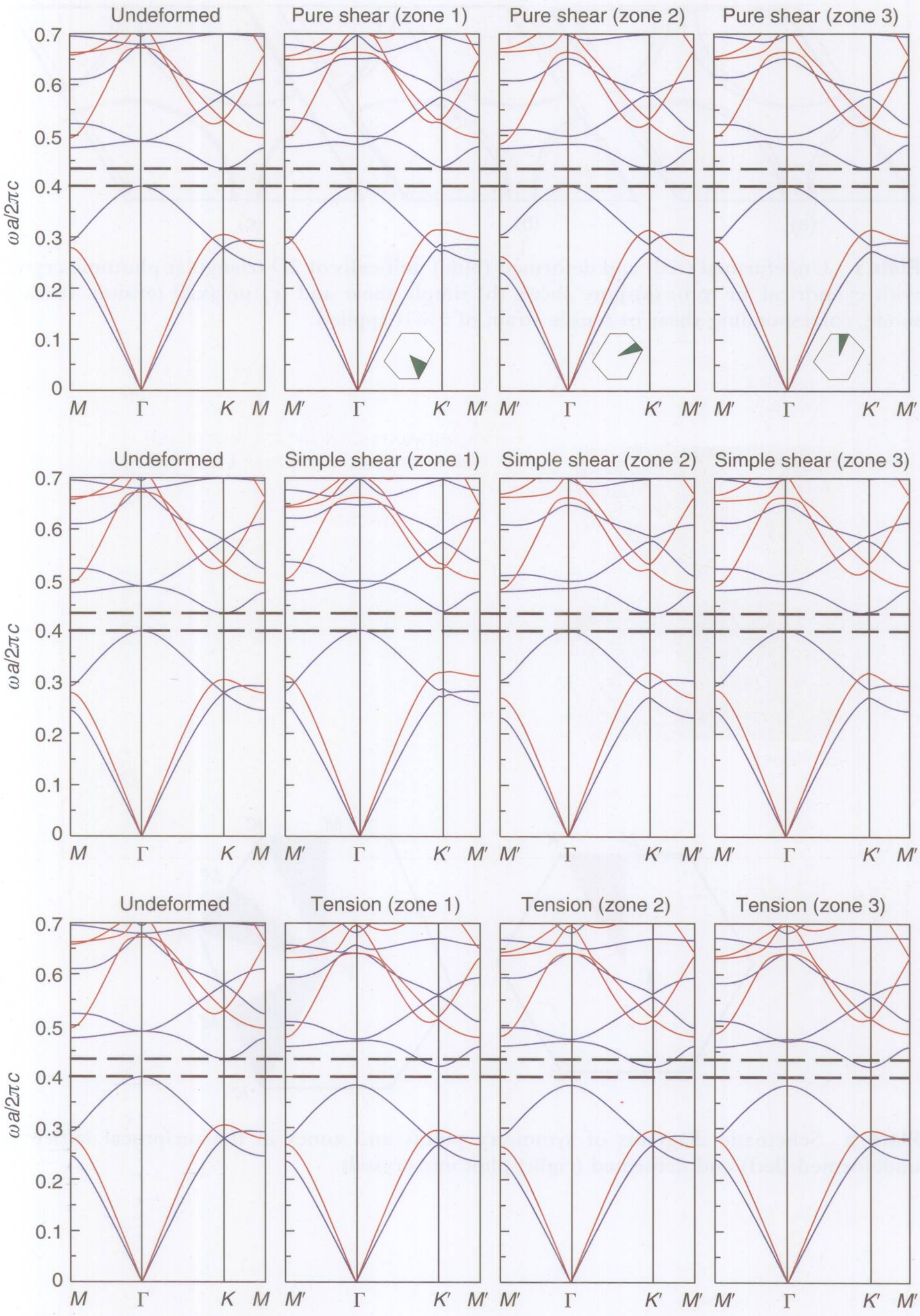

Plate 3 Photonic band structures under pure shear (top), simple shear (middle), and uniaxial tension (bottom). TM and TE modes are in blue and red, respectively. Dashed horizontal lines indicate the bandgap of undeformed original photonic crystal. Insets in top low illustrate the quasi-hexagonal symmetry zones of the deformed photonic crystal.

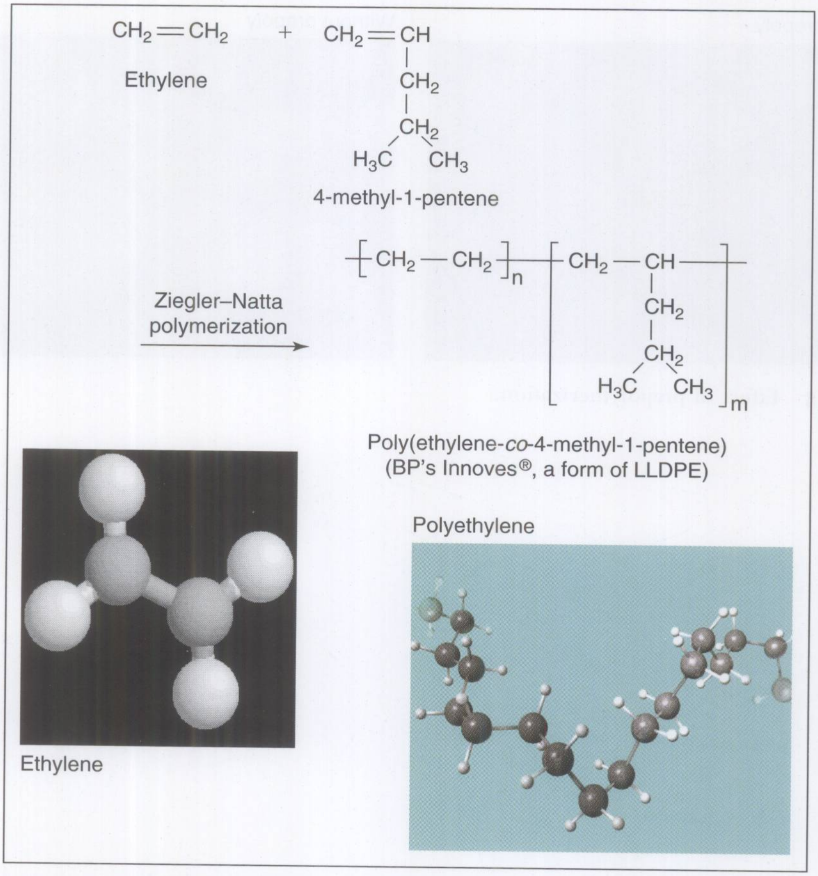

Plate 4 Polyethylene.

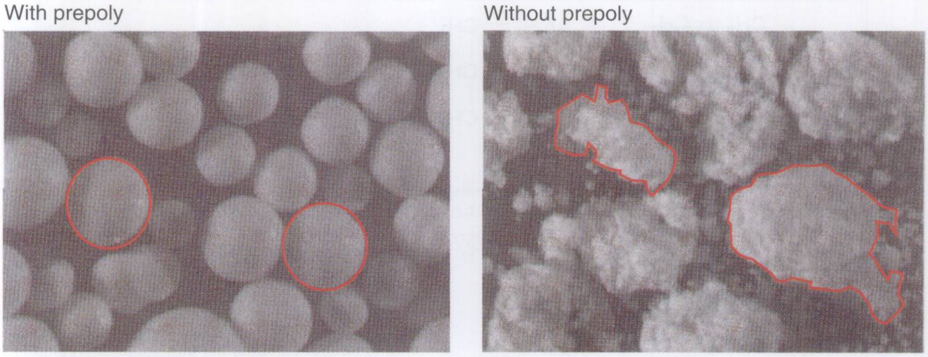

Plate 5 Effect of prepolymerization.

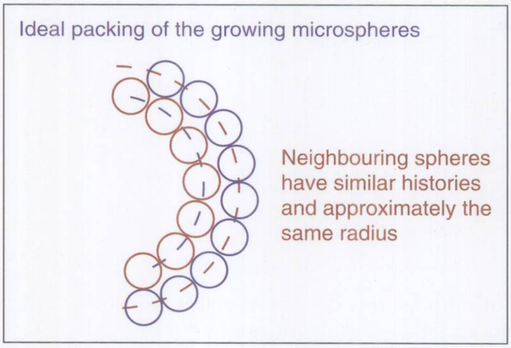

Plate 6 Porosity ε constant.

Plate 7 Schematic of three thin film growth modes. Left: Frank–van der Merwe or planar layer-by-layer growth. Center: Stransk–Krastanow or island growth on a wetting layer. Right: Volmer–Weber or island growth with no wetting of the substrate.

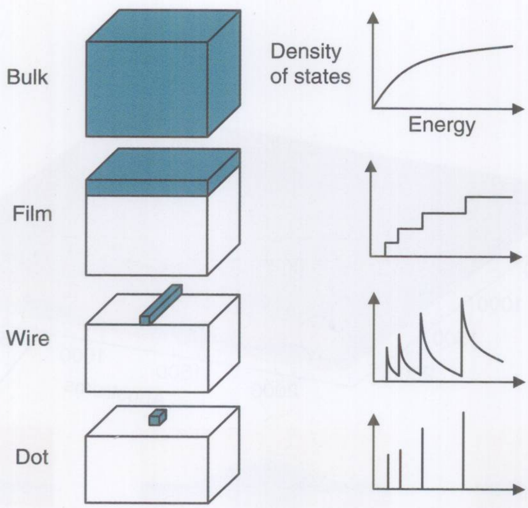

Plate 8 Schematic of the electron density of states in bulk and quantum confined material systems. The delta-function-like densities of states in quantum wire and quantum dot configurations are desirable for many nanoelectronic and optoelectronic devices.

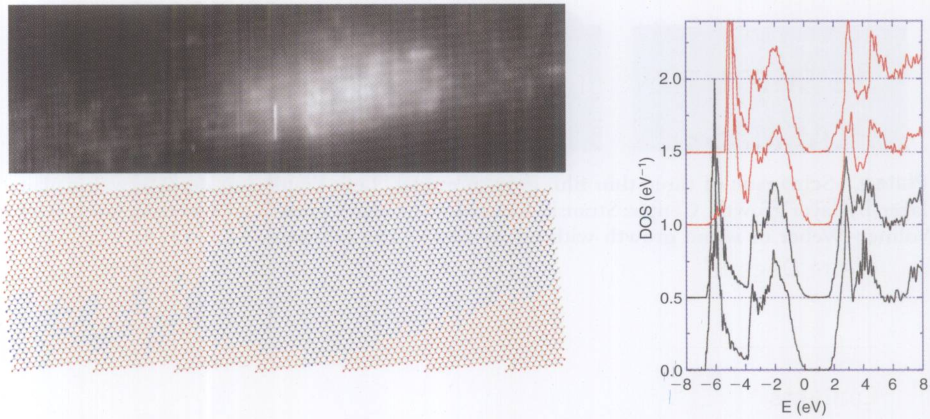

Plate 9 Combined experimental and computational study of electronic structure of individual embedded quantum dot at the atomistic scale. Atom positions are determined using high resolution cross-sectional scanning tunneling microscopy (upper left) and then converted to an atomistic computational input file (lower left). Using a novel tight-binding method, the local density of states is determined at various positions (right) and compared to experimental data [56].

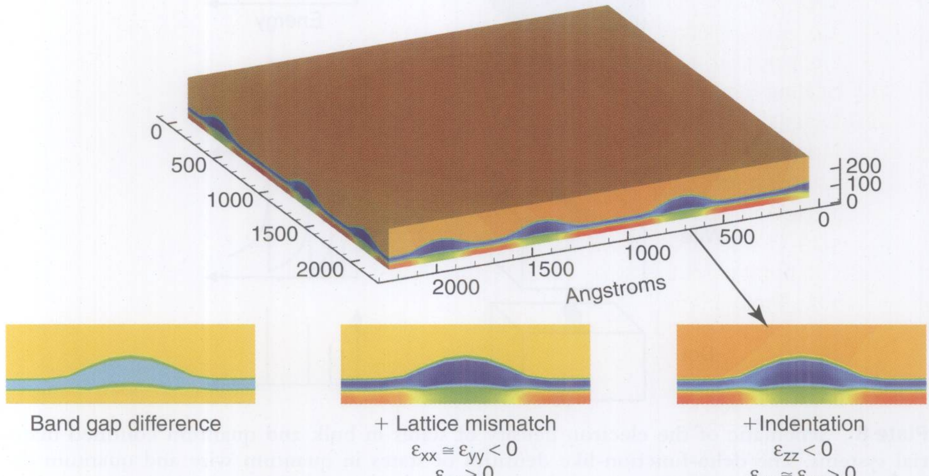

Plate 10 Embedded quantum dot array finite element mesh. The color contour shows the electrostatic potential for a single electron in the system when the surface is nanoindented to a small depth. The three inset images show how bandgap difference, lattice mismatch strain, and nanoindentation strain contribute to the total potential field [64].

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