

## Multiscale modeling of crystalline nanostructures

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**Résumé** — A finite element procedure for modeling crystalline nanostructures such as nanowires is proposed. The size effects exhibited by nano objects are captured by taking into account a surface energy, following the classical Gurtin Murdoch surface elasticity theory. An appropriate variational form and a finite element approach are provided to model and solve relevant problems numerically. The methodology is completed with a computational procedure based on ab initio calculations to extract elastic coefficients of general anisotropic surfaces.

**Mots clés** — Nano structures, Finite elements, ab initio calculations, size effects.

Studying atomistic systems at a mesoscopic scale (around 10-100 nm) is of fundamental interest, as it is usually the scale of nanosystems practical applications and elementary cells for nanocomposites. However, at this scale the system contains too many atoms to be studied directly with a full atomistic model. To reduce the costs and simplify design analysis, a continuum description of nanosystems, including all specific features (surface and quantum effects) is highly needed and of great scientific and industrial importance.

Here we present a framework aiming at modelling surface effects in nanosystems within a continuum (or coarse-grained) model. The technique is based on the Gurtin-Murdoch surface elasticity theory [1] combined with local quantum mechanical calculations (Density Functional Theory), which are used to extract the coefficients of the surface in the continuum model.

First, we formulate the weak form related to the continuum elastic model with surface energy. The additional surface terms are both associated with surface strain-independent and surface strain-dependent stresses. Second, we define an original procedure to extract by ab initio calculation (via e.g. available softwares) the surface elastic coefficients and surface residual stresses : a series of calculations on slabs associated with the surface are carried out (see figure 1). Then the surface elastic coefficients are deduced by fitting the ab initio energy results with respect to tangential strains. Eventually, the coefficients are used in the continuum equations, which are solved via the finite element method. In this framework, special surface elements must be employed. Another proposed alternative is the use of XFEM [3], which is very convenient to describe complex geometries of interfaces and avoids the use of explicit surfaces description. Moreover, the different surface operators can be constructed directly on the basis of a level-set function. The size effects are accurately captured in this framework. Applications to ionic crystalline nanowires are presented. To validate our approach, we have compared the continuum model with full ab initio models of nanowires with different sizes [2, 4]. An example is provided in Figure 2 (a), where

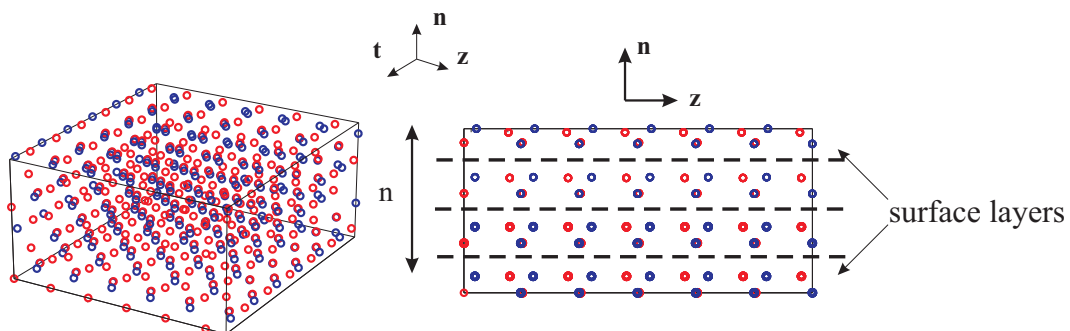


FIGURE 1 – Slab models with number of layers  $n$  used for ab initio calculations.

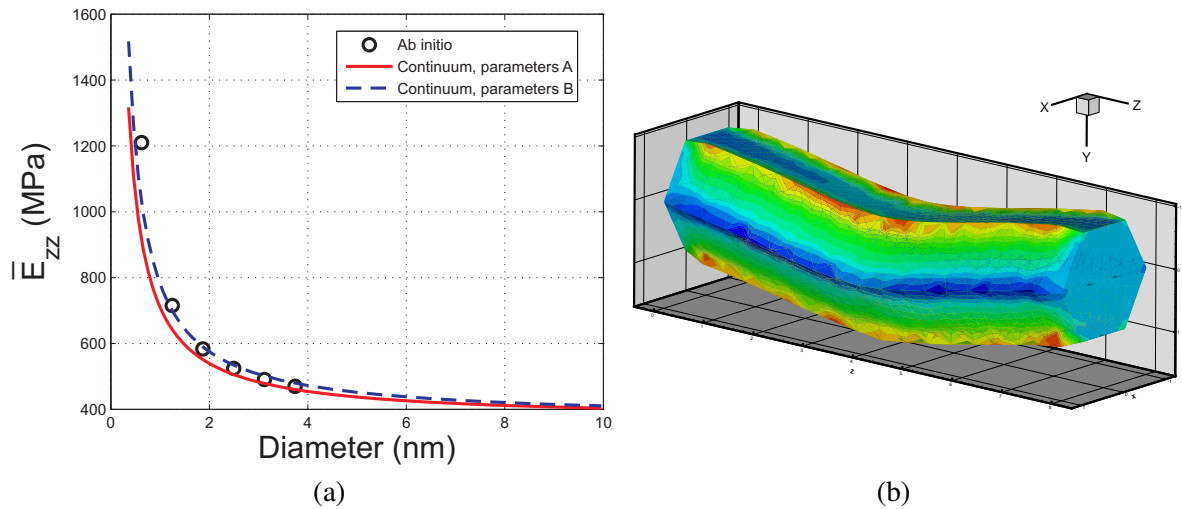


FIGURE 2 – Effective Young modulus of the nanowire : comparison between continuum FEM model and *ab initio* model (prescribed strain);  $\epsilon_{yy}$  strain field and deformed configuration of the nanowire in bending.

the effective Young modulus of the full *ab initio* nanowire model is compared with the Finite element model for different radii. very good agreement between both models is noticed. In figure 2 (b) we show a deformed configuration of a nanowire in bending including effects of surface energy.

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