Composite materials: mechanical properties

A computational lattice model describing scale effects @ nano-scale

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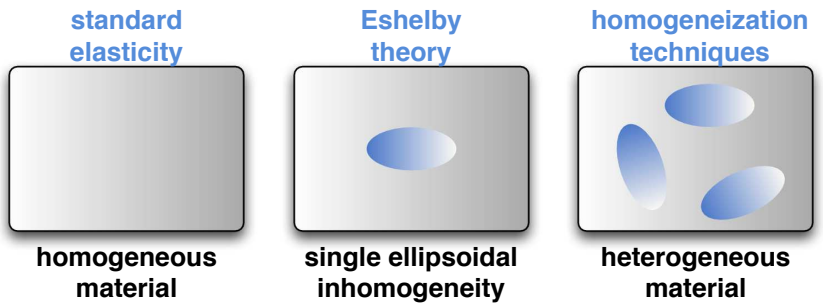
Outline

Conceptual framework

Scenario

- Heterogeneous structures central to modern science & engineering
- Structural complexity typically ranges from the microscale to the nano-scale
- Standard continuum approach



scale-invariant prediction about the elastic fields within and nearby the inhomogeneity

- Advanced models describe scale effects at surfaces and interfaces
  → *Interface Stress Model (ISM)*
- ISM applied to
  → *Eshelby configuration with interface effects - Duan et al. (2005) and (2008)*
  → *stratified particles - Duan et al. (2006)*
  → *alloyed quantum dots - Duan et al. (2006)*

Major conceptual difficulties arise by projecting continuum theories @ nano-scale

1. standard elasticity theory that can hardly work @ the nano-scale
   → *continuum picture does not apply*
2. constitutive equations @ nano-scale typically nonlinear
   → *often overlooked in standard applications since leading to severe complications*
3. only selected combinations of elastically nonlinear matrix or inhomogeneity
4. effective medium approach

Key issues for the elastic behavior of nano-structures materials

- scale effects
- nonlinear elastic response
- nano-structure induced anisotropic behavior

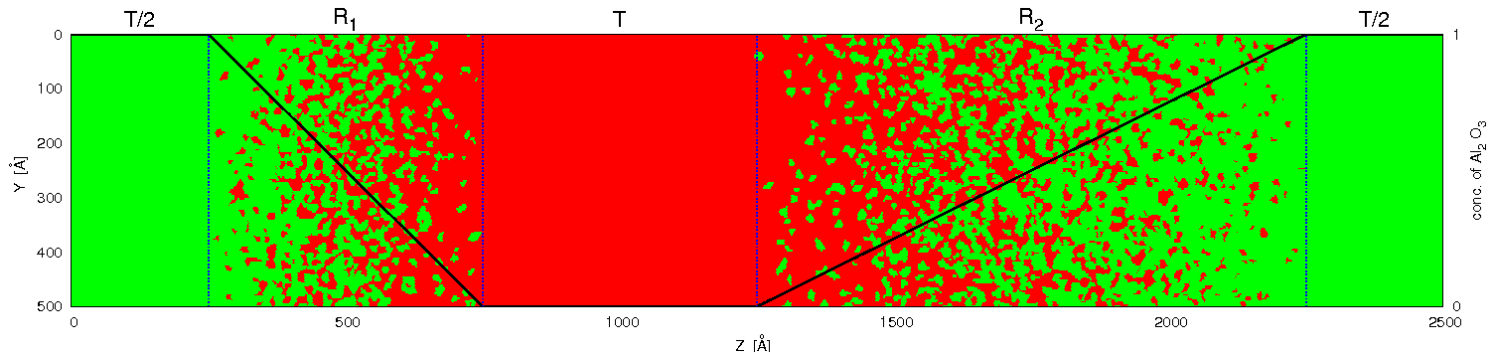
... and their possible interplay as well !

This work

- attempt a more general solution based on **an elastic lattice model** fully exploiting nanoscale features
- **no educated guess on the actual constitutive behavior** for the interface (or nonlocal continuum model) assumed
- atomic-scale degrees of freedom fully described by **constitutive force fields**

Steps

1. An **elastic lattice model is developed** such that:
   - continuum elasticity mapped onto a discrete lattice
   - a suitable interatomic distance introduced → the notion of length scale is naturally introduced and, therefore, the possible onset of scale effects can be described;
   - an arbitrary continuum constitutive law (either linear or not) translated into a simple atomistic interaction potential
2. **2D Eshelby problem used to benchmark the model**
   - simple two-body interaction potentials (harmonic, linearized and anharmonic) to govern the mechanics of a triangular (isotropic) lattice
   - extension to many-body potentials straightforward (but quite boring!)
3. model applied **to predict the elastic moduli of a nano-/alloys&graded interfaces**
   - generate a proper atomic-scale structural model
   - define a simulation protocol to address the stress-strain relation
   - compute both linear and nonlinear elastic moduli



Elastic lattice model

- **2D triangular lattice of atoms**, belonging to the hexagonal crystal symmetry
  - → *isotropic linear elastic behavior, as indeed requested by the Eshelby theory*
  - → *straightforwardly extended to 3D lattices and/or arbitrary crystal symmetries*
- **linear regime**: isotropic behavior 2 independent elastic moduli λ and μ
- **nonlinear regime**: anisotropic behavior, 3 independent elastic moduli Λ_1, Λ_2 and Λ_3

elastic energy density $\mathcal{U}(\hat{\varepsilon})$ - continuum formulation

$$\begin{aligned}\mathcal{U}(\hat{\varepsilon}) &= \frac{\lambda}{2}\left[\mathtt{Tr}(\hat{\varepsilon})\right]^2 + \mu\,\mathtt{Tr}(\hat{\varepsilon}^2) + \Lambda_1(\varepsilon_{11}-\varepsilon_{22})\left[(\varepsilon_{11}-\varepsilon_{22})^2 - 12\varepsilon_{12}^2\right] \\ &+ \frac{1}{2}\Lambda_2\,\mathtt{Tr}(\hat{\varepsilon})\left[2\,\mathtt{Tr}(\hat{\varepsilon}^2) - \mathtt{Tr}(\hat{\varepsilon})^2\right] + \frac{1}{2}\Lambda_3\,\mathtt{Tr}(\hat{\varepsilon})^3\end{aligned}$$

- elastic moduli related to **stiffness constants** of crystal elasticity through

$$\lambda = C_{12} \qquad 2\mu = C_{11} - C_{12}$$

$$\begin{aligned}\Lambda_1 &= \frac{1}{12}(C_{111} - C_{222}) \\ \Lambda_2 &= \frac{1}{4}(C_{222} - C_{112}) \\ \Lambda_3 &= \frac{1}{12}(2C_{111} - C_{222} + 3C_{112})\end{aligned}$$

- **each site of the triangular lattice is occupied by an atom**
  $\rightarrow$ *$\mathcal{U}(\hat{\varepsilon})$ given by of a suitable interatomic potential*
- **N-body force field at work - each term governed by a single parameter**
  $\rightarrow$ *2-body terms mimic bond stretching* $\rightarrow$ *3-body terms mimic bond bending*
- **this work**: interatomic interactions only described by **2-body harmonic springs** between next neighboring atoms $\rightarrow$ $U_h = \frac{1}{2}\kappa_h (r_{ij} - r_0)^2 = \frac{1}{2}\kappa_h \left(\vec{n}_{ij} \cdot \Delta\vec{u}_{ij}\right)^2 + \mathcal{O}(u^3)$

elastic energy $U_{lattice}$ - **elastic lattice formulation**

$$U_{lattice} = U_0 + \frac{1}{2}\sum_{ij}\left[U_l(r_{ij}) + U_h(r_{ij}) + U_a(r_{ij})\right]$$

By definition:

1. **linearized terms** $U_l = \mathcal{L}\left[\frac{1}{2}\kappa_l (r_{ij} - r_0)^2\right] = \frac{1}{2}\kappa_l \left(\vec{n}_{ij} \cdot \Delta\vec{u}_{ij}\right)^2$ affect only the linear elastic moduli $C_{\alpha\beta}$
2. **harmonic terms** affect both the linear $C_{\alpha\beta}$ and the nonlinear $C_{\alpha\beta\gamma}$ elastic constants
3. **anharmonic terms** $U_a = \frac{1}{3}\frac{\kappa_a}{r_0}(r_{ij} - r_0)^3$ affect only the nonlinear moduli $C_{\alpha\beta\gamma}$

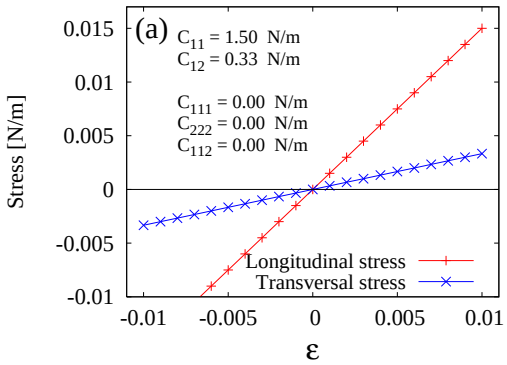
- proved that **a triangular lattice described by the atomistic potential energy $U_{lattice}$ is equivalent to the continuum described by the strain energy function $\mathcal{U}(\hat{\varepsilon})$**
- the **linear and nonlinear elastic moduli** are provided by the following synopsis

$$
\begin{aligned}
C_{11} &= \frac{3\sqrt{3}}{4}(\kappa_l + \kappa_h) \\
C_{12} &= \frac{\sqrt{3}}{4}(\kappa_l + \kappa_h) \\
C_{111} &= \frac{9\sqrt{3}}{16}\kappa_h + \frac{9\sqrt{3}}{8}\kappa_a \\
C_{222} &= \frac{3\sqrt{3}}{16}\kappa_h + \frac{11\sqrt{3}}{8}\kappa_a \\
C_{112} &= -\frac{5\sqrt{3}}{16}\kappa_h + \frac{3\sqrt{3}}{8}\kappa_a
\end{aligned}
$$

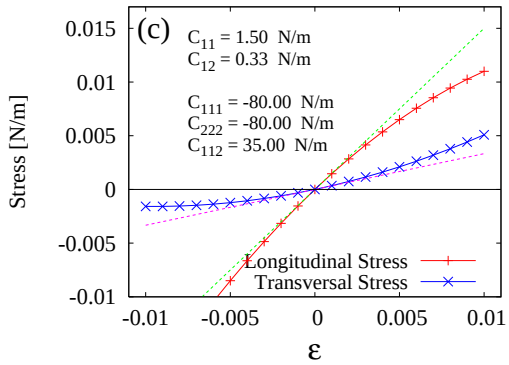
Key results

1. the continuum elastic behavior can be obtained by **properly setting the potential parameters** $\kappa_h, \kappa_l, \kappa_a$
2. such a 2-body interaction potential works as a **constitutive force field**
   same holds for any N-body potential choice: more flexibility... but much more complex

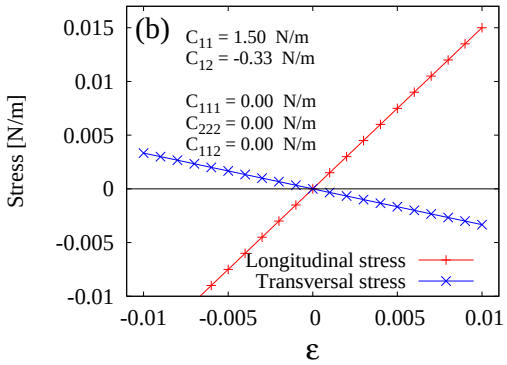
linear elastic - positive Poisson ratio



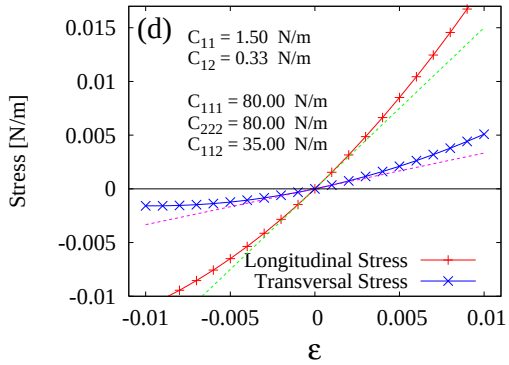
nonlinear hypoelastic



linear elastic - negative Poisson ratio

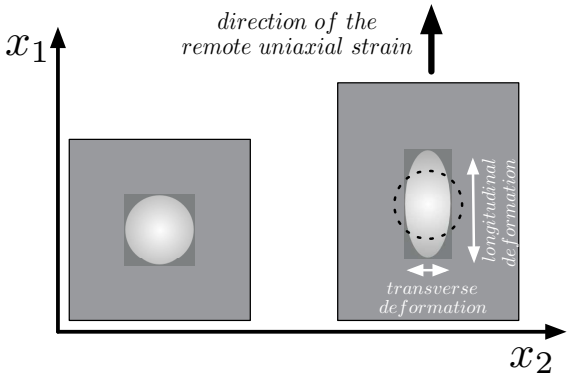


nonlinear elastic - hyperelastic



- Isotropic linear behavior is a consequence of the lattice symmetry (honeycomb)
- Isotropic nonlinear behavior ($C_{111} = C_{222}$) enforced by $\kappa_a = \frac{3}{2}\kappa_h$

2D Eshelby problem



Case study

- system under uniaxial strain along x_1
- transverse and longitudinal deformations calculated and then represented as $\varepsilon_l = L^I\epsilon + L^{II}\epsilon^2$ and $\varepsilon_t = T^I\epsilon + T^{II}\epsilon^2$ with $-0.01 \leq \epsilon \leq +0.01$

Atomistics

- 144000 atoms (120nm-large simulation cell)
- asymptotic boundary conditions
- atomic degress of freedom relaxed through dumped dynamics

Four combinations:

1. linear matrix - linear inhomogeneity
2. linear matrix - nonlinear inhomogeneity
3. nonlinear matrix - linear inhomogeneity (*)
4. nonlinear matrix - nonlinear inhomogeneity (*)

Under isotropy condition:

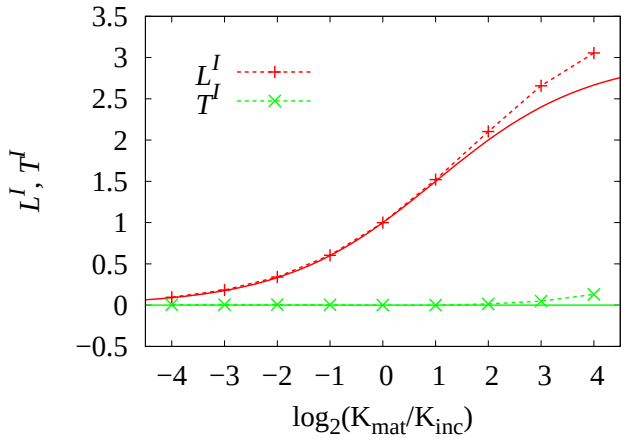
- linear material: $C_{111} = C_{222} = C_{112} = 0$
- nonlinear material: $C_{111} = C_{222}$

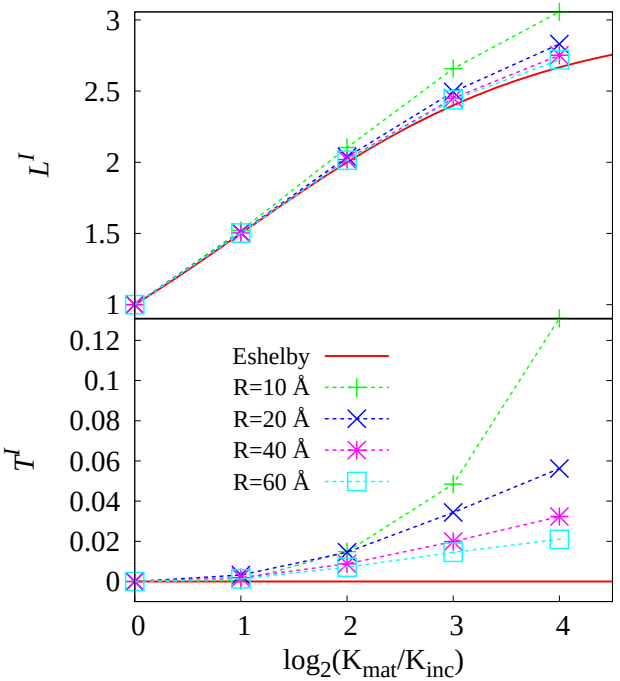
Constitutive force field

material	κ_l	κ_h	κ_a
linear	K	0	0
nonlinear	0	K	$\frac{3}{2}K$

- K: the elastic stiffness (material specific)
- different elastic contrasts $\log_2 \frac{K_{mat}}{K_{inh}}$
- different radius R values

linear matrix - linear inhomogeneity





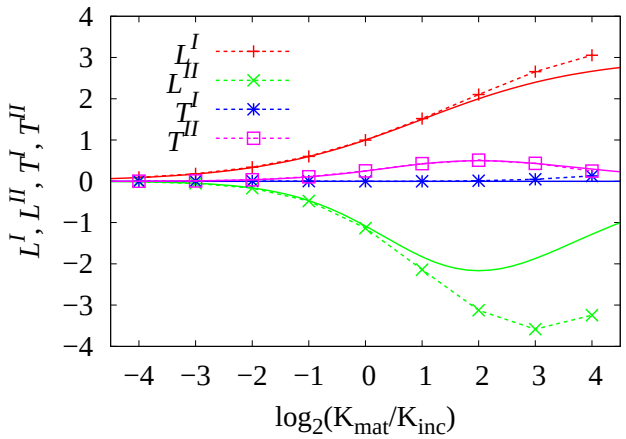
- inhomogeneity radius $R = 1$nm
- **uniform internal strain field**
- for a positive contrast (i.e inhomogeneity softer than matrix) **atomistic data differ from the continuum prediction**

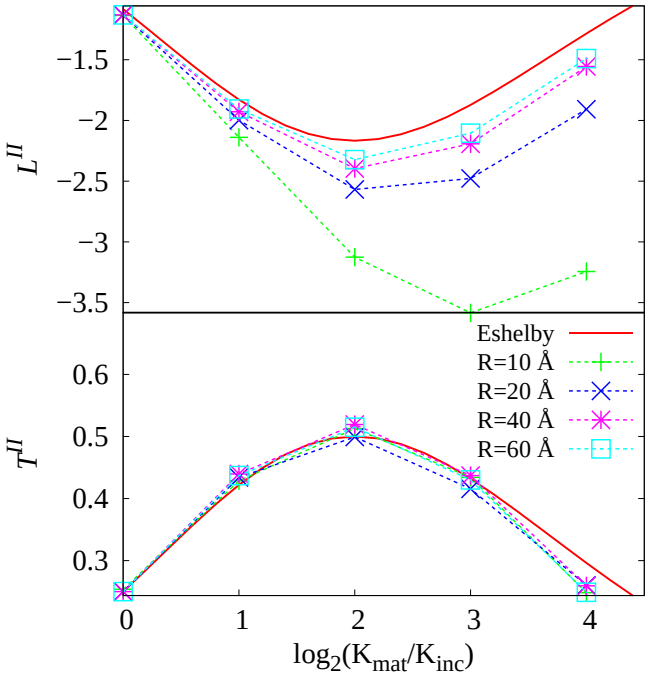
- disagreement vanishes for larger R
- effect attributed to **truly atomic-scale features**
- scale effects stronger for L^I than T^I.

Key result

The lattice elastic model sets **a lower limit of validity for the Eshelby theory**, as far as the length scale is concerned

linear matrix - nonlinear inhomogeneity

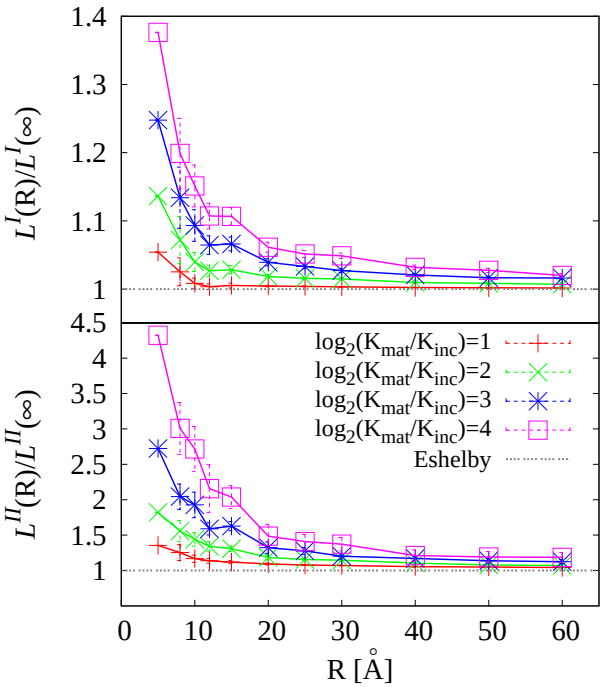




- inhomogeneity radius $R = 1$nm
- **uniform internal strain field**
- linear coefficients L^I and T^I as before
  $\longrightarrow$ *not affected by a possibly nonlinear inhomogeneity*

- nonlinear coefficient L^{II} large differences between atomistics and continuum for positve elastic contrast
- nonlinear coefficient T^{II} marginally affected by elastic contrast
- **scale effects observed even for nonlinear coefficients**

Searching for scaling laws in atomistic effects



- $L^I(R)$ (top) and $L^{II}(R)$: atomistic coefficients for different elastic contrasts.
- $L^I(\infty)$ and $L^{II}(\infty)$: continuum counterparts (Eshelby theory)

- atomistic data fitted by the power laws

$$\frac{L^I(R)}{L^I(\infty)} = 1 + \frac{a}{R^\alpha} \quad ; \quad \frac{L^{II}(R)}{L^{II}(\infty)} = 1 + \frac{b}{R^\beta}$$

- found the **same scaling exponent** for the linear and nonlinear coefficients

$$\alpha \simeq \beta \simeq 1.11 \pm 0.05$$

- **scaling exponents independent of elastic contrast**

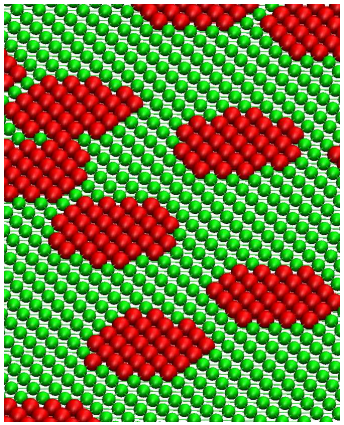
Key result of lattice elastic model

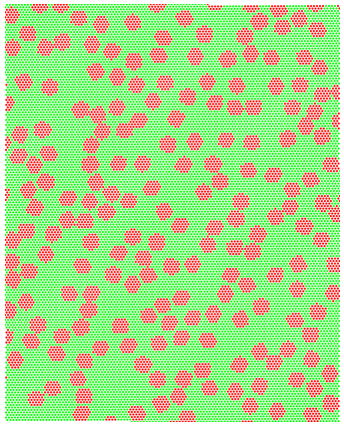
both linear and nonlinear behaviors belong to the **same universality class**

- *continuum ISM -based on competition between surface/volume- provides* $\alpha = 1$
- *present results rather suggest* α *is related to the* **discretization of the continuum equations at the atomic scale**

Nano-alloys

- **structural model**
  1. two elastically different media placed onto an honeycomb lattice
  2. random dispersions ($0\% < c < 50\%$)
  3. circular inclusions with constant radius $R \simeq 10$Å and $R \simeq 20$Å



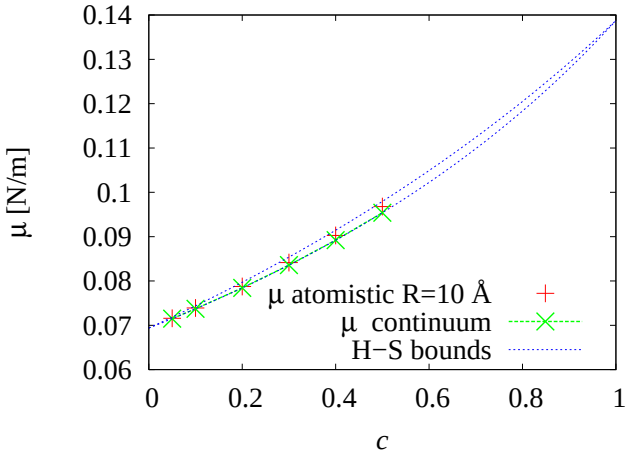


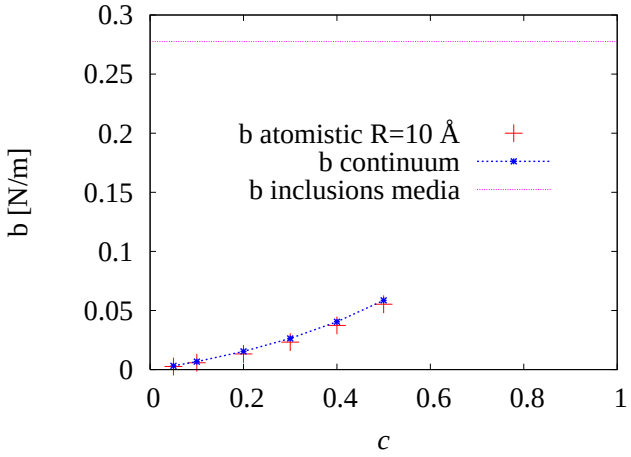
- **elasticity**
  1. *matrix*: isotropic linear material *inhomogeneities*: isotropic nonlinear material
  2. two linear moduli: μ and K
  3. two nonlinear parameters: $b = \frac{C_{111}-C_{112}}{4}$ and $c = \frac{3}{4}(C_{112} - \frac{1}{3}C_{111})$
- **simulation protocol** *large-scale simulations* ($\sim 10^5$ *atoms*)
  1. elastic moduli computed through interpolation of the stress-strain curves
  2. atomic degrees of freedom relaxed by dumped dynamics
  3. atomic-level stress tensor provided by virial

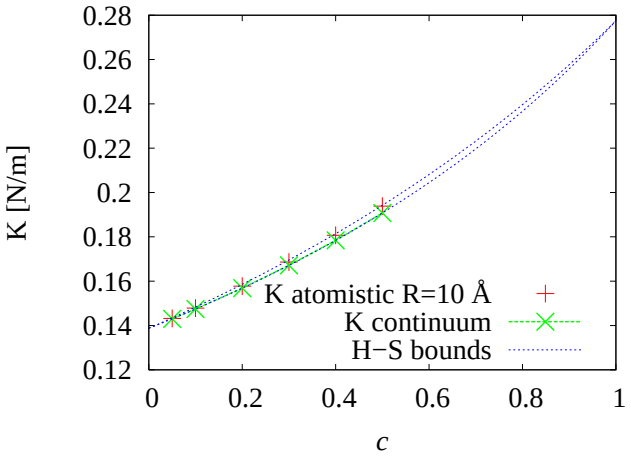
Atomistic results *vs*. continuum prediction: **inclusions stiffer than matrix**

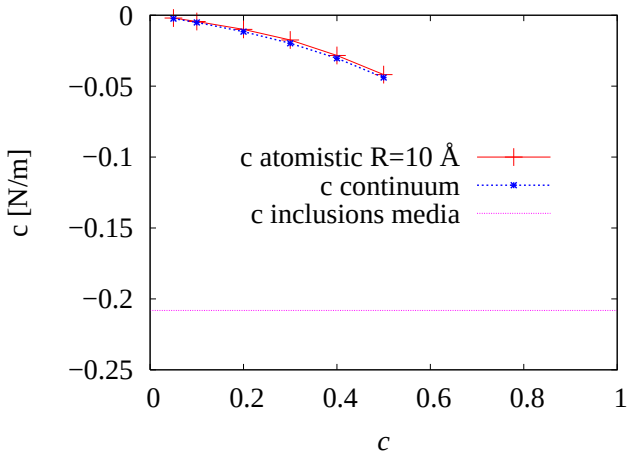
Results

- overall good agreement between atomistics and continuum
- Hashin-Shtrikman bounds fully satisfied for both linear coefficients
- interesting enough continuum predictions are well verified even for high c-values (while expected to work basically in the regime of dilute dispersions)





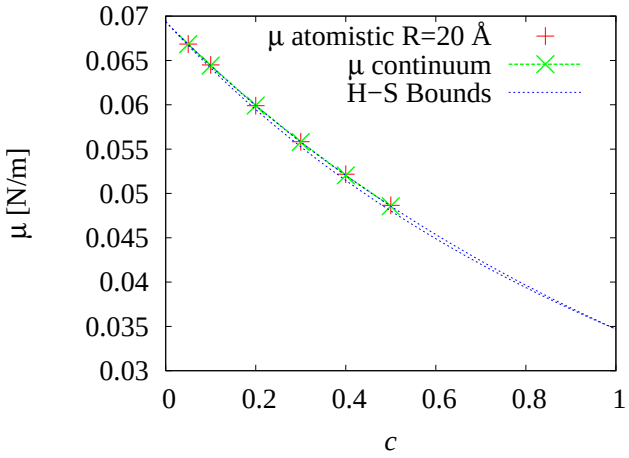


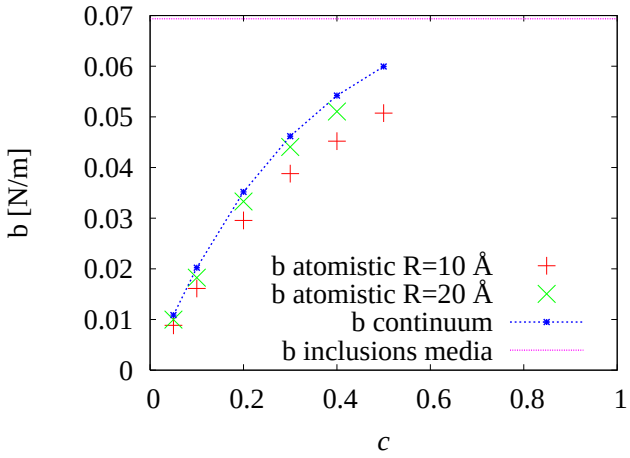


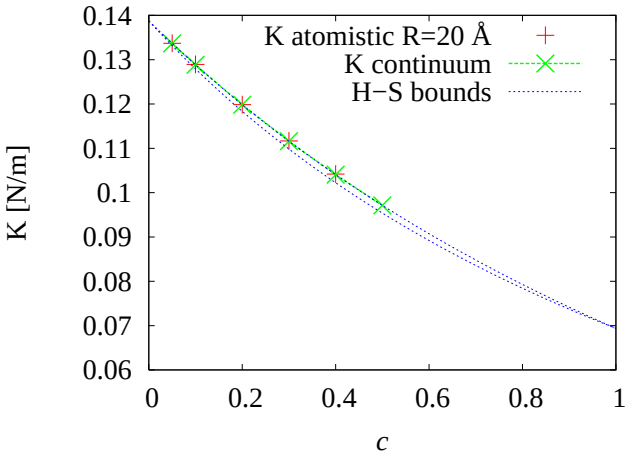
Atomistic results *vs*. continuum prediction: **inclusions softer than matrix**

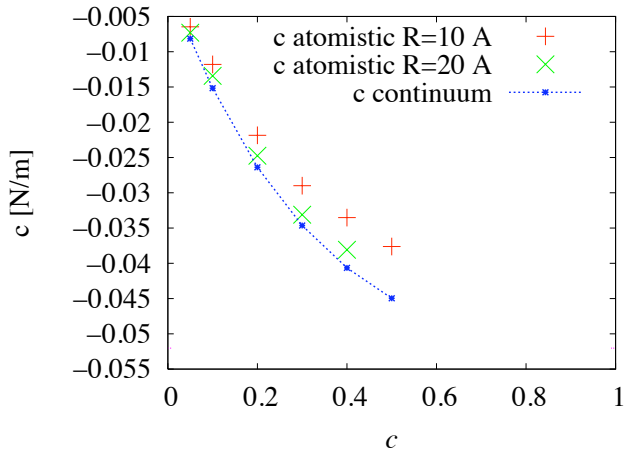
Results

- agreeemnt between continuum and atomistics found only for larger inhomogeneities $R \simeq 20$Å
- for positive elastic contrast a size-dependence of the elastic behavior observed atomistically



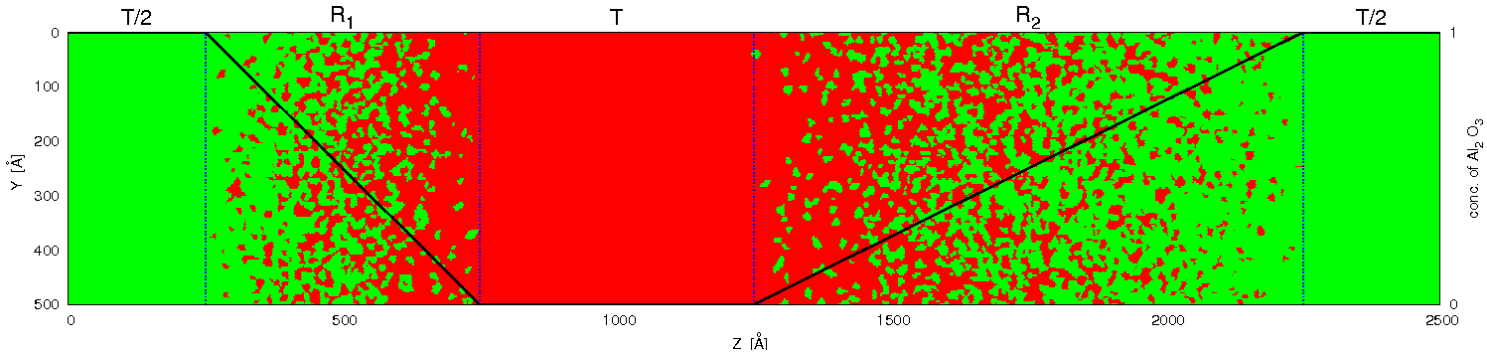




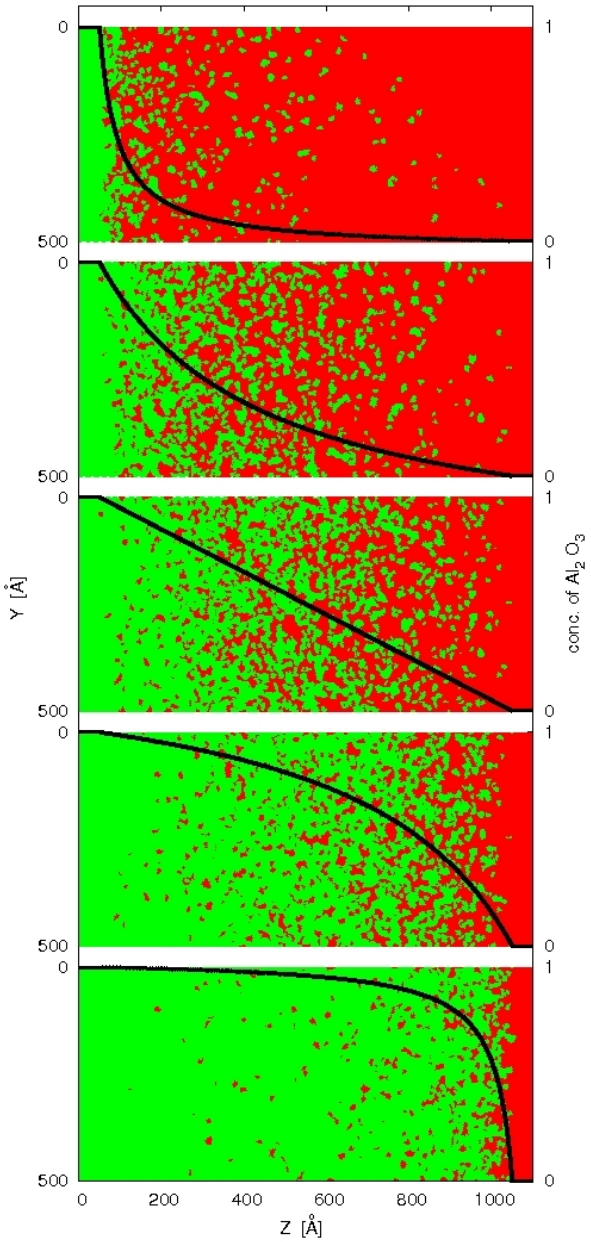


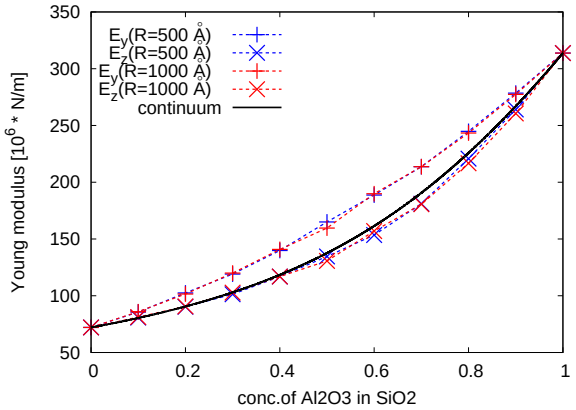
Nano-graded interfaces

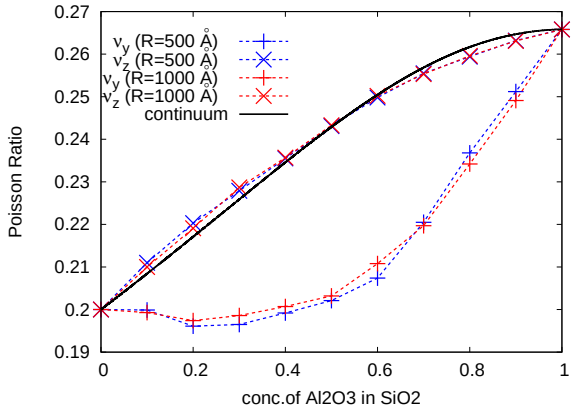
- **structural model**
  1. two elastically different media placed onto an honeycomb lattice
  2. periodic boundary conditions along z
  3. random dispersions of grains
  4. arbitrarly-shaped concentration profiles



- **elasticity**
  1. *matrix*: isotropic linear material *inhomogeneities*: isotropic linear material
  2. two linear moduli: E and ν
- **simulation protocol** *(large-scale simulations:* $\sim 10^5$ *atoms)*
  1. plane strain deformations - strain evaluated just in the interface region (after relaxation)
  2. atomic degrees of freedom relaxed by dumped dynamics
  3. stress in the interface region evaluated as average of atomic-level stresses (virial formulation)
  4. stiffness coefficient obtained by the consitutive equation $\hat{T} = \mathcal{C}\hat{\epsilon}$
  5. elastic moduli: $\nu = \frac{C_{12}}{C_{11}}$ and $E = \frac{C_{11}^2 - C_{12}^2}{C_{11}}$







Results

- continuum results obtained within an *effective medium theory* (EMT): graded interface replaced by an isotropic slab with average properties
- observed anisotropic elastic behavior
- EMT only valid for elasticity along the growth direction

Conclusions

1. **conceptual mapping** of the constitutive linear and nonlinear equations of the continuum elasticity theory onto a lattice model
2. atomistic structure exploits the **actual nano-structure** (single/multiple inhomogeneity/ies and graded interfaces)
3. **notion of length-scale** naturally introduced
4. investigate by computer experiments possible **scale effects** on the elastic behavior of nanostructured materials.
5. **anisotropic behaviors** (due to nano-structure) properly captured

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Nonlinear elasticity in nanostructured materials

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Abstract
We elaborate on a blended continuum/atomistic theoretical picture of the nonlinear elastic properties of nanostructured materials, looking at diverse aspects such as dispersions of inhomogeneities within a matrix, random or graded nanograined materials, two-dimensional atomic sheets. In particular, we discuss the possible onset of length-scale effects and we establish the limits and merits of continuum versus atomistics. While most situations here discussed correspond to model systems, the main conclusions have a paradigmatic relevance and indeed apply to most nanomaterials of current interest.

This article was invited by S Washburn.

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