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ON THE MULTI-SCALE MODELING OF THE ZHU'S NANOROD

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This paper discusses the mechanical properties of the Zhu's nanorod, undergoing a uniaxial tension, via two atomistic-continuum coupling methods. The first method is the quasicontinuum method, which bridge the length scales in a single model with the aid of the finite element method, and the second method is the embedded atom method. Both methods are adequate for multi-scale description of the nanorod properties and offer results closer to the realistic behavior of the nanorod than those furnished by the classical atomistic method.

Key words: Zhu's nanorod, multi-scale models, quasicontinuum method, embedded atom method, uniaxial tension.

1. INTRODUCTION

According to Richard Feyman, the term "nanotechnology" was first used by N. Taniguchi in his paper (1974), "*On the basic concept of nanotechnology*." In the last time, nanoengineering and nanomanufacturing have been extensively discussed by Eric Drexler through the Foresight Institute [1].

Nanoscience involves multiple length and time scales and the combination of different materials and molecules. This means that fundamental methods that were developed in separate contexts will have to be combined and new ones invented. This is why an alliance of researchers in nanoscience with those in applied mathematics and computer science will be necessary to the success of theory, modeling, and simulation in nanoscience [2]. Now, it is not very clear what theories from the disparate subdisciplines of physics, mechanics, surface science, material science and engineering, chemistry, mathematics and computational sciences will be successful in the new context being created by novel experiments.

Material structures forms spontaneously at all size scales [3]. Electrons, protons and neutrons form atoms, and atoms form clusters and molecules. These building blocks form mesostructures, examples range from the classic Guinier–Preston zones in aluminum–copper alloys [4] to lipid bilayers, and to more recently discovered strain-induced quantum dots [5, 6].

In this paper we study the uniaxial tension of the Zhu's nanorod by using two methods. The first method is the quasicontinuum method (QCM), which is an attempt to bridge the length scales in a single seamless model with the aid of the finite element method [7]. The basic idea of QCM is carried forward to dynamics, in that representative atoms are chosen, and a finite element mesh is constructed with these as nodes [8], [9]. For example, the plastic deformation of metals involves the core structure of individual dislocations, interactions of dislocations with each other and with grain boundaries. The prediction of plastic behaviour requires modeling at different scales where input to a model at a higher scale will be the output form to the model at a lower scale (nanoscale $10^{-10}-10^{-9}\,\mathrm{m}$, mesoscale $10^{-8}-10^{-6}\,\mathrm{m}$, and macroscale $>10^{-4}\,\mathrm{m}$) [7].

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All the atoms of a solid are the same species and the mass of each of them is m. The classic expression of the Hamiltonian is a sum of the potential energy, the kinetic energy and the potential of external sources [10] as

$$H(x_1, x_2, ..., x_N, p_1, p_2, ..., p_N) = E(x_1, x_2, ..., x_N) + \sum_{i=1}^{N} \frac{p_i^2}{2m} - \sum_{i=1}^{N} f_i x_i , \tag{1.1}$$

where x_i is the deformed position, p_i is the momentum, f_i is the external force of the atom i, and N is the total number of atoms. The potential energy E is obtained from an atomistic formulation. The motion equations are

$$\dot{p}_i = -H_{,x_i} = -E_{tot,x_i} + f_i , \quad \dot{x}_i = H_{,p_i} = \frac{p_i}{m} , \tag{1.2}$$

where comma means the differentiation with respect to the specified variable and dot means differentiation with respect to time.

The molecular dynamic simulations usually involves billion-atom. The goal of the dynamic quasicontinuum method is to develop an approximate Hamiltonian for a reduced degrees of freedom model [7]. So, the method selects a number of representative atoms whose positions and momenta are the reduced degrees of freedom. The position and velocity of any other atom may be obtained using a finite element interpolation from the mesh constructed with these representative atoms as nodes [7].

The second method is the embedded atom method (EAM) (Kröger *et al.* [11, 12]). The method is based on the fact that in metals the conduction electrons are not localized about the nuclei, and the energy depends on the local electron density, resulting in forces between particles that are many body in character, rather than simply pairwise additive [13–16]. Accordingly, let us consider two contributions to the potential energy E of the whole system made up of N particles. There is a binary interaction term E_b through a two-body interaction potential Φ as a function of the distance between interaction particles and a term of an embedding functional F, which produces the effect of the electronic "glue" between interaction particles [11, 12]

$$E_b = Ne_b = \sum_{i=1}^{N} \left(\frac{1}{2} \sum_{j \neq i}^{N} e_{ij} \Phi(r^{ij}) + \mathbb{F}(\rho_i) \right), \tag{1.3}$$

where e_b represents a "binding energy" per particle, $r^{ij} = r^i - r^j$ is the relative position vector between particles of coordinates r^i and r^j, and e_{ij} the interface coefficients which are set to unity for the bulk metals and different from unity in the contact zones. The quantity $\mathbb{F}$ is a nonlinear function of the local embedding density ρ_i of atoms $i = 1, 2, ..., N$, constructed from the radial coordinates of surrounding particles

$$\rho_i == \sum_{i=1}^{N} w_{ij} W(r^{ij}) = W(0) + \sum_{j \neq i}^{N} w_{ij} W(r^{ij}) , \tag{1.4}$$

where $W(r)$ is a weighting function. The coefficients w_{ij} characterize the strength of interaction between particles of the same and to different materials.

2.THE QUASICONTINUUM METHOD

We recall that the ideal goal is to simulate the behaviour of structures with the only constitutive law being the interactions between the atoms. The maximum resistance of a material to deformation can be determined by regarding the material as an assembly of interacting atoms, the cohesive or binding energy of

which is known for arbitrary interatomic separations, the strength then being specified by an inflexion point in the variation of this energy with deformation (strain).

The first step is the selection of R representative atoms whose positions will be the unconstrained degrees of freedom of the system [7]. The position x_i^h of any other atom is obtained by interpolation

$$x_i^h = \sum_{\alpha} N_\alpha(X_i) x_\alpha \,, \tag{2.1}$$

where $N_\alpha(X_i)$ is the shape function centred on the representative atom α, which is a finite element (FE) node, evaluated at the undeformed position X_i of atom i. The next step in the process is to develop an approximate potential energy E that depends only on the positions of the representative atoms. Static equilibrium at zero temperature follows by minimizing the total energy or, equivalently, finding the zero-force positions for every degree of freedom where the force on a degree of freedom is the derivative of the total energy with respect to the degree of freedom coordinate (Curtin and Miller [16]).
For this it is assumed as

$$E = \sum_{i=1}^{N} E_i = \sum_{\alpha=1}^{R} n_\alpha E_\alpha \,, \tag{2.2}$$

where n_α are the unknown weights, which can be interpreted as the number of atoms represented by the representative atom α. The energy of the representative atom E_α may be computed in two different ways, depending on the nature of the atomic environment of the atom α. Firstly, far from the defect core, the atomic environments are nearly uniform and then it is possible to make a local calculation of the energy. The state of deformation is homogeneous and is characterized by the local deformation gradient F. The Bravais lattice vectors of the deformed configuration b_α are obtained from those in the reference configuration B_α as $b_\alpha = FB_\alpha$. Secondly, in regions that suffer a state of nonuniform deformation, the energy is computed by building a crystallite that reflects the deformed neighborhood from the interpolated displacement fields. The atomic positions of each atom are given by $x = X + u(X)$, where the displacement field u is determined from finite element interpolation.

The transition region between the atomistic and continuum regions is shown in Fig. 2.1 [17]. On one side of this region is the atomistic region in which every atom is explicitly represented and treated using interatomic potentials. On the other side, there is a FE mesh with its associated nodes in which, the nodes sit on atomic lattice sites although not all atom sites are nodal positions. At the interface between the FE nodes and the atoms there is a one-to-one correspondence between atoms and nodes on the FE mesh. Away from the interface on the continuum side, the FEM nodes become increasingly sparse and the corresponding elements become larger. There is a 'pad' region where pseudoatoms exist on the continuum side of the interface and overlap physical space with the FEs. Some of the 'pad' atoms coincide with the FE nodes while others lie within the elements.

In the absence of externally applied forces, forces on each atom are obtained as

$$f_i = -\frac{\partial E}{\partial x_i} \,. \tag{2.3}$$

The availability of the total energy and the forces permits application of the conjugate-gradient method to minimize the total energy to obtain the equilibrium atomic configuration as a function of applied forces and imposed displacements on specific atoms. In the atomistic calculations, there is no direct consideration of the continuum concepts of strain or displacement. We follow the motion of individual atoms without reference to their original positions. In fact, the "deformations" that can occur in atomistic simulations explicitly violate many assumptions about the continuity of deformations, the invertibility of deformations and other hypotheses of continuum mechanics [17].

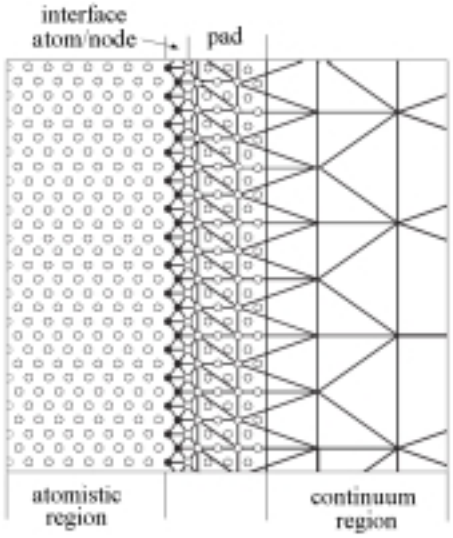

Fig. 2.1. The atomistic/continuum transition region (after Curtin and Miller [17]).

3. THE EMBEDDED ATOM METHOD

A simple model for the binary potential function $\Phi(r)$ is the radially symmetric short ranged attractive (SHRAT) potential [11, 12]

$$\Phi(r)=\frac{\phi_0}{r_0^4}\left[3(h-r)^4-4(h-r_{\min})(h-r)^3\right],\ \text{for}\ r\le h, \tag{3.1}$$

and $\Phi(r)=0$ otherwise, where ϕ_0 is an energy scale, r_0 a length scale and h an interaction range. The expression (3.1) was used by Kröger and Hess [12] to study solid friction and the mechanical behavior of metals. We will see that the same expression (3.1) will help us to analyze the mechanical behavior of the uniaxial tension of the Zhu's nanorod.

The minimum of the potential is located at $r_{\min}=2^{1/6}r_0\simeq 1.123r_0$, and the well depth of potential is $\Phi(r_{\min})=-\frac{\phi_0}{r_0^4}(h-r_{\min})^4$, as for a Lennard-Jones potential. We add the normalized Lucy's weight function [12]

$$W(r)=W_0(1+3\frac{r}{h})(1-\frac{r}{h})^3,\ \text{for}\ r\le h,\ W_0=W(0)=\frac{105}{16\pi h^3}, \tag{3.2}$$

and a simple parabolic embedding potential $\mathbb{F}$ [12]

$$\mathbb{F}(\rho)=F_0\phi_0 r_0^6[(\rho-\rho_{des})^2-(W_0-\rho_{des})^2), \tag{3.3}$$

where $\rho_{des}=\frac{1}{r_0^3}=n=\frac{N}{V}$ is the desired embedding density which equals the particle number density, for $h=1.6r_0$ and fixed temperature, and F_0 is the embedding strength.

4. THE ZHU'S NANOROD

The study of mechanical behavior of the nanorod is a good example of interatomic interactions. Consider the Zhu's nanorod constructed by Zhu *et al*. [18], and composed of 144 atoms (48 SiO_2) and shown in Fig. 4.1. The construction first involves the formation of hexagonal planar six rings, Si_6O_{18}. As shown in Fig. 4.1b, each Si_6O_{18} ring contains six corner-linked SiO_4 tetrahedra, where each tetrahedron has two bridging oxygen atoms that are shared with two neighboring tetrahedra. For each Si_6O_{18} ring, there are six Si atoms and six O atoms lying within the plane of the ring, and six O atoms each above and below the plane, respectively.

Then, the nanorod is assembled by stacking such layers one over another. Each interior ring is linked to two adjacent rings by sharing O atoms. The nanorod ends are rings in which the six Si atoms are connected alternately by a bridging oxygen or two oxygens, in the manner shown in Fig. 4.1c. Each end layer has 21 atoms, whereas each interior layer has 24 atoms. An eight-layer rod, therefore, has a total of 144 atoms. The ratio of Si to O atoms in a nanorod is 1:2. Though the nanorod is an idealized structure created by Zhu *et al*. [18] for the study of atomistic processes and mechanical behavior in structures that are neither cluster-like nor bulk. The rod is a stand-alone cylindrical assembly of hundreds of atoms, which retain the characteristic structural unit of a quartz. The geometric features can be scaled up to those of a wire, tube, or column. Similar crystal structure occurs in nature, for example, in cyclosilicate mineral beryl [18].

To characterize the stress state of the nanorod we take the sum of all forces acting on the cross section divided by the initial cross section area $A_0 = 4\pi d_\infty^2 = 88.9\text{A}^{\circ 2}$, where $d_\infty = 2.66\text{A}^\circ$ is the nominal length of a layer (ring). The mechanical behavior of the nanorod is analyzed by using atomistic-continuum coupling methods QCM and EAM. The results are compared to those obtained by using the classical atomistic method (CM), in which potentials are expressed as a sum of a short-range interaction of the form $\exp^{-6}$ and a Coulomb interaction with fixed charges. The experimental measurements of the relaxed bond distances and bond angles are $d_{\text{Si-O}} = 1.61\text{A}^\circ$, $\theta_{\text{O-Si-O}} = 109.4^\circ$ and $\theta_{\text{Si-O-Si}} = 143.7^\circ$ respectively [18].

Fig. 4.2 depicts a comparison of the stress–strain law of the nanorod obtained by using QCM and EAM. As a reference result it is considered the CM diagram. The EAM and QCM yield to higher tensile critical strength and smaller critical strain than the CM simulation. The QCM yields to lower tensile critical strength and higher critical strain than the EAM simulation. This is explained by taking into consideration into EAM of the effect of the electronic "glue" between interaction particles. We mention that the experimental value for the tensile critical stress (55.2GPa) and the critical strain (0.242) for the Zhu's nanorod are closed to the value given by EAM and QCM [18].

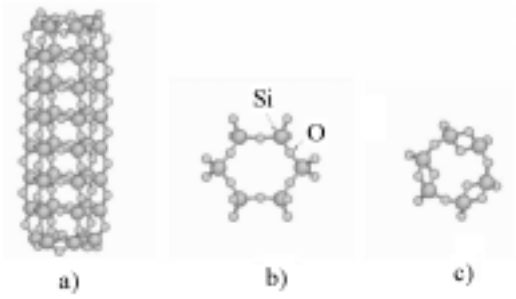

Fig. 4.1. Structure of the Zhu's nanorod: a) a relaxed nanorod, b) an interior ring, c) an end ring.

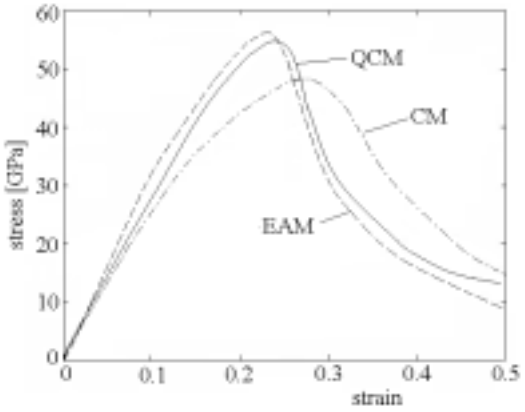

Fig. 4.2. The constitutive law for uniaxial tension of nanorod using EAM, QCM and CM.

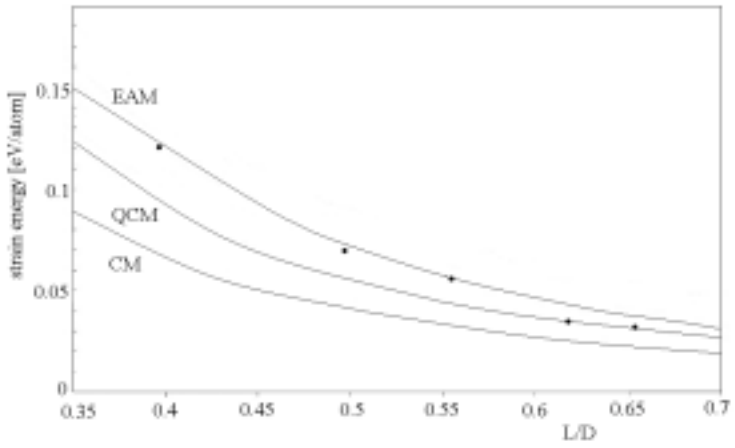

Fig. 4.3. The straia energy of the nanorod subjected to uniaxial tension.

The variation of the strain energy of the nanorod with respect to the ratio of length L to the diameter D, is presented in Fig. 4.2 for different ratios L/D for the computational methods EAM, QCM and CM. Dots represent the experimental results [18]. It is assumed that the nanorod behaves elastically in tension for all ratios. Clearly, the values of the energy strain are higher in the case of the coupling methods then those given by CM, being in a good agreement to the experimental data represented by dots.

5. CONCLUSIONS

The macroscopic theories attempt to "model" the smaller scale phenomena into "effective" properties or "constitutive laws", but the macroscopic phenomena such as fracture, depend on the details of smaller scale phenomena. On the other hand, the atomistic description does not provide for the determination of macroscopic behaviour, since the higher scale interactions operate to drive large-scale behaviour. The methods of coupling the length scales are intensively developed to a realistic modeling of materials [12].

This paper has compared two different atomistic-continuum coupling methods, QCM and EAM, by studying the mechanical properties of the Zhu's nanorod subjected to uniaxial tension.

The comparison shows the main differences between these methods and CM [18]. As we see from Fig. 4.2, the results agree to the experimental tensile critical stress which is 55.2GPa, and to the experimental critical strain which is 0.242. Also, the coupling methods QCM and EAM offer results closer to the realistic

behavior of the nanorod (Fig. 4.3). The study of mechanical behavior of nanorods plays an important role in nanotechnology, in the prospect of actual specimens on which mechanical deformations can be performed. For example, the silica nanowires, with 5–100nm diameters, are recently synthesized by Pan *et al.* [19].

The QCM and EAM has been used to investigate a large range of problems such as fracture, nano-identation, dislocations and grain boundary structure [17].

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