A Multi-Scale Computational Method Integrating Finite Element Method with Atomic Interactions of Materials

Bin Gu^{1,2,3}, L. C. Zhang², Weifeng Yuan¹ and Youjun Ning¹

Abstract: Bridging the atomic and continuous analyses is an important aspect in multi-scale mechanics. This paper develops a computational method to integrate the atomic potential of a material with the finite element method. The novelty of this method is that strain energy is calculated from the atomic potential without the assumption in the Cauchy-Born rule that deformation in a virtual atomic cell is homogeneous. In this new method, the virtual atomic cell deformation is interpolated according to the continuum displacements associated with the shape functions. The applications of the method to single crystal Si and Ge bars under uniaxial tension and compression show that with a proper construction of the virtual atomic cell, the Young's modulii in the <100>, <110> and <111> directions obtained are in good agreement with the experimental measurements and MD simulations in the literature. Moreover, the simulated material's response to tension and compression is consistent with the interatomic interactions.

Keywords: Multi-scale computation, FEM, Atomic potential, Virtual atomic cell

1 Introduction

It has been very common that scale effect spans from meter to nanometer in length and from hour to femto-/pico-second in time. Due to their intrinsic disadvantages, computational methods suitable for a specific scale are unable to correctly capture the behavior of materials across multiple scales. For instance, a molecular dynamics (MD) simulation, limited by its computational capacity and error truncation/accumulation hurdle, can only model the size under micrometer while the continuum assumption in the finite element method (FEM) becomes invalid when

¹ School of Manufacturing Science and Engineering, Southwest University of Science and Technology, Sichuan 621010, China

² School of Mechanical and Manufacturing Engineering, The University of New South Wales, NSW 2052, Australia

³ Corresponding author: Prof. Bin Gu. Tel: +86-816-6089898, Email: gubin@swust.edu.cn

the scale reaches the atomic range [Zhang (2010)]. Therefore, multi-scale modeling which aims to bridge the gap has triggered tremendous research attention in the past decades [Ghanbari and Naghdabadi (2009); Ojeda and Cagn (2010)].

Following the strategy of direct coupling, many methods have been proposed to address the atomistic/continuum coupling problems, such as the quasi-continuum (QC) methods with and without a ghost force correction [Tadmor, Ortiz and Phillips (1996); Shenoy, Miller, Tadmor, Phillips and Ortiz (1998); Shenoy, Miller, Tadmor, Rodney, Phillips and Ortiz (1998); Miller and Tadmor (2002)], the concurrent coupling of length scale (CLS) method [Broughton, Abraham, Bernstein and Kaxiras (1999); Rudd and Broughton (2000)], the FEAt model [Curtin and Miller (2003)] and the coupling of atomistics and discrete dislocation (CADD) method [Curtin and Miller (2003); Shilkrot, Miller and Curtin (2002); Shilkrot, Miller and Curtin (2003)]. In these direct coupling methods, a domain for analysis is divided into multiple regions handled by different computational methods respectively. In general, MD is applied on atomistic regions to explore complicated mechanisms, and continuum computational methods such as FEM are applied in continuum regions to model large volumes so as to provide an appropriate background for the MD simulation. Because MD is a non-local computational method, transition regions are established between the atomistic and continuum regions so that all atoms in the atomistic regions have full complement of neighboring atoms. Usually, the atomic scale deformation in the transition regions, called pad atoms, is interpolated from the displacements of continuum regions. The difference among these methods is in their ways to treat the continuum and the transition regions. In the QC methods, the continuum region is simulated using the FEM incorporating the interatomic potential in terms of the Cauchy-Born (C-B) rule. In the CLS method, the traditional linear elastic FEM is applied to treat the continuum region. In the FEAt model, the transition region and continuum region are dealt with nonlocal and nonlinear FEM, respectively. In the CADD method, on the other hand, the plasticity in the continuum region is accounted by discrete dislocations. A meshless computational method [Gu and Zhang (2006)] has also been adopted to model the continuum regions in the direct coupling methods on the basis of the QC method. By using bridging scale decomposition, Wagner and Liu (2003) realized the coupling of atomistic and continuum simulation, in which the deformation of the entire domain is first solved from the C-B rule based FEM, followed by obtaining the supplementary deformation from MD simulation and superposing to the atomistic region. The difference between the direct coupling methods in terms of the treatment of the transition region depends on whether the pad atoms are included in the atomistic energy calculation. When the pad atoms are excluded, such as in the QC and CLS methods, a unified total energy functional can be obtained. It requires much less computational resources to find its solutions, but inevitably gives rise to the physically meaningless ghost force. When the atomic potential accounts for the contribution of the pad atoms, these atoms are treated as fixed atoms in MD simulations. Meanwhile, the interface atoms are regarded as fixed boundary conditions in the modeling of continuum regions. In so doing, the ghost force can be eliminated while an iterative computation scheme between the atomistic and continuum solutions is needed. Although the direct coupling methods can cope with different scales separately, it is difficult in the simulation to foresee the atomistic and continuum regions when deformation in a material is complicated, especially when the region boundaries change during a deformation process. The size of the atomistic regions may exceed the limit of the MD simulation, leading to low computational efficiency. Moreover, the gap between different time scales is unlikely to be eliminated.

Much effort has been dedicated to develop multi-scale methods in the continuum mechanics framework where both the length and time scales are computationally practical and efficient. To this end, the basic equations in continuum mechanics are often modified to accommodate the information extracted from smaller scales. Including the work conjugates of the slip rate and slip rate gradient in the principle of virtual work, Fleck and Hutchinson (2001) established a strain gradient theory in which the higher-order stresses and additional boundary conditions were introduced to investigate the size effect problem. McVeigh and Liu (2009) derived a set of multi-resolution governing equations with the introduction of microstresses in different scales within a material. This continuum approach was used to analyze the fracture toughness of ductile reinforced brittle composites. Due to the intrinsic link between the atomic potential and the strain energy, the strain energy in continuum mechanics is often replaced by the atomic potential to achieve the atomistic/continuum coupling. To date such replacement is generally implemented in terms of the C-B rule [Milstein (1980)] by which the strain energy is assumed to be equal to the atomic potential of atoms in a material and all the atoms in the virtual atomic cell (VAC) constructed around a material point undergo homogeneous deformation. Based on the C-B rule, the equilibrium equations of a continuum model can be derived from the principle of the minimum potential without the need of a constitutive relationship. On the contrary, the constitutive relationship and material constants can be deduced from the interatomic potential via the work conjugate of stress and strain. The C-B rule based FEM was firstly applied in the QC method to handle the deformation of continuum regions. It was further extended to the virtual internal bond (VIB) model by Klein and Gao (1998) in which the real lattice structure of material was replaced by the bond density distribution function while maintaining the assumption of homogeneous deformation of bonds in the VAC. As has been pointed out in [Zhang, Huang, Geubelle, Klein and Hwang (2002)], homogeneous deformation in the VAC is appropriate only when lattice structure of materials is centrosymmetric, as otherwise the assumption may give rise to unphysical or incorrect results. For a non-centrosymmetric crystal structure, an interpenetration technique using simple Bravais lattices as sublattices should be applied to construct an assembly [Zanzotto (1996)]. In this method, atoms belonging to the same sublattice undergo uniform deformation and the difference of deformation between two sublattices can be represented with a rigid body displacement deduced according to the minimum energy of the VAC. Compared with the direct coupling methods which are merely a mathematical combination of different methods, the information transfer methods are more physically meaningful. Difficulty in this kind of methods is to establish the correct link between two scales through properly selected parameters, which requires a deep understanding of the mechanisms and physics of the behavior of a material.

This paper develops a continuum computational method (CCM) incorporating atomic potential which does not need the assumption of uniform deformation in the VAC. Instead, atom displacements in the VAC will be obtained through nodal displacement interpolation using the shape functions. It is therefore suitable for both centrosymmetric and non-centrosymmetric crystal structures. The basic idea and procedure of our CCM will be depicted in the next section. A bar subjected to a uniaxial tension/compression will be used as an example to illustrate the application of the method. Numerical results will be discussed and compared with the experimental and MD results to verify the feasibility of this new method.

2 Principle and Procedure

Our CCM is based on the traditional FEM. For simplicity and convenience, we use a single element to demonstrate the implementation procedure and principle of the method.

First, the displacement field within an element can be approximated by the shape functions and nodal displacements as

$$u = \sum_{i=1}^{N_{EN}} N^{i}(X) U^{i}$$
(1)

in which U^i and $N^i(X)$ denote the displacement vector and shape function of node i. N_{EN} is the number of element nodes. Neglecting the dynamic effect, the potential energy in the material can be expressed as

$$\Pi = \sum w(u) \, dv - \sum_{i=1}^{N_{EN}} U^{iT} . F^{i}$$
(2)

where w(u) represents the strain energy density and F^i is the nodal force vector. Then the principle of the minimum potential energy gives

$$\delta \Pi = \sum_{j=1}^{N_{GP}} \left[\alpha^{j} (\delta u^{T} \cdot \frac{\partial w^{j} (u)}{\partial u}) \right] - \sum_{i=1}^{N_{EN}} \delta U^{i^{T}} \cdot F^{i} = 0$$
(3)

when the Gauss integration scheme is adopted. In Eq. (3), α^{j} and N_{GP} are the weight of Gauss point j and the number of Gauss points, respectively. In our CCM, the strain energy density in Eq. (3) is not calculated from the stress and strain at the Gauss point, and therefore the constitutive relationship of continuum mechanics is not needed. Instead, it is deduced from the energy equivalence that the strain energy is equal to the interatomic potential of a material according to the C-B rule. To do so, a virtual atomic cell in which the atoms before deformation are arranged according to the crystal structure of material is constructed with the Gauss point in the centre. The strain energy density can then be calculated by

$$w(u) = \frac{1}{V_{VAC}} \sum_{\substack{m,n=1\\m \neq n}}^{N_{RA}} E_{mn}(u)$$
(4)

where V_{VAC} is the volume of the VAC before deformation with N_{RA} being the number of atoms in the VAC and $E_{mn}(u)$ is the interatomic potential function.

Rewriting Eq. (3) in terms of the displacement of the VAC atoms and using Eq. (1), the balance equations associated with the strain energy density can be obtained as

$$\sum_{j=1}^{N_{GP}} \left[\alpha^j \sum_{k=1}^{N_{RA}} \left(N^i(X^k) \frac{\partial w^j(u)}{\partial u^k} \right) \right] = F^i \quad (i = 1, 2, \dots N_{EN}).$$
⁽⁵⁾

Substituting Eq. (4) into Eq. (5), the equilibrium equations of our new CCM for one element finally becomes

$$\sum_{j=1}^{N_{GP}} \left[\frac{1}{V_{VAC}} \alpha \sum_{k=1}^{j} \left(N^{i}(X^{k}) \sum_{\substack{m,n=1\\m \neq n}}^{N_{RA}} \frac{\partial E_{mn}^{j}(u)}{\partial u^{k}} \right) \right] = F^{i} \quad (i = 1, 2, \dots N_{EN}).$$
(6)

The above equations are nonlinear; thus a numerical method, such as the Newton-Raphson method or the arc-length method, should be applied for a solution.

Compared to the computational methods based on the C-B rule, our CCM stated above has the same form of equilibrium equations. The difference lies in the way

to obtain the bond length after deformation, i.e., the atom position after deformation. According to the C-B rule, when a lattice structure is centrosymmetric, the bond length after deformation can be described by $r^{mn} = |F.R^{mn}|$ in which R^{mn} is the undeformed vector from atom m to atom n and F denotes the deformation gradient at the central point of the VAC. In our CCM, however, $r^{mn} = |R^{mn} + u^n - u^m|$. It is easy to see that our CCM and the methods based on the C-B rule give rise to the same results when the deformation gradient in the VAC is uniform. When deformation gradient becomes non-uniform in the VAC, nevertheless, the formula in our CCM is more accurate than that from the C-B rule where only the deformation gradient at the central point is involved. As can be seen from the procedure, meshless technique can be readily incorporated into our CCM, provided that the displacement field is constructed in the same way as in meshless methods. Moreover, any dynamic effect can be taken into account when the kinematic term is added in the potential energy. It is noted that the term $\sum_{m,n=1}^{N_{RA}} \frac{\partial E_{mn}^{j}(u)}{\partial u^{k}}$ in Eq. (6) $m \neq n$ represents the force on the kth atom in the VAC. Therefore, the equilibrium equa-

tions of the CCM are also similar to those in the fully non-local QC method [Knap and Ortiz (2001)] where the internal force on a node was mathematically assumed to be approximated by the forces of a cluster of atoms around the node. Hence, the equilibrium equations of our CCM are physically more reasonable.

3 Results and Discussion

First, let us apply the CCM to simulate and predict the mechanical response of a bar to uniaxial tension and compression, using the Young's modulus of the bar material as a measure to validate this method. Assume that the bar has a length of L and cross-section area of A with one end fixed and force F on the other end, as shown in Fig. 1.



Figure 1: Configuration of a bar subjected to uniaxial tension

Assumed that only the displacement component in X direction is non-zero and is the function of coordinate variable X. The whole bar can then be modeled as a two-node element with the following shape functions

$$N^{1}(X) = (L - X)/L \text{ and } N^{2}(X) = X/L.$$
 (7)

With the consideration of the boundary conditions, the equilibrium equations for this case can be simplified from Eq. (6) and has the form of

$$\sum_{j=1}^{N_{GP}} \left[\frac{A}{V_{VAC}} \alpha \sum_{k=1}^{j} \left(N^1(X^k) \sum_{\substack{m,n=1\\m \neq n}}^{N_{RA}} \frac{\partial E_{mn}^{j}(u)}{\partial u^k} \right) \right] = F.$$
(8)

If the bar material is single crystal Si which has a diamond cubic lattice structure, the three dimensional virtual atomic cell can be constructed around each Gauss point by piling up the unit cell of Si crystal structure along three basic lattice vectors, i.e., [100], [010] and [001] directions. The numbers of the unit cells in the three directions are N_1 , N_2 and N_3 , respectively. Fig. 2(a) schematically illustrates the construction of the VAC on the (a) plane for <100> Si where the [100] direction of the VAC is the same as the coordinate *X*-axis. Since monocrystalline Si is an anisotropic material, Young's modulii in three directions, namely <100>, <110> and <111> directions, will be different. To build up the VACs for <110> Si and <111> Si, the VAC of <100> Si is rotated around the center point of the VAC, i.e., Gauss point, so that the *X* direction is aligned with the <110> and <111> directions respectively, as shown in Fig. 2(b) for <110> Si.



Figure 2: Schematic illustration of the construction of VAC on (001) plane (a) For <100> Si, and (b) For <110> Si

Generally, the Tersoff potential is the proper interatomic potential for Si-Si bond [Zhang and Tanaka (1998); Zhang and Tanaka (1999)], and is therefore adopted in

the present CCM. Hence [Tersoff (1989)],

$$E_{mn}(u) = E(r^{mn}) = \frac{1}{2} f_c(r^{mn}) \left[f_R(r^{mn}) + b_{mn} f_A(r^{mn}) \right]$$
(9)

Where

$$f_{R}(r) = Ae^{(-\lambda r)}, \quad f_{A}(r) = -Be^{(-\mu r)},$$

$$f_{c}(r) = \begin{cases} 1 & r < R \\ \{1 + \cos\left[\frac{\pi(r-R)}{S-R}\right]\}/2 & R < r < S \\ 0 & r > S \end{cases}$$

$$b_{mn} = [1 + (\beta \zeta_{mn})^{\eta}]^{-1/2\eta}, \quad \zeta_{mn} = \sum_{l \neq m,n} f_{c}\left(r^{ml}\right)g\left(\theta_{mnl}\right)$$

$$g(\theta_{mnl}) = 1 + \left(\frac{c}{d}\right)^2 - \frac{c^2}{d^2 + [h - \cos(\theta_{mnl})]^2}, \quad \cos(\theta_{mnl}) = \frac{r^{mn^2} + r^{ml^2} - r^{nl^2}}{2r^{mn}r^{ml}}.$$

In the calculation, If not specified, $L = 1 (\mu m)$, $A = 1.0 \times 10^{-14} (m^2)$, $N_{GP} = 20$, $N_1 = N_2 = N_3 = N = 1$, and the Newton-Raphson method can be used to solve the nonlinear Eq. (8). Parameters of the Tersoff potential for Si together with the lattice constant a are listed in Table 1.

Table 1: Parameters in Tersoff potential and lattice constants for Si and Ge [Tersoff (1989)]

	Si	Ge
A (eV)	1.8308×103	1.7690×103
<i>B</i> (eV)	4.7118×102	4.1923×102
λ (Å-1)	2.4799	2.4451
μ (Å-1)	1.7322	1.7047
β	1.1000×10-6	9.0166×10-7
η	7.8734×10-1	7.5627×10-1
С	1.0039×105	1.0643×105
d	1.6217×101	1.5652×101
h	-5.9825×10-1	-4.3884×10-1
<i>R</i> (Å)	2.7	2.8
S (Å)	3.0	3.1
a (Å)	5.430	5.657

The stress-strain curves of single crystal Si under uniaxial tension and compression along <100>, <110> and <111> directions are plotted in Fig. 3, with the maximum strain less than 0.8%. As can be seen, at the small deformation stage, Si under both tension and compression exhibits explicit linear behavior in the three directions. It is at this stage that the Young's modulus is calculated when the stress is ± 0.1 GPa. Here the Young's moduli from tension and compression are found to be the same, indicating that single crystal Si has symmetric tensile and compressive behavior when the deformation is linear. Numerical results are summarized in Table 2 and compared with the experimental measurements in the literature [Ono, Kitamura, Nakajima and Shimanuki (2000)]. As expected, the maximum Young's modulus is in the <111> direction and the minimum in the <100> direction. We can see that the predicted Young's modulus is in good agreement with the experimental results along the <100> direction, has considerable discrepancy in the <110> and <111> directions. Numerical simulation is also carried out on monocrystalline Ge under uniaxial tension and compression with relevant parameters in Table 1. Similarly, the Young's moduli of Ge predicted by the CCM simulation showed the same phenomenon in comparison with the reported testing results [Wortman and Evans (1956)], as shown in Table 3. In addition, the MD simulation on the uniaxial tension of <100> Si and Ge [Komanduri, Chandrasekaran and Raff (2003)] gave the Young's modulus of 130GPa for Si and 103GPa for Ge respectively, which agree well with our numerical results.

Table 2: Young's modulii of Si from the CCM simulation and literature

E(Gpa)	CCM	Ref.
<100>	127.48	130
<110>	224.56	169
<111>	261.72	188

Table 3: Young's modulii of Ge from the CCM simulation and literature

E(Gpa)	CCM	Ref.
<100>	113.21	103
<110>	173.49	138
<111>	194.60	155

It is suspected that inaccurate prediction of Young's modulii in <110> and <111> directions may be attributed to the configuration of the VAC, including the size and



Figure 3: Stress-Strain curves at the linear deformation stage of Si under uniaxial tension and compression in <100>, <110> and <111> directions

shape. With increasing the number of unit cells in the VAC, Young's modulii of Si in three directions are obtained from our CCM and listed in Table 4. Numerical results indicate that the effect of the volume of the VAC is very small and therefore does not contribute to the discrepancy between the CCM simulation and the experimental measurements. When the VACs of <110> Si and <111> Si are constructed in the way mentioned above, its facets are not perpendicular to the coordinate axes. It may lead to errors in the atomic potential calculation because some atoms do not have proper environment of neighboring atoms, such as atom A in Fig. 2(b). Inspired by the case of <100> Si, we conclude that a VAC of which facets are normal to the coordinate axes, rather than the basic lattice vectors, can be more appropriate. Following this, a large volume of single crystal Si is first constructed using the previous method with $N \ge 10$. Then a cube of side length a' is cut from the center of the large Si crystal structure as the VAC, as demonstrated by the square at the center in Fig. 2(b) for <110> Si. With the newly-constructed VAC, numerical simulations are carried out to predict the Young's modulii of anisotropic monocrys-

talline Si when a'/a = 1, i.e., the VAC is the same size as the unit cell. The results in Table 5 show that the predicted all the Young's modulii of Si in <100>, <110>and <111> directions are in good agreement with the reference values in the literature. This means that a proper construction of the VAC has a vital influence on the numerical prediction. This new way of VAC construction will be used in the following sections.

Table 4: Young's modulii of Si from the CCM simulation with different volume of the VAC

E(Gpa)	N=1	N=2	N=3	Ref.
<100>	127.48	134.00	136.58	130
<110>	224.56	225.94	226.49	168
<111>	261.72	259.22	258.20	185

Table 5: Young's modulii of Si from the CCM simulation when the VAC is built in different methods

E(Gpa)	a'/a=1	N=1	Ref.
<100>	127.48	127.48	130
<110>	166.94	224.56	168
<111>	197.10	261.72	185

Apart from all above, the effect of the assumption that each node has only one degree of freedom (DoF) is investigated. Here a new element type is used which is still two-node element and therefore has the same forms of shape functions in Eq. (7); but now each node of the element has three DoFs, and hence three displacement components (U_x , U_y and U_z). Using the new element in the modeling, our CCM gives quite close Young's modulii of anisotropic Si in comparison to those under the one DoF assumption and to the experimental measurements, as shown in Table 6. In the case of uniaxial tension and compression, therefore, the assumption of one DoF at each node is feasible and does not reduce the simulation accuracy. However, it can be expected that an element with multiple DoFs could be more appropriate for complicate deformation status.

The response of single crystal Si to large deformation is displayed in Figs. 4 and 5 when it is subjected to uniaxial tension and compression along <100>, <110> and <111> directions. The stress-strain curves in the two figures clearly show that with

Table 6: Young's modulii of Si from the CCM simulation for different elements (NE represents the element with three DoFs at each node)

E(Gpa)	<i>a'/a</i> =1(NE)	a'/a=1	Ref.
<100>	140.67	127.48	130
<110>	167.10	166.94	168
<111>	197.56	197.10	185

the increase of deformation, the deformation linearity no longer maintains, so does the symmetry of deformation between tension and compression. A comparison between Figs. 4 and 5 indicates that the resistance to compressive deformation is much higher than that to tension when the deformation is beyond the linear phase. This material behaviour is consistent with the interaction between atoms. In the vicinity of the balance position, i.e., when the deformation is small, the repulsive force and attractive force are linear to the interatomic distance and almost equal. When the distance is far from the balance position, the repulsive force rises much faster than the attractive. Moreover, it can be seen from Fig. 4 that <100> Si has the ultimate tensile strength (UTS), of about 28GPa, which is again reasonably close to the MD result ($^{2}5$ GPa) [Komanduri, Chandrasekaran and Raff (2003)]. The UTS of Si in <110> and <111> directions are 19GPa and 15GPa respectively. In compression, the maximum ultimate compressive strength of Si crystalline is along the <111> direction but the minimum is in the <100> direction.

4 Conclusions

This paper has developed a new continuum computational method (CCM) based on the finite element method. Compared to the currently available multi-scale computational methods, the new method does not need the unreasonable assumption of uniform deformation in a virtual atomic cell. Therefore this CCM is expected to be more feasible for different length and time scales and more accurate for problems where high deformation gradient exists. Its application to a bar under uniaxial tension and compression showed that when the VAC is properly constructed, the CCM can provide good Young's modulii of single crystal materials such as Si in the <100>, <110> and <111> directions when compared to the experiment and MD simulation. It is also applied to predict the ultimate tensile strength and the anisotropic material behavior through the stress-strain curves. The comparison with the MD results indicates that the predicted material response to the uniaxial tension and compression is consistent with the atomic interaction.



Figure 4: Anisotropic stress vs strain curves of Si under uniaxial tension



Figure 5: Anisotropic stress vs strain curves of Si under uniaxial compression

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