Journal of Computational Science 10 (2015) 1–12

Contents lists available at ScienceDirect

Journal of Computational Science

journal homepage: www.elsevier.com/locate/jocs

Investigation of surface stress effect in 3D complex nano parts using FEM and modified boundary Cauchy–Born method

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ARTICLE INFO

Article history:
Received 11 May 2014
Received in revised form 29 January 2015
Accepted 21 April 2015
Available online 23 April 2015

Keywords:
Multi-scale
MBCB (modified boundary Cauchy–Born)
Molecular dynamics
Surface effects

ABSTRACT

In this paper the surface effects in 3D complex parts are investigated via classical FEM and the modified boundary Cauchy–Born method, which are continuum based theories, and the results are compared with molecular dynamics simulations. The boundary Cauchy–Born covers the weakness of the surface Cauchy–Born in modeling edge and corner elements, so the results are in better agreement with molecular dynamics simulations. Using super convergent patch recovery method, MBCB shows more precise results in comparison with BCB as it can model acute and obtuse angles which cannot be modeled via BCB. The flexibility of MBCB in modeling 3D complex and non-right angle geometries are utilized to model industrial examples under free relaxation condition. Unlike samples in previous works, the complexity of geometry proposed here results in highly nonlinear problems where the MBCB method can no longer guarantee convergency of the solutions. Therefore, a new and modified arc-length method is developed and utilized to overcome this nonlinearity.

1. Introduction

Modeling of material at nano-scale is investigated with atomistic methods such as molecular dynamics (MD) and Monte Carlo (MC). These methods suffer from high computational cost. The various multi-scale methods are proposed to link continuum and atomic region. The Cauchy–Born (CB) hypothesis is a well-known multi-scale method; based on the CB hypothesis [1–4], the equilibrium in media will be obtained by gradient deformation which minimizes potential energy of lattice. The CB hypothesis is successful in reduction of computational cost, so it is very popular in nano-scale modeling of materials.

The multi-scale models are generally categorized into hierarchical and concurrent methods. In the hierarchical approach, information at the smaller scale is bridged to the larger one. The contents of information can include any physical observable such as elasticity, stress, viscosity, thermal conductivity, diffusion tensors and many others. The main limitation of this approach is a loss of accuracy of transferred data between scales. In concurrent methods, two scales simultaneously exist in the simulation domain; among the most notable are Quasi-continuum [5,6], bridging scale [7,8] and bridging domain [9] methods.

The surface Cauchy–Born model is the first application of the CB hypothesis in hierarchical methods to capture the surface effects. In this method, the potential energy is decoupled to surface and bulk terms [10]. Also, a temperature-related surface Cauchy–Born model is developed to simulate temperature effect [11–13]. Park and Klein implemented this method to study silicon nano-wires [14], resonance behavior of nanowires [15] and electromechanical behavior of nano-materials [16]. Recently, Qomi et al. [17] proposed a new hierarchical multi-scale method for modeling surface stress using BCB rule. They captured the surface stress along the surface, edges and corners of plain and curved objects while the CB model cannot trace stress on surface. Further studies were done to the proposed method to include thermal effects [18] and improve the accuracy which results in modified-boundary CB (MBCB) method [19]. In this method the super convergent patch recovery (SPR) method was utilized to interpolate atomic properties in Gauss points. Also, the MBCB was utilized in modeling polygonal cross-section silicon nanowires [20].

As it have been denoted, to overcome the insufficiency of BCB in modeling obtuse and acute geometries, MBCB method has proposed using real atomic structure in surfaces to calculate material properties and stresses. In that regard, there is no need to define elements to simulate surface effects, which are used in BCB.

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http://dx.doi.org/10.1016/j.jocs.2015.04.031
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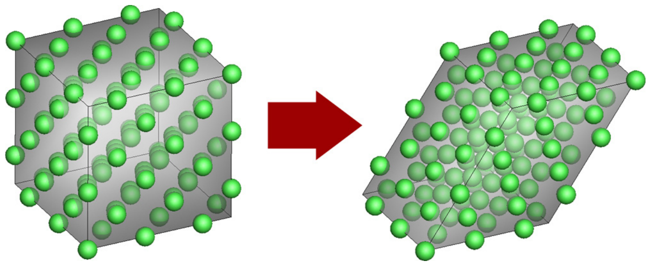

Fig. 1. The undeformed/deformed lattice structure.

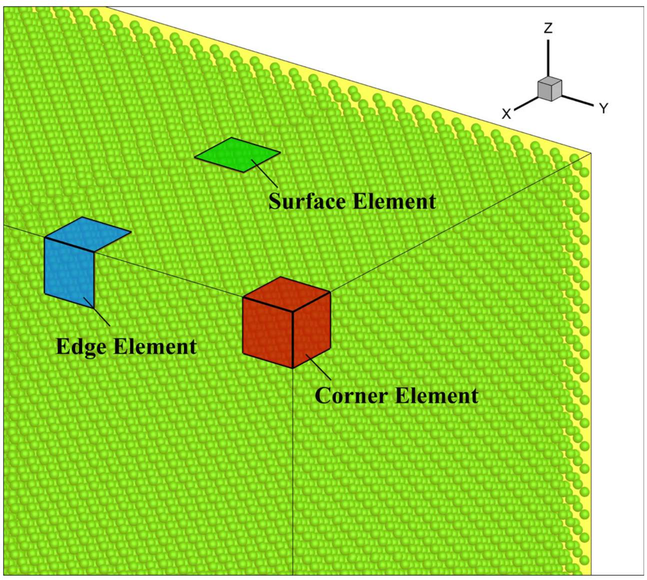

Fig. 2. Different types of elements in BCB methods.

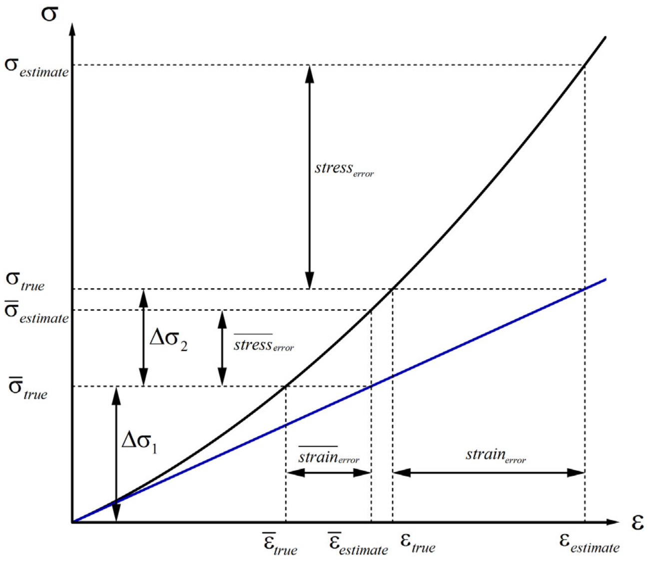

Fig. 3. Arc-length scheme.

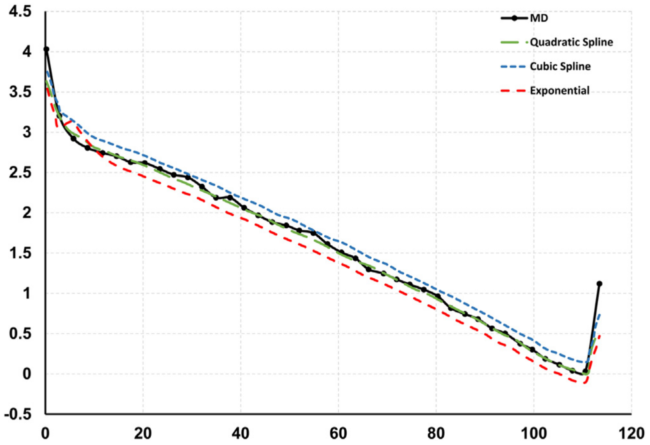

Fig. 4. The evolution of stress σ_x along the line passed through the surface of structure using different weighting functions [19].

Furthermore, by utilizing radial quadrature or SPR, the material properties and stresses can be estimated more precisely in MBCB method.

In this paper the MBCB method is used to model complex and industrial examples. In the previous works the MBCB method was utilized to simulate 2D transition metals [19] and 3D silicon nano-wires [20]. However, it was never used to model 3D transition metals where surface stresses are so much more severe than silicon nano-wires. In this study, some modifications to the method are proposed to harvest admittable convergence in real industrial examples. The efficiency of the method is shown through numerical simulations of three complex industrial examples and comparison of their results with MD simulations. The detailed description of how the MD simulation is implemented is out of the scope of this paper and the exact implementation can be found in [1]. Also it is worth noting, to achieve higher levels of convergence in numerical simulations, a modified arc-length method is implemented to overcome instabilities in nonlinear modeling approach.

2. The Cauchy–Born hypothesis, BCB, and MBCB

The Cauchy–Born (CB) hypothesis relates atomic and continuum deformations [6,21]. In other words, two scale deformations via

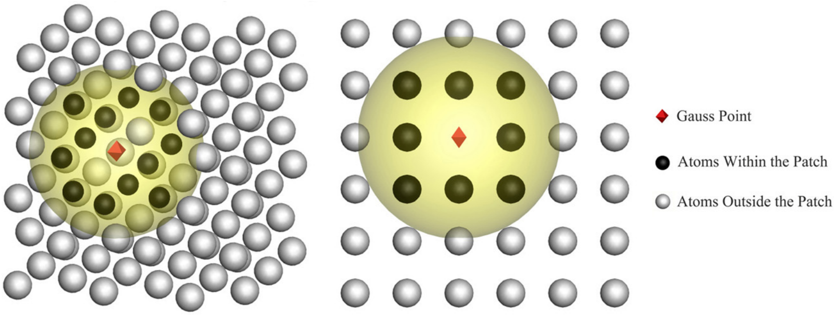

Fig. 5. Sample patch of atoms around a Gauss point (yellow sphere represents boundaries of sample patch). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)