한국기계가공학회지, 제8권 제1호, pp. 43～47 (2009. 3)
Journal of the Korean Society of Manufacturing Process Engineers, Vol.8 No.1, pp. 43～47 (2009. 3)

A New Approach of Multi-Scale Simulation for Investigating Nano-Scale Material Deformation Behavior

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나노스케일 재료 변형 거동을 위한 새로운 멀티스케일 접근법

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(Received 3 March 2009; received in revised form 26 March 2009; accepted 28 March 2009)

ABSTRACT

Recently, an approach for nano-scale material deformation has been developed that couples the atomistic and continuum approaches using Finite Element Method (FEM) and Molecular Dynamics (MD). However, this approach still has problems to connect two approaches because of the difference of basic assumptions, continuum and atomistic modeling. To solve this problem, an alternative way is developed that connects the QuasiMolecular Dynamics (QMD) and molecular dynamics. In this paper, we suggest the way to make and validate the MD-QMD coupled model.

Key Words : Molecular dynamics, Quasimolecular dynamics, Multi-scale simulation

1. Introduction

Traditionally, two kinds of approaches to model nano-scale material deformation have been used. The continuum theory, under the assumption that the material deformation can be treated as continuum material, and the molecular dynamics (MD) aiming the detailed behavior of each individual atom based on quantum mechanics are those approaches. The continuum theory has been impressively successful in solid mechanics. However, this approach is no longer valid for the nano-scale material deformation due the violation of continuum assumption[1]. Therefore, molecular dynamics to study the properties and defects of micro- and nano-systems has been suggested. It is already proved that this approach returns good quantitative results of studies for nano-scale materials. This study has been enable due to the recent advancement in computer that treats a large amount of data with high speed CPU. Nevertheless, the material size that can be analyzed is limited since the material of actual size includes an astronomic number of molecules.

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Recently, the alternative approaches have been developed that couples the atomistic and continuum approaches. One such approach to make coupling of length scales (CLS) is suggested by Abraham, Broughton, Bernstein and Kaxiras[2]. In that approach, all single scale simulations run at the same time, while dynamically transferring and receiving relevant information from the other single scale simulations. Other approach, the most successful and best-known implementation, is the quasicontinuum method by Tadmor, Ritiz and Philips[3]. The main idea of this study is to couple atomistic modeling and the continuum approach by connecting the adaptive finite element procedure and atomistic evaluation of the potential energy of the system. Park, Karpov and Liu also suggest an approach to couple length scales[4]. In this approach, by using a projection operator to decompose the displacement field into orthogonal coarse and fine scales, they are able to derive a coupled set of equations of motion describing the evolution of the MD and FE systems. Another method combining MD and FEM for silicon is proposed by Izumi, Kawakami and Sakai[5]. For simultaneous simulation, isoparametric element embedding the combined atoms was used to exchange displacement information.

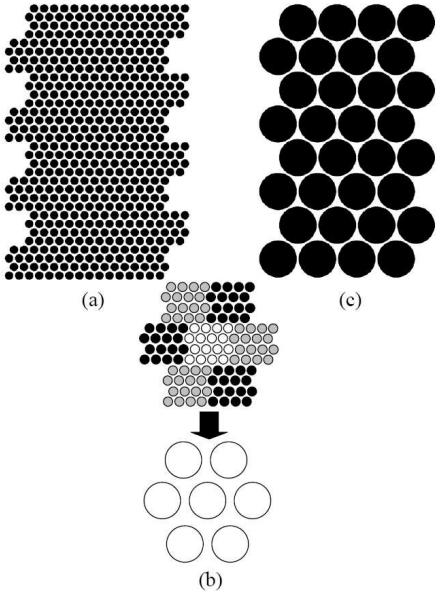

Fig. 1 Schematics of (a) MD model, (b) a method to make a quasimolecule, and (c) QMD model.

However, these alternative approaches still have problems to connect two approaches because of the difference of basic assumptions, continuum and atomistic modeling. In addition, the movement of each atom during material deformation is prone to cause the distorted elements producing numerical error at the connected area.

Recently, Greenspan suggests a new approach, quasimolecular dynamics (QMD), to model real size material. In quasimolecular dynamics, atoms (or molecules) are aggregated into large units, called virtual quasimolecules[6]. Greenspan, Choi and Ryu[7], Kim and Park[8], and Kim et al[9] have modeled material deformation successfully. The main advantages of QMD are time saving and the inactive movement of each quasimolecule since the weight of quasimolecule is rather heavier than that of atom.

In this paper, we explore the possibility to make seamless coupling of quasimolecular dynamics to molecular dynamics. More detail process will be discussed in next section.

2. Computational Modeling

2.1 MD modeling

Let us consider a rectangular Cu-plate with about 43.06(Å)×66.06(Å) that has step shape at both sides like Figure 1(a). The step shape is chosen to make the same geometry with the quasimolecular model. This plate consists of 512 atoms (16 atoms and 32 atom lines). A 6-12 Lennard-Jones potential for two copper atoms r(Å) apart is given by,

$$\phi_{md}(r) = 4\varepsilon_{md}\left[\left(\frac{\sigma_{md}}{r}\right)^{12} - \left(\frac{\sigma_{md}}{r}\right)^{6}\right] \quad (1)$$

where σ_{md} is the distance when $\varphi_{md}(r)=0$, and ε_{md} is the cohesive energy. The least-square fitted values for the Morse potential of copper are σ_{md}=2.19(Å) and ε_{md}=3.15×10^3(gÅ^2/s^2). From this equation, the force F interacting between two atoms can be derived by the differentiation of $\varphi(r)$ as follows

$$F_{md}(r)=\frac{d\phi_{md}(r)}{dr}=\frac{4\varepsilon_{md}}{\sigma_{md}}\left[6\left(\frac{\sigma_{md}}{r}\right)^{7}-12\left(\frac{\sigma_{md}}{r}\right)^{13}\right] \quad (2)$$

The minimum results when $F(r)$=0, that is, at $r_{eq(md)}$=2.46Å.

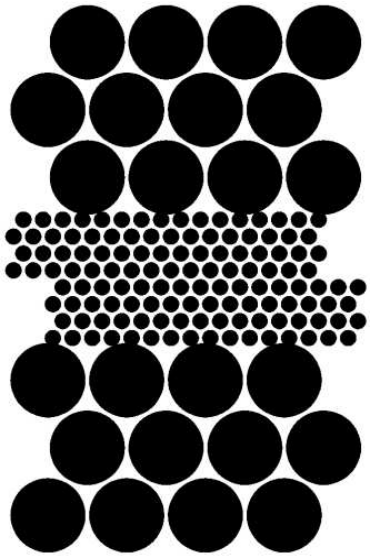

Fig. 2 Schematics of MD and QMD coupled model.

2.2 QMD modeling

It is assumed that the structure of Cu quasimolecules is Faced Centered Cubic (FCC) as is in reality. It is also assumed that 16 atoms with 4 atoms×4 atom lines are treated as a quasimolecule (refer Figure 1(b)). Hence, the equilibrium distance $r_{eq(qmd)}$=9.84Å equal to 4 times of $r_{eq(md)}$. Then the resulting arrangement is shown as in Figure 1(c). The total number of quasimolecules in the plate is 32 (4 quasimolecules×8 quasimolecules line). The total energy of the system of atoms at the equilibrium position is

$$E_{md}=\sum\sigma_{md}(r) \quad (3)$$

Here the measured E_{md} is -4.96×10^6(gÅ^2/s^2). Now we assume that the potential of quasimolecules (φ_{qmd}) has the same shape with that of atoms. Then, we have two unknowns ε_{md} and σ_{md}, and two equations, E_{md}= E_{qmd} and $F_{md}(r_{md})$= $F_{qmd}(r_{qmd})$. From these conditions, two unknowns can be acquired as follows,

$$\sigma_{qmd}(r)=\frac{r_{eq(qmd)}}{\sqrt[6]{2}} \quad (4)$$

and

$$\varepsilon_{md}(r)=\frac{E_{md}}{E_{qmd}}=\frac{E_{md}}{4N\left[\left(\frac{\sigma_{qmd}}{r_{eq(qmd)}}\right)^{12}-\left(\frac{\sigma_{qmd}}{r_{eq(qmd)}}\right)^{6}\right]} \quad (5)$$

where N is the number of potential relationship among quasimolecules in system. The obtained values are ε_{md}= 6.80×10^4(gÅ^2/s^2) and σ_{md}= 8.77(Å) since N is 73. Lastly, the mass of quasimolecule is 16 times of that of Cu-atom, in that, 1.69×10^{-21}(g).

2.3 MD and QMD coupling

To connect MD and QMD, the locations of 4th and 5th quasimolecules lines are filled with 128 atoms instead of quasi-molecules as shown in Figure 2. When calculating the force between atoms and quasimolecules, quasimolecule is assumed as a bunch of atoms. The force acting on a molecule near quasimolecule is represented by the summation of forces acting on each molecule in the quasimolecules as follows

$$F_{on\ a\ quasimolecule}=\sum_{i}^{16}F_{on\ molecules\ \in\ a\ quasimolecule} \quad (6)$$

All positions of each molecule in a quasimolecule are fixed when the position of quasimolecules is obtained.

3. Results and Discussion

In order to validate coupling MD and QMD, two models, MD and QMD, consisting of pure atoms and pure quasimolecules, and a coupled model consisting atoms and quasimolecules are subjected to tensile test. Constant velocity of 10m/s is given to 4 atom lines of MD model and 1 quasimolecule line at both ends until 34.63Å displacement. From this study, local strain, local stress and potential energy after deformation are measured. Note that relaxation process for thermal equilibrium is not applied to

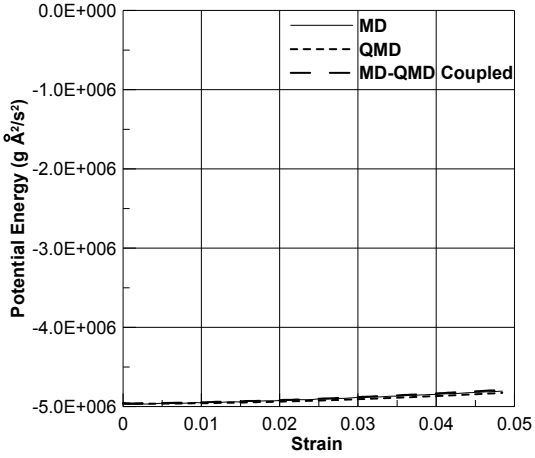

Fig. 3 Potential energy measured during material deformation

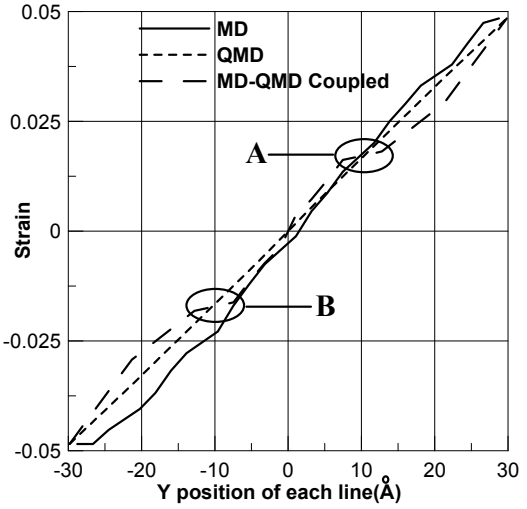

Fig. 4 Measured strain distribution at final stage along the vertical direction of the model

these models for the convenience of calculation. Also note that the Verlet algorithm is chosen to save calculation time.

3.1 Potential Energy

Figure 3 depicts total potential energy as a function of strain. The potential energy for each step is measured while strain is applied. The total potential energy increases as the strain increase, since the averaged distance among atoms increases. In addition, the energies for the MD, QMD and coupled model are almost identical.

3.2 Strain distribution

To know the strain distribution on the models, local strains for each atom and quasimolecule are evaluated at the final stage. Then, the local strains are averaged for each line. The averaged strain for each line is represented in Figure 4 as a function of original Y coordinate of each line. The acquired strain is proportional to the original coordinate as can be expected. The plots for MD, QMD and coupled model show a relatively good agreement. However, at points A and B, the strain of the coupled model of MD and QMD is flat for the Y-coordinate of atom lines. Since the atoms much lighter than quasimolecule move with the quasimolecules, the strain of MD part is similar to that of QMD part. Since the strain represents linear relationship with Y-position of each line except two points, the deformation is uniformly applied to the models.

4. Conclusion

In the present study, a new approach for simulating a nano-scale material behavior is developed that connects the quasimolecular dynamics (QMD) and molecular dynamics (MD). In the Verlet algorithm to solve the system, the time to examine all pair separations is proportional to N^2 where N is the total number of atom or quasimolecules in the system. Therefore, the proposed MD-QMD coupled model is 256 times faster than pure MD model in simulating the nano-scale material behavior for the case of the present study. It means the same results can be acquired with much smaller effort for modeling and time consuming.

Acknowledgements

This paper was supported by Research Fund, Kumoh National Institute of Technology

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