7-11

A FEM-MD combination method for silicon

Satoshi Izumi[1] , Takashi Kawakami[1] , Shinsuke Sakai[2]
[1] Mechanical and System Research Lab., Research and Development Center, Toshiba Corporation, JAPAN
satoshi.izumi@toshiba.co.jp
[2] Department of Mechanical Engineering ,University of Tokyo, JAPAN

Abstract- A new method combining the finite element method (FEM) and the molecular dynamics (MD) for silicon is proposed. For simultaneous simulation, the patch model was used to exchange displacement information in both directions. A one-to-one correspondence of atoms and nodes is impossible for silicon lattice, therefore the atom was embedded in isoparametric element. The influence of internal displacement which is the additional displacement to the continuum one was taken into consideration. Martin's method was applied to calculate internal displacement and elastic constants. The verification model showed that the smooth transition of displacement and stress was realized in the boundary region of FEM and MD. These value showed good agreement with elastic solution.

1. Introduction

"Dislocation loops" are generated due to high stress concentration around nano-scale structures of semiconductor devices. However, the generation mechanism of dislocation is not fully understood. Molecular Dynamics (MD) is expected to provide useful results for such a nano-scale phenomenon. Simulation of the entire device structure is impossible even by recent parallel supercomputer. It is effective to simulate only the important region by MD and the other region by Continuum approach, for example Finite Element Method (FEM). This work focuses on the mechanical (elastic) combination of FEM and MD for silicon that realizes the accurate stress distribution.

2. Proposed method

Until now, a combination method has not been proposed for silicon because of the difficulty posed by silicon's complicated diamond-like structure. A new method is proposed as follows.

The non-local property of interatomic force precludes the direct combination of FEM and MD. To avoid that problem, simultaneous simulation is carried out by exchanging only displacements through transition region. That method, first proposed by Kohlhoff et al.[1] for b.c.c. crystal, is employed.

In their method, the whole system consists of four regions (I,II,III,IV) as shown in Fig.1. MD regions are from I to III, and FEM regions are from II to IV. Each transition region (II,III) provides the displacement boundary conditions for the other. The displacement of atoms in II supplies the boundary conditions of FEM (continuum), and conversely the displacement field of elements in region III supplies those of MD (atoms). The non-local atomic forces are transmitted to region I and II by fixing the atoms in region III. The local reaction forces are transmitted to region III and IV by fixing the nodes in region II. Therefore mechanical balance is established between MD (I,II) and FEM (III,IV).

Elastic constants must be equal in MD region and FEM region for complete compatibility. Those obtained by MD simulation are employed.

However, there are two problems regarding the application of this method to silicon.

(1) A one-to-one correspondence of atoms and nodes is impossible for silicon lattice.

(2) In addition to continuum displacement, internal displacement occurs in silicon lattice and affects the

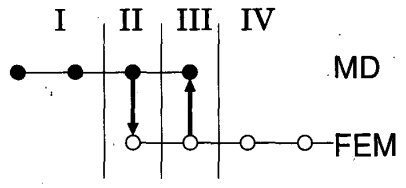

Fig. 1. Schematics of patch model

elastic constants.

For the first problem, in the transition region, atoms are embedded into FEM isoparametric elements[2] as shown in Fig.2. Every node must coincide with atom. In the case of transformation from FEM to MD, the displacements of atoms are fixed by using the FEM interpolation function. Conversely, nodes are fixed by atoms with which they coincide.

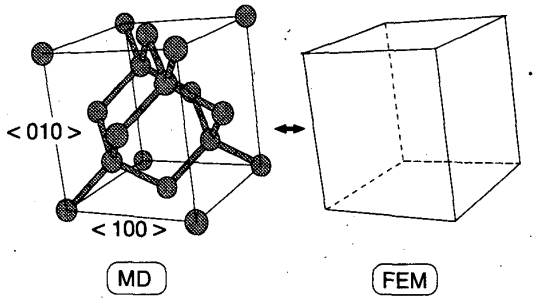

Fig. 2. The correspondence of atoms and a mesh

For the second problem, the effect of internal displacement, i.e., nonlinear displacement due to the deformation, is taken into account. Total displacement of atoms is equal to the sum of continuum (FEM) and internal displacement. Thus, to establish the method of determining the internal displacement and its effect on the elastic constants, Martin's formulation[3] was newly applied to MD.

According to Martin's formulation, internal displacement vector $\boldsymbol{\xi}^p$ is the product of the inverse of force constants tensor $\boldsymbol{g}$, the third-rank tensor $\boldsymbol{D}$ related to the piezo-effect and strain $\boldsymbol{\eta}$, as shown in Eq.(1). Elastic constants $\boldsymbol{C}$ are expressed in Eq.(2). The second term of the right-side represents the effect of internal displacement. Here ϕ indicates the potential energy of a system. Ω shows volume. δ_{rq} is the Kronecker delta, equal to unity if $r = q$ and zero otherwise.

$$\xi_i^p = -g_{im}^{pq} D_{mkl}^q \eta_{kl} \quad (1)$$

$$C_{ijkl} = C_{ijkl}^0 - D_{ijm}^p g_{mn}^{pq} D_{nkl}^q \quad (2)$$

$$E_{ji}^{rp} g_{im}^{pq} = \delta_{rq}\delta_{jm} \quad (3)$$

$$C_{ijkl}^0 = \frac{1}{\Omega}\frac{\partial^2\phi}{\partial\eta_{ij}\partial\eta_{kl}} \quad (4)$$

$$E_{ji}^{rp} = \frac{1}{\Omega}\frac{\partial^2\phi}{\partial\xi_j^r\partial\xi_i^p} \quad : \quad D_{mkl}^q = \frac{1}{\Omega}\frac{\partial^2\phi}{\partial\xi_m^q\partial\eta_{kl}} \quad (5)$$

Convergent calculation method is as follows.

(1) Set the initial displacement of both MD and FEM

(2) Fix the atomic displacement of region III by using the FEM result and compute the stable state of MD region (I,II) by the conjugate gradient method.

(3) Fix the nodal displacement of region II by using the MD result and compute the stable state of FEM region (III,IV).

(4) Check the convergence. If failed, return to procedure (2).

3. Verification model and analysis method

To verify the proposed method, a square model was adopted as shown in Fig.3. MD regions were set at the center of the model under the periodic boundary condition in the z-direction and were surrounded by FEM regions. The number of atoms was 133 (region I) , 152 (region II) and 280 (region III). The number of nodes was 32 (region II, it corresponds the innermost atomic row), 280 (region III), 920 (region IV). The number of elements was 560. Uniform displacement was enforced on the right-side nodes (Ux=0.01[A],Uy=0.1[A]), and the left-side nodes were fixed. All the z-displacements were fixed (plain strain condition). For MD simulation, three-body Tersoff[4] potential was used to realize silicon lattice structures and the conjugate gradient method was used to find the atomic stable state. The FEM program for 3D elastic analysis based on infinitesimal deformation theory was prepared[2]. The isoparametric element which includes 8-nodes and 8-integration points was used. Stress was averaged and evaluated at nodes.

The significant advantage of this proposed method is that the information transmits to FEM region from MD region which includes the unpredictable phenomenon. How ever in this paper, it dealt with the problem that a solu-

tion was obtained by only FEM for the purpose of high accurate verification.

4. Results and Discussions

Simultaneous calculation was completely convergent with 30 iterations. The normalized norm of residual force became less than 1.0 $\times 10^{-4}$. Displacement (U_x, U_y) and stress (σ_{xy}) distribution along a plot line (see. Fig.3) are shown in Fig.4, Fig.5. Smooth transition of displacement and stress was realized at the boundary. These values showed good agreement with the elastic solution (FEM prediction). Errors of displacement and stress were 0.18 % and 0.4 %, respectively.

The slight disorder of stress distribution may be due to the use of FEM interpolation function and be concentrated near the boundary due to the short-range property of potential.

In order to examine the effect of internal displacement, calculation that ignored its effect was conducted. Stress distribution (σ_{xy}) was shown in Fig.6. It should be noted that distribution was remarkably confused near the boundary in comparison with Fig.5. It appears that the neglect of the internal displacement might introduce those errors and the consideration of internal displacement might be necessary.

5. Conclusion

A method combining the finite element method and the molecular dynamics was proposed that could deal with the silicon lattice structure. The use of isoparametric element and the incorporation of internal displacement effect realized the combination. The validity of the proposed method was confirmed by use of a verification model.

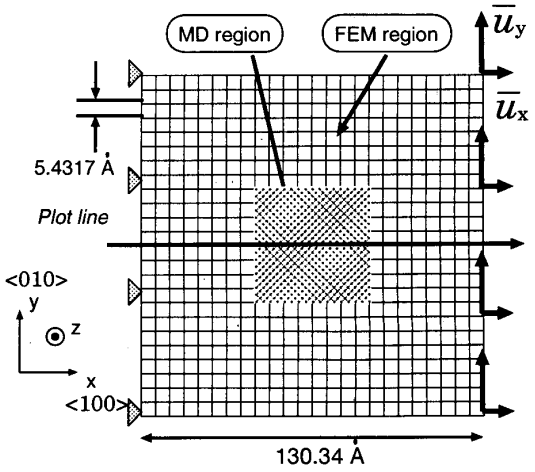

Fig. 3. Schematics of verification model

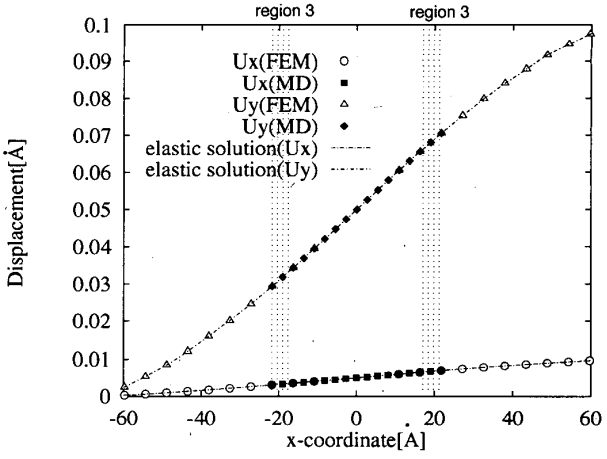

Fig. 4. Displacement distribution along a plot line (See Fig.3).

References

[1]Kohlhoff,S.,Gumbsch,P.,Fischmeister,H.,Philo.Mag.A64 (1991)p851-878

[2]Zienkiewicz,O.C.,Taylor,R.L.,"The finite element method 4th-ed."1989,McGraw-Hill Book Company(UK)

[3]Martin,J.W.,J.Phys.C,8(1975),2858

[4]Tersoff,J.,Phys.Rev.B38(1988),9902

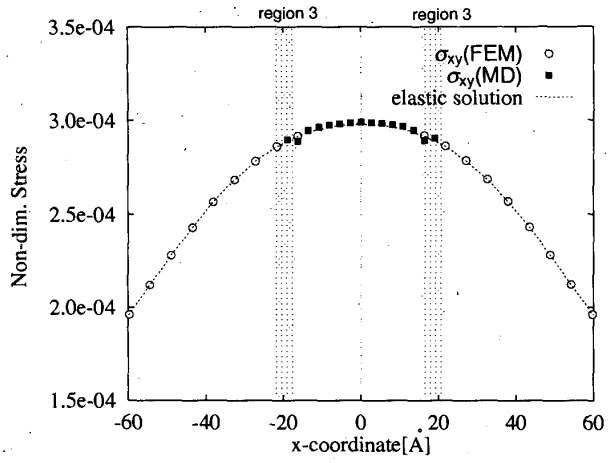

Fig. 5. Stress distribution along a plot line (See Fig.3).

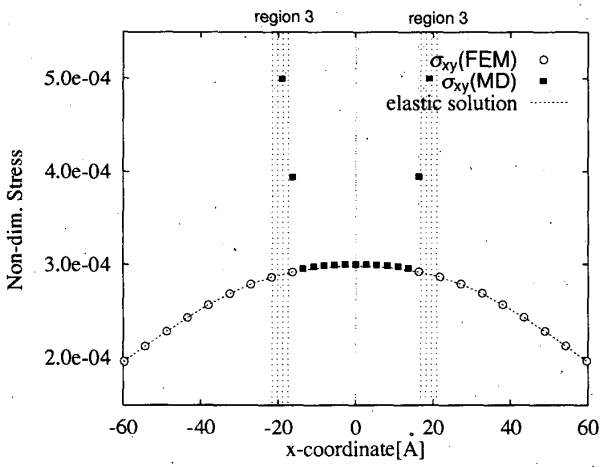

Fig. 6. Stress distribution along a plot line (See Fig.3), but the effect of internal displacement was ignored