Study of a Combined FEM-MD Method for Silicon*

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A new method combining the finite element method (FEM) and the molecular dynamics (MD) for the complicated diamond-like structure of 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 a silicon lattice, therefore, the atom was embedded in an isoparametric element. The influence of internal displacement which is a additional displacement to the continuum one, was taken into consideration. Martin's method was applied to calculate the internal displacement and elastic constants. The conjugate gradient method was used for MD, the Newton-Raphson method was used for FEM to efficiently find the stable state, and the acceleration condition was set to raise convergence. The verification model showed that the smooth transition of displacement and stress was realized in the boundary region of FEM and MD. These values showed good agreement with the elastic solution.

Key Words : Molecular Dynamics, Finite Element Method, Elasticity, Micro Mechanics, Internal Displacement, Lattice Dynamics, Elastic Constants

1. Introduction

In recent years, the atomic level evaluation of materials has attracted considerable attention, and many approaches have been attempted. The molecular-orbital method and the first principle molecular-dynamics method, which calculate potentials semi- or non-empirically, have been used for the design of new materials and the mechanism elucidation of phenomena which cannot be evaluated by experimental approaches. However, their deficiency is that they can treat only several tens of atoms. Since molecular dynamics (MD) approximates potentials with empirical functions, the accuracy becomes lower than the first principle calculation. However, calculation of significantly large systems becomes possible. Recently, calculation of no less than 100,000,000 atoms was performed[(1)]. However, it is still impossible to deal with real system size, and thus for the application of MD to real systems, it may be effective to simulate only the important regions by MD and the other regions by the continuum method, such as finite element method (FEM). In this paper, we focus on the mechanical combination of FEM and MD. In particular, an effective method for complicated lattice structures (non-Brave lattice) such as silicon, which is an important material for semiconductor devices, is proposed.

Various combination methods have been already proposed. Mullins[(2)] proposed a method using "force". In the FEM-MD boundary, the atoms were embedded into FEM elements, and atomic force was converted to the concentrated load of FEM. However, since the atomic force was long-range and had non-local property, it could not maintain the balance of the force in the boundary, and non-physical and discontinuous stress distribution was introduced. Moreover, it is doubtful whether the strong-directive atomic force of the covalent bond can be converted to the concentrated load. By the use of displacement instead of force, the problem of non-local property and bond directivity can be avoided. Therefore the displacement-constrained method which provides the boundary atoms with the

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elastic solution has been applied[3]. However, since the action in the atomic region cannot be transmitted to FEM region by using this method, simultaneous combination of FEM and MD is impossible. In this paper, in order to solve this problem the patch model first proposed by Kohlhoff et al.[4] was applied. FEM-MD combination for homogeneous lattice structures, such as the FCC and BCC, has already been investigated. However, for complicated lattice structures such as diamond-like, amorphous types, etc., there are some typical problems. Firstly internal displacement which is the difference between the atomic and continuum displacement prevents the consistency of the displacement between FEM and MD[5]. Secondly, a one-to-one correspondence of atoms and nodes as Kohlhoff et al. achieved[4], is impossible for complicated lattices. Because of these difficulties, the FEM-MD combination method for diamond-like structures and others has not been proposed until now. In this paper, a FEM-MD combination method which can solve these problems is proposed. Thus, in order to establish the method for determining the internal displacement and it's effect on elastic constants, Martin's formulation[6] was newly applied to MD. Atoms are embedded into FEM isoparametric elements in the normalized coordinate system (ξ, η, ζ). The FEM-MD combination method for the complicated lattice which contains internal displacement is realized. Moreover, in the convergence calculation for finding a stable state, an excellent accurate and efficient technique is proposed. In this paper, only the static analysis was carried out for the purpose of mechanical (stress) combination. The treatment of heat vibration needs to be investigated independently (separately). The details of the proposed FEM-MD combination method are shown in Chapter 2. The model used for the verification of the proposed method and the concrete analysis technique are shown in Chapter 3, and the result is shown in Chapter 4. In Chapter 5, the effects of internal displacement and convergence of the method are discussed.

2. Proposed method

The FEM-MD combination method for complicated lattice structures such as diamond structure which contain the internal displacement is described.

2·1 Correspondence of nodes and atoms In the overlap region of FEM and MD, nodes and atoms need to correspond to one another. One-to-one correspondence is difficult due to structural problems in the case of diamond-like or amorphous structures. It is considered that non-physical distortion is generated if nodes exist at the point where atoms do not exist. For example, in the case of silicon, 8 atoms in a unit cell are embedded into an isoparametric element in the normalized coordinate system (ξ, η, ζ coordinates), as shown in Fig.1. In the case of transferring displacement from FEM to MD, the interpolation is conducted by the use of shape function for atoms which are not correspondent with nodes. In the opposite case, the displacement of nodes is equal to that of corresponding atoms. The extrapolation from neighboring atoms is required if the node exists in the non-existing point of atoms. However, it is desirable for the node to correspond to atoms, if possible, from the viewpoint of the calculation accuracy.

The patch method[4] which realizes simultaneous simulation by exchanging only the displacements of FEM and MD through the transition region, is employed. In this method, the whole system consists of four regions. Regions 2 and 3 are transition regions (Fig.2). MD regions are from 1 to 3, and FEM regions are from 2 to 4. The displacement of atoms in region 2 supplies the boundary conditions for FEM, and conversely the displacement field of elements in region 3 supplies those for MD. It is necessary that region 3 is larger than the cutoff distance of the atomic force to eliminate the surface effect. Region 2 may be a row of atoms because it is the boundary of FEM. By exchanging the displacement in both directions iteratively, the stable system is realized with continuous stress and displacement distribution through the boundary of FEM and MD.

2·2 Consideration of internal displacement effect It is necessary to take the internal displacement effect into consideration in the case of lattice structures where atomic displacement is

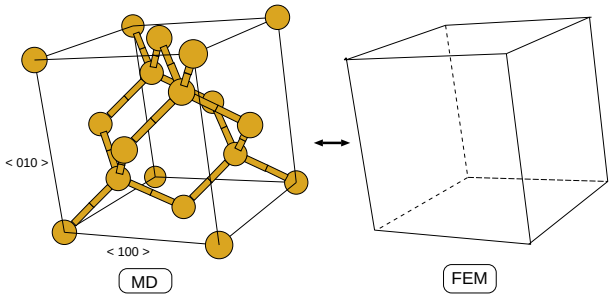

Fig. 1 The relationship between Si atoms and FEM mesh

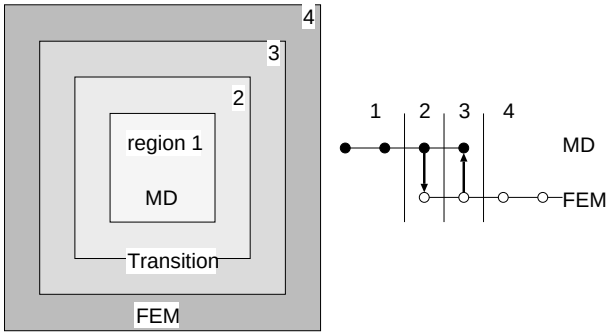

Fig. 2 The patch model[4]

nonlinear to the deformation (for example, silicon and amorphous structures). According to Martin's formulation, the internal displacement vector $\boldsymbol{\xi}^p$ is the product of the inverse of the force constants tensor $\boldsymbol{g}$ and the third-rank tensor $\boldsymbol{D}$ related to the piezo-effect, as shown in Eq.(1). Therefore atomic displacement is the sum of the elastic displacement and internal displacement. Here ϕ indicates the potential energy of a system and Ω is the volume.

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

$$E_{ji}^{rp} g_{im}^{pq} = \delta_{rq}\delta_{jm} \quad (2)$$

$$E_{ji}^{rp} = \frac{1}{\Omega}\frac{\partial^2\phi}{\partial\xi_j^r \partial\xi_i^p} \quad : \quad D_{mkl}^q = \frac{1}{\Omega}\frac{\partial^2\phi}{\partial\xi_m^q \partial\eta_{kl}} \quad (3)$$

When the displacement of FEM transforms to MD atoms, it is necessary to add an internal displacement, and to subtract one in the opposite case. The strain value required to obtain the internal displacement vector $\boldsymbol{\xi}$ is derived from the product of the atomic stress and compliance matrix as for MD. The averaged node strain is used as for FEM. Although the atomic stress of MD has non-local property, it seems that the effect can be ignored by setting the boundary region of FEM-MD in small strain-gradient region. In such a case, it is expected that the atomic stress is almost the same as the continuum stress. Atomic stress σ_{ij}^p was defined by formula(4), where r^{pq} expresses the distance between atom p and q and Ω^p is the volume per one atom. It was defined so that the average value of the atomic stress was equal to the stress of the whole system. In order to examine the validity of the definition, the atomic stress distribution was calculated for the model where the displacement of all atoms was fixed by the result of FEM analysis of the whole system as shown in **3·1**, and then compared with the stress of FEM. The deviations of atomic stress from FEM stress were 0.08 % for σ_x and 0.22 % for σ_{xy}. It was found that both stresses were coincident within remarkable accuracy limits.

$$\sigma_{ij}^p = \frac{1}{\Omega^p}\sum_q \frac{\partial\phi}{\partial r^{pq}}\frac{\partial r^{pq}}{\partial\eta_{ij}} \quad (4)$$

Since the deviation of MD and FEM elastic constants introduces nonphysical strain in the boundary region, the elastic constants of MD region were calculated separately[5], and provided for FEM region.

2·3 Method for convergence Kohlhoff et al. used the Newton-Raphson method for the convergence calculation to find the stable state of FEM-MD system[4]. However, Newton-Raphson method is not suitable for MD calculation with many-body potential such as silicon, because of the difficulty of the Hessian calculation, thus, the conjugate gradient method without the Hessian calculation is more suitable. Therefore, for MD calculation, the conjugate gradient method was adopted. FEM calculation was able to use the Newton-Raphson method in the form including the interaction with MD calculation. In order to combine the two different analyses, the following iteration was applied.

1. Set the initial displacement of MD and the boundary condition of FEM
2. Obtain the atomic strain from the atomic stress in region 2, then calculate the internal displacement.
3. Fix the nodal displacement of region 2 by using the MD result and compute the reaction force vector of FEM ($\boldsymbol{f}_{i-1}$). Note that the fixed nodal

displacement is obtained to subtract the internal displacement from the atomic displacement

4. Compute the stable state of FEM regions 3 and 4 and obtain the displacement of all nodes
5. Obtain the internal displacement from the nodal strain in region 3
6. Fix the atomic displacement of region 3 by using the FEM result and compute the stable state of MD regions 1 and 2 by the conjugate gradient method, and obtain the atomic displacement of all atoms. Note that the fixed atomic displacement is the sum of the nodal and internal displacement.
7. Check the convergence. If failed, return to procedure 2.

The displacement of the i-th iteration can be derived as in Eq.(5).

$$\begin{aligned} \boldsymbol{a}_i &= \boldsymbol{a}_{i-1} + \alpha_i \Delta \boldsymbol{a}_i & (5) \\ \Delta \boldsymbol{a}_i &= -\boldsymbol{K}'^{-1} \boldsymbol{\Phi}_{i-1} & (6) \\ \boldsymbol{\Phi}_{i-1} &= \boldsymbol{K}\boldsymbol{a}_{i-1} - \boldsymbol{f}_{i-1}(\boldsymbol{a}_{i-1}, MD) & (7) \end{aligned}$$

Here, $\boldsymbol{K}$ is the global stiffness matrix, and $\boldsymbol{\Phi}$ is the residual force vector. $\boldsymbol{f}_{i-1}(\boldsymbol{a}_{i-1}, MD)$ expresses that $\boldsymbol{f}_{i-1}$ is introduced by the result of MD calculation with the boundary condition obtained from the former FEM result. Later, it simply abbreviates to $\boldsymbol{f}_{i-1}$. From the definition of the Newton-Raphson method, $\boldsymbol{K}'$ is written as follows

$$\boldsymbol{K}' = \frac{\partial \boldsymbol{\Phi}_{i-1}}{\partial \boldsymbol{a}_{i-1}} = \boldsymbol{K} - \frac{\partial \boldsymbol{f}_{i-1}}{\partial \boldsymbol{a}_{i-1}} \quad (8)$$

Since $\frac{\partial \boldsymbol{f}_{i-1}}{\partial \boldsymbol{a}_{i-1}}$ cannot be solved analytically and inverse matrix must be calculated for each step of the change in $\boldsymbol{K}'$, here $\boldsymbol{K}'^{-1} = \boldsymbol{K}^{-1}$ is approximately assumed.

Additionally, using Eq.(5) and Eq.(6), Eq.(7) is rewritten in the simple form as Eq.(9).

$$\begin{aligned} \boldsymbol{\Phi}_{i-1} &= \boldsymbol{K} \cdot (\boldsymbol{a}_{i-2} + \alpha_{i-1} \Delta \boldsymbol{a}_{i-1}) - \boldsymbol{f}_{i-1} \\ &= \boldsymbol{\Phi}_{i-2} + \boldsymbol{f}_{i-2} - \alpha_{i-1} \boldsymbol{\Phi}_{i-2} - \boldsymbol{f}_{i-1} \\ &= (1 - \alpha_{i-1}) \cdot \boldsymbol{\Phi}_{i-2} + \boldsymbol{f}_{i-2} - \boldsymbol{f}_{i-1} \quad (9) \end{aligned}$$

Since α_i is set to unity in the case of the normal Newton-Raphson method, the accelerated technique is adopted in order to raise the convergence. The potential energy of FEM system is differentiated with respect to α_i in order to obtain the α_i to reduce the potential energy as much as possible.

$$\frac{\partial \pi(\boldsymbol{a}_i)}{\partial \alpha_i} = \frac{\partial \pi(\boldsymbol{a}_i)}{\partial \boldsymbol{a}_i} \cdot \frac{\partial \boldsymbol{a}_i}{\partial \alpha_i} \quad (10)$$

Using Eq.(5) and $\pi(\boldsymbol{a}_i) = \frac{1}{2}\boldsymbol{a}_i^t \boldsymbol{K} \boldsymbol{a}_i - \boldsymbol{f}_I \boldsymbol{a}_i$, it follows that

$$\Gamma = \frac{\partial \pi(\boldsymbol{a}_i)}{\partial \alpha_i} = (\boldsymbol{K}\boldsymbol{a}_i - \boldsymbol{f}_i - \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{a}_i}\boldsymbol{a}_i) \cdot \Delta \boldsymbol{a}_i \quad (11)$$

Since $\frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{a}_i}$ cannot be calculated analytically as with Eq.(8), it is assumed to be zero. The potential energy will become minimum with respect to α_i, which leads to $\Gamma = 0$. For efficiency, the approximate value of α_i is obtained by the linear interpolation of two calculation results for $\alpha_i = 0$ and $\alpha_i = 1$[7]. For α_i=0, using $\boldsymbol{a}_i$=$\boldsymbol{a}_{i-1}$, $\Gamma = \boldsymbol{\Phi}_{i-1}\Delta \boldsymbol{a}_i$ is obtained. As for α_i=1, using Eq.(9) $\Gamma = \boldsymbol{\Phi}_i^* \cdot \Delta \boldsymbol{a}_i = (\boldsymbol{f}_{i-1} - \boldsymbol{f}_i^*) \cdot \Delta.\boldsymbol{a}_i$ is obtained. $\boldsymbol{\Phi}_i^*, \boldsymbol{f}_i^*$ are the residual and force vectors respectively for calculating $\boldsymbol{a}_i$ as $\alpha_i = 1$. Moreover, for the stability of the calculation, the maximum value of α is set at 4.0.

Here, it is considered that convergence will increase through initial displacement in MD region. For example, it will be effective that initial displacement is set to be the same as the result of FEM calculation for the whole region.

3. Analysis condition

To verify our method, crystal silicon which was fully investigated in a former report[5] was used as the analysis subject. Crystal silicon has a diamond-like structure and internal displacement occurs due to the shear deformation. Therefore, the shear-strain dominant field was set. The analysis condition and FEM and MD technique are shown in detail.

3·1 Analysis model The analysis model (meshes and atoms) is shown in Fig.3. The division of regions 1-4 is shown in the lower part. The outermost size of region 3, region 2 and region 1 is 8×8, 6×6 and 4×4(unit cell), respectively. For the correspondence of the atoms and nodes in region 2 and 3, a unit basic lattice is set up with 1 mesh (1 mesh per eight atoms), as shown in Fig. 1. For simplicity, the thickness of the z-direction was set

one mesh layer and all the z-displacements were fixed (plain strain condition). To eliminate the surface effect of MD region, a periodic boundary condition was adopted in the z-direction. To introduce the shear-strain dominant field, uniform displacement was enforced on the right-side nodes, $\overline{u}_x$=0.01[Å], $\overline{u}_y$=0.1[Å], and the left-side nodes were fixed. The number of atoms was 133 (region 1
2) and 280 (region 3). The number
32 (region 2, corresponding to the inn
row), 280 (region 3) and 920 (region 4
s 560.

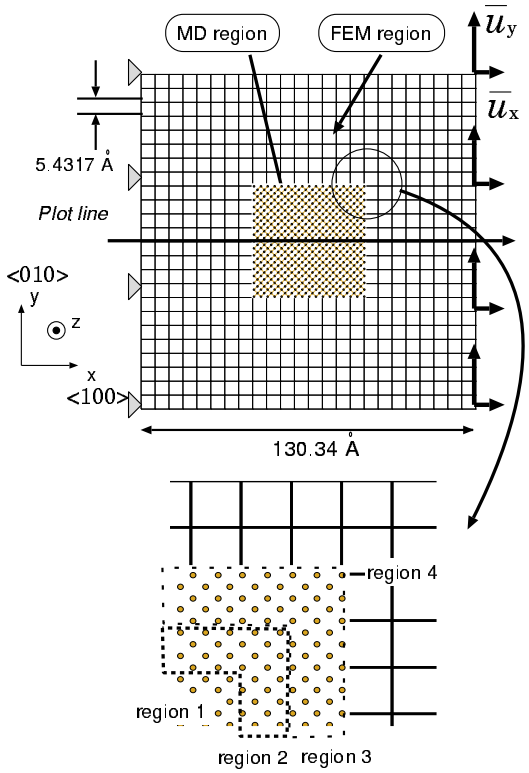

Fig. 3 Analysis model and setup of the transition region

The significant advantage of this proposed method is that the information transmits to FEM region from MD region, which includes unpredictable phenomena from the use of FEM, and that those transmission realize the mechanical stable state of the whole system. However, this paper deals with the problem that the solution was obtained by only the FEM for the purpose of highly accurate verification of the FEM-MD combination method. Additionally, all displacements of MD region were set to zero so that there might be no correlation of displacement between MD and FEM regions in the initial state. Since the initial displacement is very different from an elastic solution, and the stable state needs to be found by exchanging displacement information between FEM-MD iteratively, it is considered that verification of our proposed method is possible.

3·2 Molecular-dynamics method The Tersoff potential[8] was used for MD calculation of silicon. Refer to the reference[5] in details, as for the calculation of the atomic force, stress, elastic constants, and internal displacement.

The conjugate gradient method was used for the optimization of structure. Generally, for the highly accurate many-body potential (for example, Tersoff potential, etc.), the calculation of the Hessian is difficult. Therefore, β in the straight-line search formula (12) required in order to obtain atomic position $\boldsymbol{x}$, was calculated by the use of the 2-divided method so that the condition of Armijo was fulfilled[9]. $\boldsymbol{d}$ is the search direction.

The condition of Armijo means that β which satisfies $\phi(\boldsymbol{x}_k + \beta\boldsymbol{d}_k) \leq \phi(\boldsymbol{x}_k) + \nu\beta\nabla\phi(\boldsymbol{x}_k)^T\boldsymbol{d}_k$ is selected as β_k, where ν is a constant which satisfies $0< \nu <1$, and is independent of k (step number of conjugate gradient method). At first, a suitable ν was set, then β was reduced to half from unity until it fulfilled the condition of Armijo. ϕ indicates potential.

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \beta_k\boldsymbol{d}_k \tag{12}$$

The Fletcher-Reeves formulation shown in Eq.(14) was used in order to obtain γ_k in Eq.(13), which is required to find search direction $\boldsymbol{d}$.

$$\boldsymbol{d}_{k+1} = -\nabla\phi(\boldsymbol{x}_{k+1}) + \gamma_k\boldsymbol{d}_k \tag{13}$$

$$\gamma_k = \frac{\|\nabla\phi(\boldsymbol{x}_{k+1})\|^2}{\|\nabla\phi(\boldsymbol{x}_k)\|^2} \tag{14}$$

As soon as the rate of energy variation became less than 1.0×10^{-14}, or the number of trials reached 60, the trial was closed. This condition was determined by trial and error so that full convergence could be realized.

3·3 Finite element method The FEM program for 3D elastic analysis based on the infinitesimal deformation theory was newly prepared. To avoid the higher-order interpolation of strain

in the non-existing region of atoms, the higher-order element was not used, but the isoparametric hexahedral element which contained 8-nodes was used. The 2nd order integration (8 integration points) was adopted. For iterative calculation, the LU decomposition by the correction Cholesky method was conducted in order to calculate the inverse matrix[10]. Since nodes were fitted to atoms, averaged node strain and stress were required. They were obtained by extrapolating strain and stress at integration points into the nodes by the use of shape function and taking the average about all those elements to which those nodes belonged.

4. Results

After 30 iterations of the procedures **2.∼7.** in **2·3**, the norm of the residual vector $\|\mathbf{\Phi}\|$ had become less than 1.0×10^{-4} times the initial norm $\|\mathbf{\Phi}_0\|$. Displacement distribution along a plot line (see Fig.3) is shown in Fig.4 and stress distribution $\sigma_x \cdot \sigma_{xy}$ (atomic stress in MD region, averaged node stress in FEM region) is shown in Fig.5 and Fig.6, respectively. Here, the stress of the surface region was eliminated from the plot, because of the surface influence. Moreover, the value (henceforth elastic solution) calculated by FEM analysis for the whole region, was also shown for verification. Smooth transition of displacement was realized at the boundary (region 3) identified as the hatched area, and almost the same value as the elastic solution was obtained in all regions.

The mean error of $U_x \cdot U_y$ compared with the elastic solution was 0.18 % in MD region. In the case of stress, a small disorder at the boundary was generated, but transition was smooth, and almost the same value as the elastic solution was obtained. The mean error of $\sigma_x \cdot \sigma_{xy}$ was 0.4 %. Therefore, it could be proved that the FEM-MD combination method was appropriate. As for the disorder of shear stress distribution at the boundary, it is considered that the errors were caused by some disagreement of the model, for example the application of the infinitesimal deformation model, or the difference in definition between atomic stress and continuum stress, etc. Further examination is required, for example, the application of a finite deformation model.

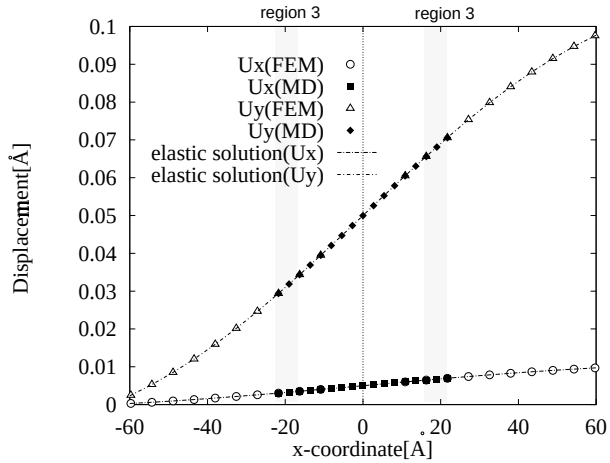

Fig. 4 Displacement($U_x \cdot U_y$) distribution along a plot-line (see Fig.3)

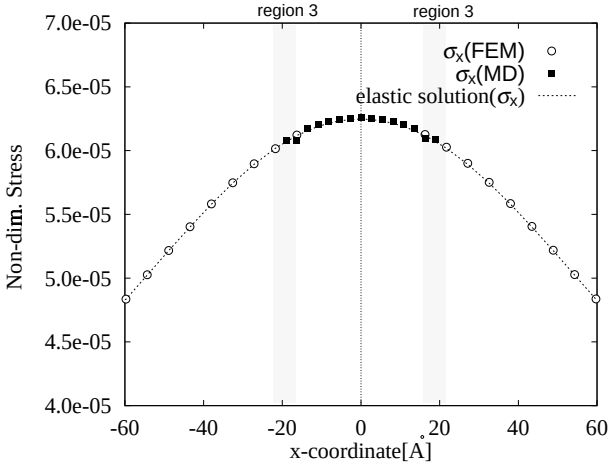

Fig. 5 Averaged node stress(FEM) and atomistic stress(MD)σ_{xx} distribution along a plot-line (see Fig.3)

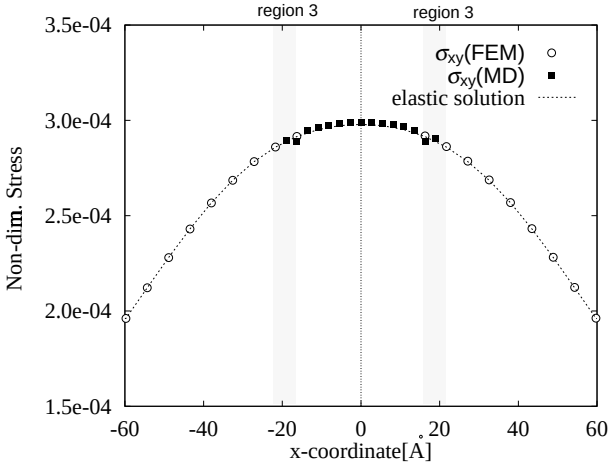

Fig. 6 Averaged node stress(FEM) and atomistic stress(MD)σ_{xy} distribution along a plot-line (see Fig.3)

5. Discussion

5·1 The effect of internal displacement In order to consider the validity of the proposed FEM-MD combination method in which the effect of internal displacement was taken into consideration, a calculation which ignored that effect was conducted. Stress distribution (σ_{xy}) along a plot line in Fig.3 is shown in Fig.7 as a result. It should be noted that stress distribution was remarkably disordered near the boundary in comparison with that in Fig.6. This was considered to be due to the neglect of the internal displacement effect. However, the value inside MD region was almost coincident with the elastic solution. Inconsistency of the model was thought to be concentrated on the boundary region, since the Tersoff potential was a short-range potential only considering the first neighbor force. In any case, the disordered stress distribution in the boundary region is a severe problem, therefore the consideration of the internal displacement was necessary.

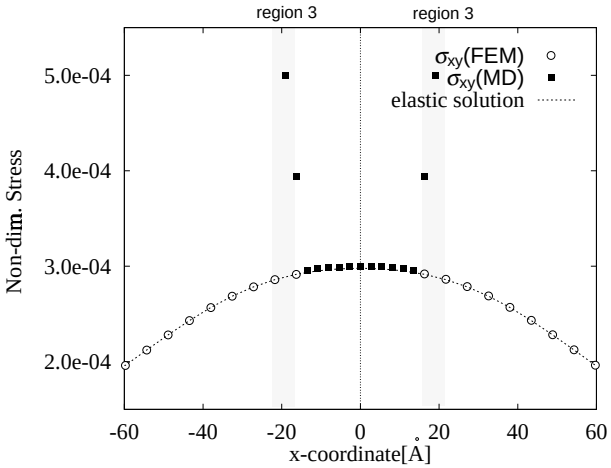

Fig. 7 Same as Fig.6 but the effect of internal displacement was ignored

5·2 Convergence

5·2·1 The effect of the accelerated condition In order to consider the effect of the proposed accelerated condition of Newton-Raphson, comparison with a normal Newton-Raphson ($\alpha = 1$) was conducted. The histories of the norm of the residual force normalized by initial value are shown in Fig.8. It should be noted that the convergence of the proposed accelerated method was about 2 times faster, therefore effectivity was proved. The errors after 30 iterations of the normal Newton-Raphson method became 2.2 % for $\sigma_x \cdot \sigma_y$, and 1.2 % for $U_x \cdot U_y$. It was found that convergence was slow and the correct result could not be obtained.

5·2·2 The influence of MD maximum trial number The number of trials (60 steps) of MD calculation was chosen from the condition which realized full convergence. For the calculation efficiency, reduction in the number of trials is effective as well as iteration. The histories of the norm of the residual force in the cases where the number of maximum trials was set at 10, 30, and 60 steps are shown in Fig.9 (failed to converge in the case of 5 steps). The errors of displacement were 0.5 % and 0.03 %, in the case of 10 and 30 steps, respectively, and those of stress were 0.6 % and 0.4 %. Complete convergence was obtained for 30 steps, but not 10 steps. However, the reduction in the number of trials made the convergence tendency unstable. It appeared that there was a correlation between instablility and α. Although, in the case of 60 steps, α was stable and between 1 and 2, and not exceeding 4. In the case of 10 and 30 steps, α frequently exceeded 4. Since accurate estimation of α was impossible due to poor convergence of MD calculation, that inaccurate estimation made the convergence of combination unstable. It is necessary to estimate the optimum number of trials for calculation efficiency.

5·2·3 Application of the conjugate gradient method Comparisons with the combination method which also adopted the conjugate gradient method for FEM as in Gumbsch et al. [11], were performed. The PCG method which contains imperfect Cholesky decomposition for the pretreatment of the conjugate gradient method was used[10]. For the simultaneous calculation, when the residual force vector was calculated for every FEM conjugate gradient step, the force vector was updated by using the result of MD calculation as in procedure **3.** in **2·3**. As soon as MD steps reached 10, or the energy variation rate became 1.0×10^{-14} or less, MD calculation was closed. Since an increase in MD steps, for example 30 steps, could make the calculation more stable, the calculation amount also increased. The smallest possible number of steps which did not lose the convergence was adopted practically (failed to converge in the case of 5 steps).

The history of the normalized norm of the residual vector is shown in Fig.10. The result where the maximum MD step in **5·2·2** was set to 10 steps is also shown. The errors of displacement $U_x \cdot U_y$ and $\sigma_x \cdot \sigma_{xy}$ were 0.1 % and 0.43 %, respectively, after 200 iterations. Therefore, it can be said that the convergence was realized. Since the convergence of the conjugate gradient method was slow, about 6 times the number of iterations were required in comparison with the accelerated Newton-Raphson method. The ratio of FEM calculation to all the calculations was small since the applied model size was so small. Therefore, it was found that the accelerated Newton-Raphson method which needed less MD steps was the more efficient method.

In the case of a large system, if the ratio of MD calculation is larger, the accelerated Newton-Raphson is still effective since it needs fewer iterations. Conversely, if the ratio of FEM becomes larger, the speed-up by the sparse-matrix method or the excellent pretreatment of the conjugate gradient method introduces a variation in the ratio of FEM and MD. A separate general discussion on this is necessary.

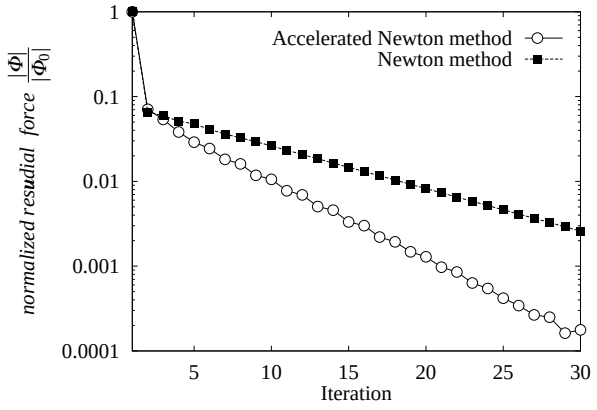

Fig. 8 The convergence of the accelerated Newton-Raphson method

6. Conclusion

A new method combining the finite element method and the molecular dynamics method was proposed, for dealing with complicated lattice structures such as the diamond-like structure of silicon.

(1) Embedding of atoms into isoparametric elements and the incorporation of the internal displacement effect realized the combination.

(2) The conjugate gradient method which was suitable for MD property was adopted for MD calculation, and the Newton-Raphson method was adopted for FEM calculation. Then, the accelerated technique for the Newton-Raphson method was proposed in order to realize the high accuracy and convergence of FEM-MD combination simultaneous calculation.

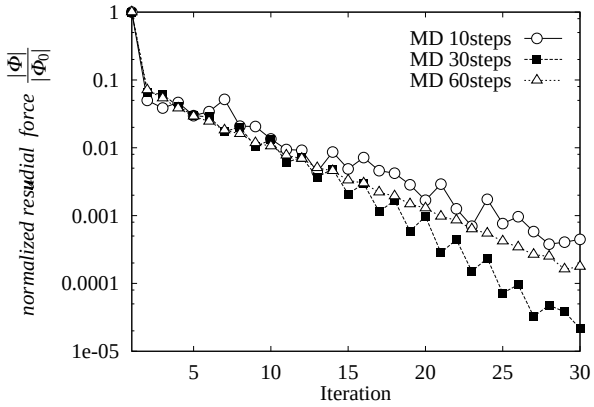

Fig. 9 The influence of the number of MD steps on convergence

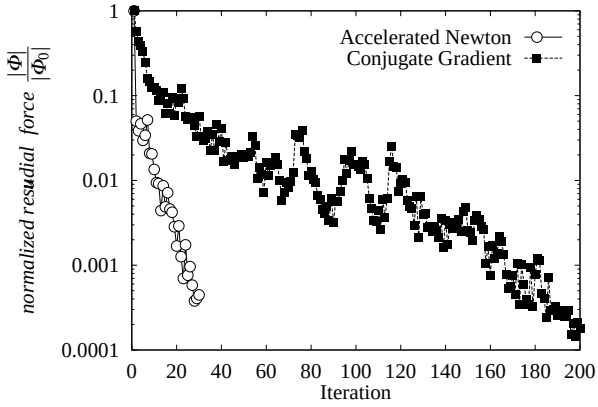

Fig. 10 Convergent difference between the accelerated Newton-Raphson method and the conjugate gradient method

By this proposed method, the smooth transition of displacement and stress was realized at FEM-MD boundary, moreover those quantitative values coincided with the theoretical ones. Therefore, the validity of the proposed method was confirmed.

The iterative calculation between FEM and MD was adopted in order to realize the consistency of the solution in the proposed method. In the case of treating heat vibration, it is necessary to

perform iterative calculation of FEM-MD for every MD step, however, it is considered to be unrealistic due to the large amount of calculation required. The approximation-technique might be possible, which satisfies the averaged balance by providing temperature with the MD region using scaling-method etc. and conducting iterative calculations for every particular time step. However, it might not be a rigorous FEM-MD combination. Further examination is required in order to treat heat vibration more rigorously.

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