Multiscale strain simulation for semiconductor devices base on the valence force field and the finite element methods

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***Abstract*—This paper presents a new methodology for multiscale strain simulations of semiconductor devices based on the valence force field (VFF) method and the finite element method (FEM). By coupling the atomistic and the continuum methods, only advantages such as the atomistic description and accuracy of the VFF method and the flexibility and numerical efficiency of the FEM can be obtained.**

Keywords—valence force field method; strain simulation; multiscale simulation; semiconductor stress

I. INTRODUCTION

The FEM-based strain simulation method has been widely used for semiconductor device researches because of its simplicity and numerical efficiency. However, the accuracy of the FEM-based simulation is limited when it is applied to nanoscale or highly strained structures because of its continuum description of simulation domains and its linearized theory of elasticity. So, when more accurate analysis is required, people are using atomistic methodologies such as ab initio, molecular dynamics (MD), or VFF simulations.

The VFF method describes the energy of a system as functions of atom positions, so it is regarded to be more accurate than the linearized FEM strain simulations [1, 2]. The VFF method also allows us to analyze the system in atomistic level, which is useful for atomistic variation analysis and the other atomistic simulations like tight-binding (TB) or extended-Huckel (EH) methods. On the other hand, although the VFF simulation is much faster than the MD simulation, it still requires more computational resources than the FEM because of its nonlinearity and atomistic resolution. Also, it is hard to take into account amorphous materials because the atomic interaction models in the VFF are basically suitable for crystalline structures.

We therefore develop a coupled-VFF-FEM method to take only advantages of the atomistic and the continuum methods. There are some atomistic-continuum strain simulation methods reported previously [3, 4] but mostly for MD simulations. Our VFF-specialized method is simpler than the previously reported methods in terms of coupling process and implementation. Also, the coupled-VFF-FEM equation can be solved by a few Newton-Raphson iterations just as an ordinary VFF method, which is more efficient than the reported VFF-FEM iterative scheme [5].

The coupled-VFF-FEM method is presented in section II, and some example simulation results are shown and discussed in section III.

II. SIMULATION METHOD

The VFF method describes the system energy (U) as a function of positions of atoms ($\vec{x}$), and the VFF strain simulation calculates such atom positions that minimizes the system energy. The equation system is nonlinear and can be written in the Newton-Raphson method form as

$$\frac{\partial^2 U(\vec{x}^{(n-1)})}{\partial \vec{x}^{\,2}} \delta\vec{x}^{(n)} = -\frac{\partial U(\vec{x}^{(n-1)})}{\partial \vec{x}} \qquad (1)$$

In the FEM simulations we usually solve the linearized elasticity equation, $K\vec{\mu} = F$, to obtain the displacement field ($\vec{\mu}$) over the FEM nodes. To couple the linear FEM and the nonlinear VFF equations we rewrite the FEM equation in a nonlinear form as

$$K\,\delta\vec{\mu}^{(n)} = F - K\vec{\mu}^{(n-1)} \qquad (2)$$

where $\delta\vec{\mu}^{(n)} = \vec{\mu}^{(n)} - \vec{\mu}^{(n-1)}$. Now the physical meanings of the system matrix and the solution and the right-hand side vectors of the nonlinear FEM equation became the same to those of VFF. We also prepare a set of pairs of atom and FEM node on the interfaces between the atomistic and the FEM domains as shown in Fig. 1. Then, the two equations can be coupled by introducing a constraint that each and every pair of atom and FEM node has the same displacement in all directions,

$$\delta\vec{x}^{(n)} = \delta\vec{\mu}^{(n)} \text{ at interfacial atom-node pairs} \qquad (3)$$

Since the constraint does not change the original equations, no distortion is involved during the coupling process. The coupled nonlinear system can be solved just as ordinary VFF strain simulations, during which any additional nonlinear models can

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be put into the FEM equation if needed without further computational burden.

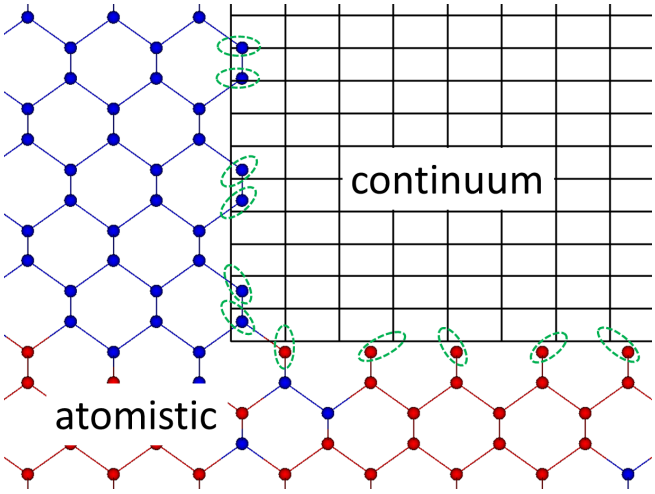

Fig. 1. Coupling of an atomistic (VFF) and a continuum (FEM) simulation domains. Here the interface atoms are paired to their nearest interface FEM nodes (marked with green circles). The atomistic and the continuum domains may have small overlap or gap, and not all interfacial atoms have to be coupled with FEM. Test simulations show that results are good enough as long as the sizes of the interfacial FEM mesh spacing are not too big and the pairing distances are close enough.

III. Results and Discussions

In this section two example applications of the coupled-VFF-FEM method are demonstrated: a Si FinFET strain simulation and a stress memorization technique (SMT) process [6] simulation. Both are the examples which are hard to be simulated by VFF-only method because of the size of simulation domains and/or the involvement of non-crystalline materials.

A. Application to Si FinFET strain simulation

The effect of atomistic-level variations on device performances is becoming more important as the critical dimensions are scaled down to few nanometers. In the case of FinFETs, for instance, there are only about 20 atom layers across the channel width so any changes in some of the atoms may result in significant device performance variations. The VFF method can be used for such atomistic-level strain analysis. Also, the results can be used for TB (or EH) electronic transport simulations [7].

Fig. 2 shows a simulated Si FinFET structure with raised epitaxial SiGe source and drain (S/D). The VFF method is applied only to the epitaxial S/D and a core part of the Si channel region because it is difficult for VFF to model the non-crystalline oxide material and solve the bulky substrate region. In VFF simulation the SiGe alloy is created by random number generations. The initial structure is generated assuming that the lattices of all the materials are the same to that of silicon substrate and the stress effect from previous process steps is not considered here. A Dirichlet boundary condition is applied to the bottom of the substrate and a periodic boundary condition is applied along the channel direction.

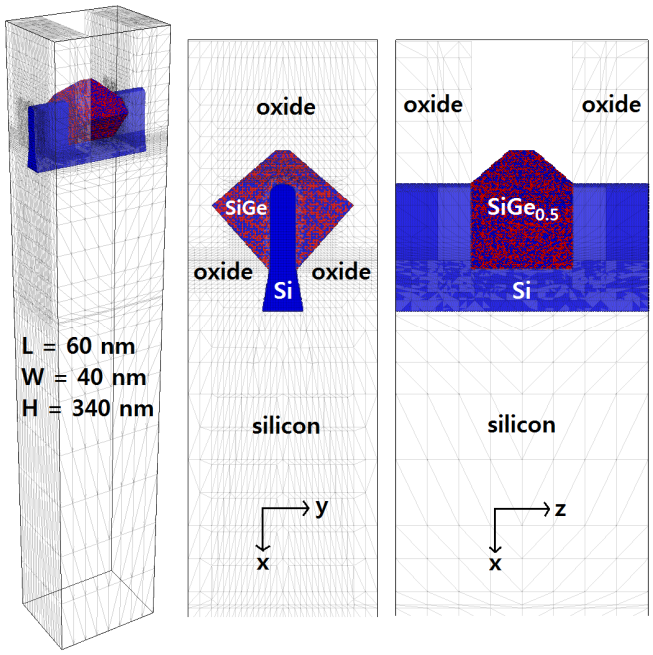

Fig. 2. Simulated silicon FinFET structure. The epitaxial S/D ($SiGe_{0.5}$ alloy) and a part of silicon channel region are solved by VFF method, and the silicon substrate and the oxide regions are solved by FEM.

Fig. 3 shows the calculated displacement field and stress profiles for the FinFET structure shown in Fig. 2. The displacement field is continuous over the entire simulation domain, which means the atomistic and the continuum methods are coupled well. We also obtained a good agreement wth the results of a FEM-only stress simulation (not shown here) where the SiGe alloy is assumed to have averaged lattice constant and elasticity. Note that the local stress values in the SiGe alloy region fluctuate with larger magnitude than the plot legends. It is also confirmed that the averaged value of the fluctuation is similar to that of FEM result. There are small errors at the atomistic-continuum interfaces which seem to be caused by uncoupled interfacial atoms since the mesh spacing is larger than inter-atom distances. It seems that the errors happen only locally and do not significantly affect the overall solution quality.

This coupled-VFF-FEM simulation has reached a good convergence after 7 Newton-Raphson iterations. The computation has been parallelized by the message-passing-interface (MPI) and an ordinary iterative sparse linear solver has been used. The simulation took about 10 minutes using 12 CPUs.

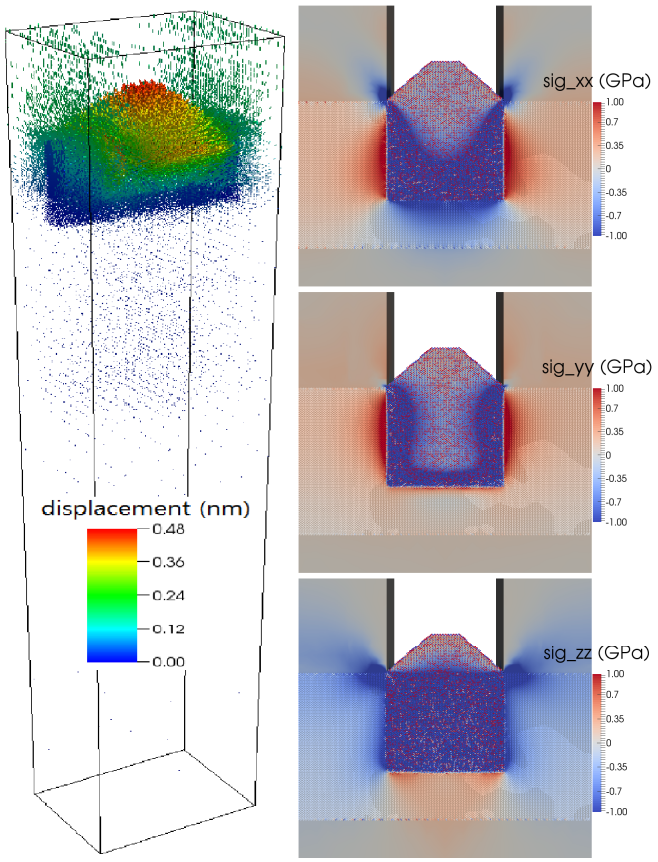

Fig. 3. Calculated displacement vector field (left) and stress profiles in the S/D epi and channel regions (right). The results have been validated by comparing with FEM-only simulation results.

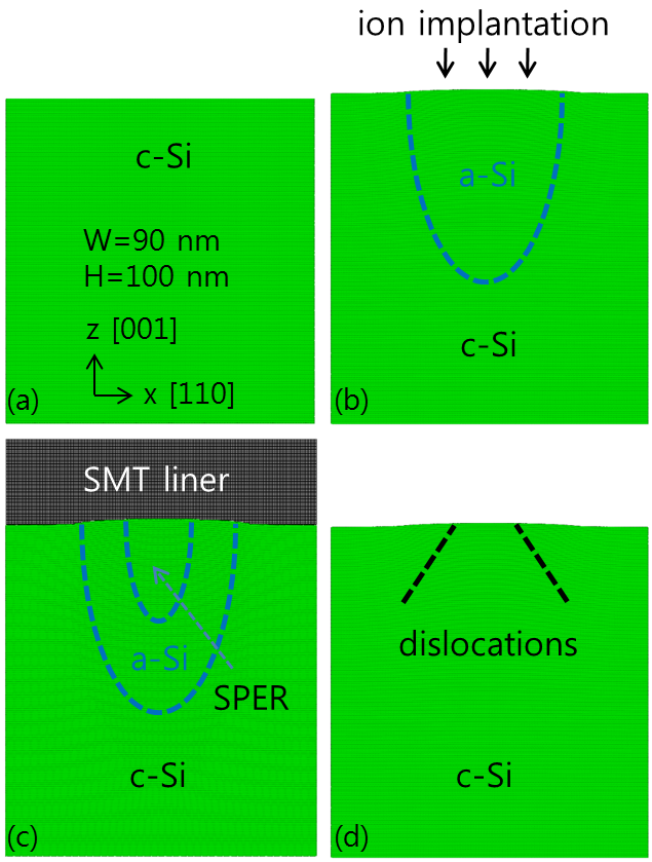

Fig. 4. Schematics of SMT process simualtions: (a) initial crystalline structure, (b) swollen structure due to ion implantation, (c) SPER snap shot simulations with SMT liner attached on top of the swollen surface, and (d) the final structure with dislocations.

B. Application to SMT process simulation

The formation of dislocations during solid phase epitaxial regrowth (SPER) is a complicated phenomenon in which many materials (crystalline Si, amorphous Si, nitride or oxide) and multiple process steps (ion implantation, over-layer deposition, SPER, and etch) are involved. There are existing SMT models [8, 9] providing valuable insights. In Ref [9], experimentally observed defect formation and evolution during SPER is nicely reproduced using the stress information of a-Si from FEM simulation. In this work, stress in a-Si is calculated by VFF.

Our approach to the SMT processes is shown in Fig. 4. The simulations start from an initial crystalline substrate shown in Fig. 4(a). The atoms at the bottom are fixed and the structure is assumed to be periodic along the x and y directions. By the ion implantation process c-Si near the top surface is turned into a-Si and the region is swollen, which is simulated by VFF method and shown in Fig. 4(b). In the VFF simulation a-Si region is treated as a material having a larger lattice constant and smaller elastic stiffness than c-Si. Experimentally, it is observed that both the average inter-atomic distance and the atomic density of a-Si formed by ion implantation are a little bit smaller than those of c-Si [10].

This apparent inconsistency is explained by vacancy type defects generated by ion implantation [10, 11]. In Ref. [10], vacancy in a-Si is defined as "unoccupied network site" which is similar to "morph-vacancy" suggested by Cowern *et al*. [12]. So, in our VFF simulation, the excessive vacancy with ~2% volume expansion is taken into account by using a large virtual atom for a-Si.

The expanded volume tends to reduce as recrystallization proceeds during SPER and leaves a residual expansion due to volume holding nitride over-layer as shown in Fig. 4(c). Without the nitride overlayer, the swollen a-Si region turns back into c-Si completely with no stress effect remaining, which is not the case with SMT. The shape of a-Si region can be simulated by the kinetic lattice Monte Carlo (KLMC) simulations for more rigorous a-c interface evolution. In this work, SPER snapshots were arbitrarily chosen to calculate stress distribution during SPER. Then, the shape of a-Si region, stress values, and/or vacancy profile during the SPER process can be used to determine the onset criteria of dislocation formation. For example, the shear stress component shown in Fig. 5(a) have some correlation with the dislocation formation [9]. In this simulation the sites corresponding to the

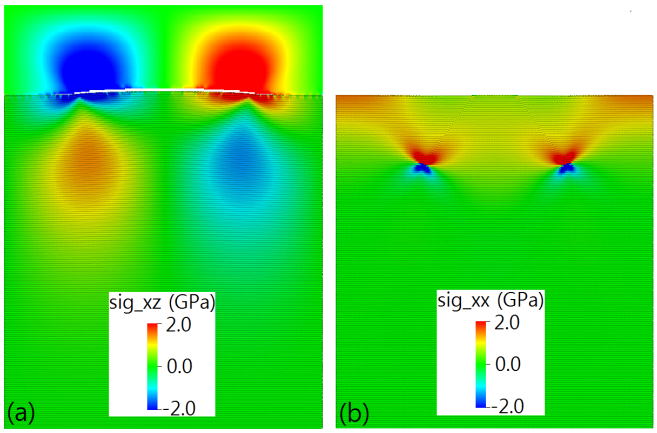

Fig. 5. (a) Shear stress distribution calculated from Fig. 4(c) by the coupled-VFF-FEM simulation. The gap between the top FEM and bottom VFF domains is just a visualization artifact since VFF changes atom positions but FEM does not. Actually, the solution is smoothly connected over the two domains. (b) normal (xx: lateral direction) stress distribution calculated from Fig. 4(d) by VFF simulation.

highest shear stress are chosen to be the centers of edge dislocations as shown in Fig. 4(d).

After the formation of dislocations is determined, we remove the SMT liner and run the final VFF simulation with the dislocations to calculate the desired stress profile. In the VFF simulation the dislocations are introduced atomistically. Fig. 6 shows the way that an edge dislocation is simulated within VFF method. The other dislocation types such as screw and mixed dislocations can also be simulated in a similar manner. We validated the correctness of the methods by comparing with MD simulation results (now shown here). The resulting stress profile is shown in Fig. 5(b). In this particular example it is observed that high tensile stress is applied to the channel region (both sides of the top surface) due to dislocations.

Note that the presented simulation results are performed to show feasibility of VFF-FEM application to SMT and the used parameter values of material properties are somewhat arbitrary. For quantitative simulations, more accurate information about a-Si and overlayer materials are required.

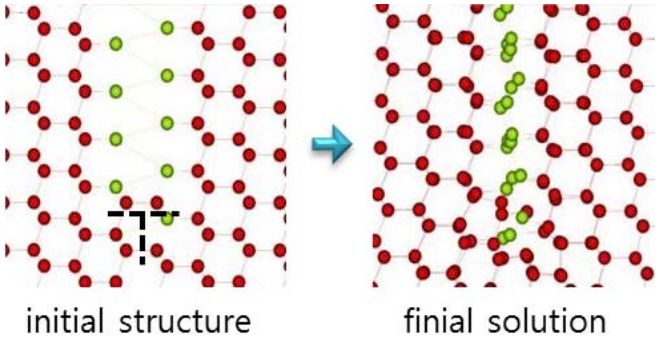

Fig. 6. VFF simulation of edge dislocation. Two atomic layers are removed from perfect crystaline structure and the inter-atomic bonding connectivities are redefiend (left). After a few iterations the atoms find their optimal positions (right).

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