Atomistic simulations of phonon- and alloy-scattering-limited mobility in SiGe nFinFETs

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***Abstract*—This paper presents atomistic simulation results about the performance limits of electron mobility in SiGe-channel nFinFETs, where phonon- and alloy-scattering-limited mobility are calculated based on the empirical tight-binding and the valence force field methods without any mobility fitting parameters. The effect of the changes in the fin thickness and sidewall orientation, SiGe alloy mole fraction, and external stress on the low-field electron mobility is investigated.**

Keywords—mobility; SiGe; FinFET; valence force field method; tight-binding method

I. INTRODUCTION

The calculation of electronic mobility has become an important device modeling issue to determine the expected device performance of SiGe channel FinFETs. In conventional approaches the mobility calculations often require many fitting parameters because of lacking detailed descriptions of electronic and phonon bandstrcutures and their interactions. Those approaches are easy, fast, and convenient when dealing with validated issues but do not guarantee the calculated results. It can be a big problem especially when the devices under investigation have different materials and/or operation conditions from conventional devices. Since SiGe FinFETs have different quantization, channel material, and stress conditions from conventional planar MOSFETs, the application of more rigorous theoretical models to the mobility calculation is accordingly required.

For accurate estimation of electronic mobility in SiGe nFinFETs we use atomistic simulations based on the empirical tight-binding (TB) and the valence force field (VFF) methods, which do not require any fitting parameters for mobility calculations other than parameters for bulk materials. The genetic algorithm (GA) method is used to obtain the bulk Si and Ge parameters.

In this paper we investigate the effects of quantum confinement, sidewall orientation, stress, and alloy mole fraction on the low-field electron mobility in SiGe-channel nFinFETs. Here, only the phonon and alloy scattering limited mobility are considered to assess the performance limit of the device.

II. SIMULATION METHOD

A. Material paramters from the genetic algorithm

First of all, TB parameters for bulk Si and Ge are extracted using the genetic algorithm method [1]. Several important bulk properties are used as the fitting targets, and the GA method, by evolving the model parameters, minimize the deviation between targets and extracted results. The details are explained in this section as follows.

In mobility calculations we need to capture accurately the band structure of both electrons and phonons, the matrix element of electron-phonon interactions and effect of strain. To ensure this, our TB and VFF models are parameterized so as to reproduce important band properties like band edges, effective mass, sound velocities and phonon energies at high symmetry k-points. In the case of electron-phonon interaction, we choose to calibrate the acoustic and optical deformation potentials of both conduction and valence bands. These are all carried out within our generic genetic algorithm (GA) framework. Here we briefly introduce GA for the sake of completeness of the paper.

Generally speaking, Genetic Algorithm employs stochastic methods based on the principle of natural selection and the evolution of biological systems. It is a powerful optimization method which does not have constraints like the continuity of solution space. The method is widely used in various engineering fields such as design of electromagnetic antennas and filters. The introduction of GA in semiconductor field is much recent.

A typical genetic algorithm contains several ingredients such as evaluation of object functions, selection, crossover, mutation and replacement. The solution space is sampled in the beginning of the algorithm and is evolving generation to generation towards optimized results.

Here we show the results of GA in terms of phonon band structures as well as deformation potentials, for both Silicon and Germanium. For electron band structure, we got similar results as [2], which will not be repeated here. The target values of phonons are from [3-4], GA results as shown in table

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1 match well with reference for both sound velocities and phonon energies. It is worth to point out that here we use a modified VFF model (MVFF) [5], which added 3 more terms to the standard Keating model (KVFF) [5]. The inclusion of these terms is necessary since KVFF model tends to give inaccurate phonon energies at zone boundaries, especially for X3 and L3 phonon modes.

For deformation potentials, the target values are from classical references like [6-7]. Our results are calculated from the response of electron band structure under certain strain conditions, in the same spirit as [6]. The GA method minimizes the deviation between our results and the target values. The results of deformation potentials for Si and Ge are summarized in Table 2. Here, we only show acoustic deformation potentials which are calculated from the band respond to uniform strain. These deformation potentials are relatively important since they determine not only scattering due to acoustic phonons but also the stress response of the material. For optical phonon scattering, the corresponding optical deformation potentials are important [8]. However, due to limited understanding of those deformation potentials to transport properties, we do not fit them in GA.

Phonon properties	Silicon		Germanium	
	Target	GA	Target	GA
$v_{100,l}$	8.43	8.51	4.87	4.95
$v_{100,t}$	5.84	5.79	3.57	3.45
$v_{110,l}$	9.13	9.12	5.36	5.31
$v_{110,t\parallel}$	5.84	5.80	3.57	3.46
$v_{110,t\perp}$	4.67	4.74	2.77	2.85
$v_{111,l}$	9.36	9.34	5.51	5.44
$v_{111,t}$	5.10	5.10	3.06	3.05
$\hbar\omega_{LTO}(\Gamma_{25'})$	64.16	66.11	37.33	38.02
$\hbar\omega_{TA}(X_3)$	18.63	18.63	9.87	9.33
$\hbar\omega_{LAO}(X_1)$	50.91	49.45	29.55	27.60
$\hbar\omega_{TO}(X_4)$	57.53	57.15	33.82	32.61
$\hbar\omega_{TA}(L_3)$	14.28	13.17	7.74	6.60
$\hbar\omega_{LA}(L_{2'})$	46.77	42.71	27.44	23.48
$\hbar\omega_{LO}(L_1)$	52.15	50.57	30.09	28.37
$\hbar\omega_{LO}(L_{3'})$	60.84	61.79	35.39	35.42

Table 1. Phonon properties of Si and Ge, where target values are according to [3-4] and fitted results are realized by GA method for the optimization of VFF parameters for Si and Ge. The unit of sound velocities is km/s, and unit of phonon energies is meV.

Deformation Potentials (eV)	Silicon		Germanium	
	Target	GA	Target	GA
a_c^{Δ}	3.82	3.78	7.75	4.55
a_c^{L}	-1.0	-0.95	-0.78	-0.78
a_c^{Γ}	1.62	1.71	-7.48	-7.79
Ξ_u^{Δ}	8.7	8.7	9.75	9.76
Ξ_u^{L}	18	17.3	15	15.3
a_v	2.1	2.1	2.0	2.0
b	-2.33	-2.32	-2.16	-2.15
d	-4.75	-4.75	-6.06	-6.05

Table 2. Deformation potentials of Si and Ge, where target values are according to [6-7] and fitted results ar realized by GA method for the optimization of empirical tight-binding parameters for Si and Ge. Δ- and L-valleys are well fitted for Si and Ge, respectively.

B. Phonon- and alloy-scattering-limited mobility models

The atomistic calculation of phonon-scattering-limited mobility is based on the empirical TB and VFF methods. The electron-phonon scattering rate can be written as

$$\frac{1}{\tau(\vec{k})}=\frac{2\pi}{\hbar}\sum_{k'}\left|\left\langle\vec{k}'\right|\sum_{nl}\frac{\partial H_{nl}}{\partial(\vec{R}_l-\vec{R}_n)}\cdot(\vec{u}_l-\vec{u}_n)\left|\vec{k}\right\rangle\right|^2\left(N_q+\frac{1}{2}\pm\frac{1}{2}\right)\delta(E_{k'}-E_k\pm\hbar\omega_q)\delta_{k'-k\pm q}$$

, where the electronic Hamiltonian (H_{nl}), energy (E_k), and wavefunction ($|k\rangle$) are calculated from TB method, and the phonon energy ($\hbar\omega_q$) and the displacement of atom (u_n) due to phonon vibration are obtained from VFF method. More details of the model can be found in [9-11]. Our approach is similar to the references but a little bit improved in that we calculate the microscopic deformation potential accurately from the TB strain model without relying on Slater-Koster formalism [12] and consider on-site Hamiltonian contributions as well as the nearest neighbor interactions due to phonon vibrations. Also, by checking and compensating the phase differences between the electron and phonon wavefunctions, the number of required phonon q-points can be reduced significantly and the computation speed becomes much faster than that of [9]. The calculated phonon-scattering-limited mobility values for bulk Si and Ge are show in the following table.

cm^2/Vs	Silicon	Germanium
$\mu_{e,phonon}$	1404	3860
$\mu_{h,phonon}$	426	1813

Table 3. Calculated phonon-scattering-limited mobility for unstrained bulk Si and Ge at 300 K.

For the alloy-scattering-limited mobility calculation, we generalized the atomistic approach for bulk SiGe shown in [13] to be able to simulate general device structures under stress condition. The alloy scattering rate is expressed as

$$\frac{1}{\tau_x(\vec{k})} = \int d\vec{k}' \left\langle \frac{2\pi}{\hbar} \left| \langle \vec{k} | H_{alloy}(\vec{k}) - H_{VCA}(\vec{k}) | \vec{k}' \rangle \right|^2 \delta(E(\vec{k}) - E(\vec{k}')) \right\rangle_{ens} \left(1 - \frac{v_x(\vec{k}')}{v_x(\vec{k})} \right)$$

, where the scattering potential is modelled as the deviation of the Hamiltonian of a certain alloy configuration (H_{alloy}) from the averaged Hamiltonian (H_{VCA}). The electron density, velocity, and wavefunctions are obtained from the averaged Hamiltonian system. The calculation requires an ensemble average of the transition rate from randomly generated alloy structures. Typically, at least 100 samples are needed to get a stable and converged result. The details of the atomistic alloy calculation can be found in [14]. When the approach is applied to thin layer structures, it seems that the surface roughness due to random alloy results in more scattering of electrons and decrease in mobility. However, the effect of surface roughness due to alloy is not investigated thoroughly in this paper.

III. Results and Discussions

In this section the behavior of the electron mobility of SiGe nFinFETs with different crystal orientations, fin thickness, and stress conditions is studied. Since the doping and bias conditions are usually rather uniform at any location in a rectangular fin channel and only the low-field mobility is interested, the simulation domain can be reduced to 1D structure with periodic boundary conditions along the transport (<110>) and the top of the fin directions, and there is a confinement only due to the sidewalls of the fin as shown in Fig. 1. For fair comparisons the flat-band with low channel doping condition is assumed and the simulation temperature is set to 300K for all the cases. sp3d5s* empirical TB model and the modified VFF model including bond stretching, bond bending, cross bond stretching, cross bond bending-stretching, and coplanar bond bending interactions are considered. A single mobility calculation takes about 40~70 CPU hours. The computations are parallelized based on the message passing interface (MPI).

Figure 2 shows the calculated phonon-scattering-limited electron mobility with different fin thicknesses and sidewall orientations. While Si-nFinFETs show higher mobility for {100} sidewalls than that of {110}, Ge-nFinFETs show better mobility for {110} sidewalls than that of {100}. The mobility of Si-nFinFETs with {100} sidewalls shows lesser sensitivity to the thickness changes than the other cases. The effect of the fin thickness changes on mobility cannot be fully understood within the conventional theories based on the effective-mass

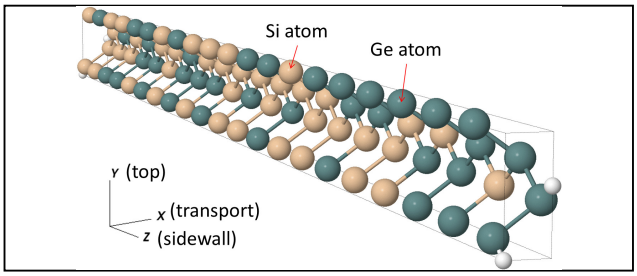

Fig. 1. Simulated atomistic structure for $Si_{0.5}Ge_{0.5}$ alloy channel with <101> transport and {110} sidewall directions.

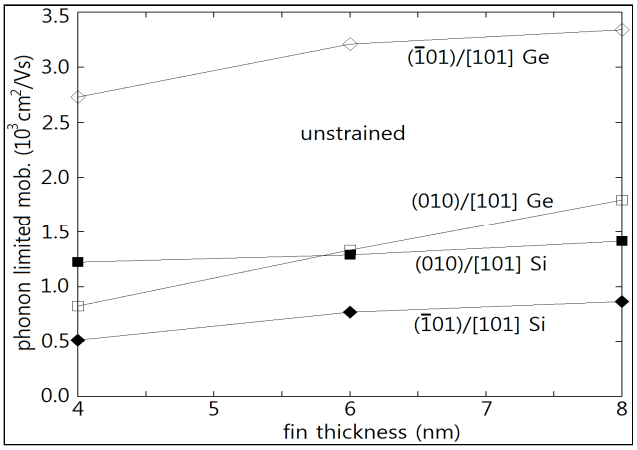

Fig. 2. Calculated phonon-scattering-limited mobility for unstrained Si- and Ge-channel nFinFETs with different fin thicknesses and sidewall orientations.

approximation because the effect of atomistic full-band structure becomes significant in the case of strong quantum confinement. The mobility values are also a little bit affected by the choice of passivation potential in the case of thin fin channels.

Figure 3 shows the calculated electron mobility for Si- and Ge-nFinFETs under different uniaxial stress conditions and sidewall orientations. In the simulations uniform stress profiles are assumed and the effect of the stress on the phonon system is not considered. For all the cases applying uniaxial tensile stress results in the increase of electron mobility but the gain starts to be saturated at about 2GPa, which is similar to the behavior of bulk mobility. The saturation of the stress gain is mainly due to the carrier population saturation in the lowest valleys, and the full-band description is needed to correctly capture the changes of valley edges and shapes. Ge nFinFETs show higher stress sensitivity than Si nFinFETs.

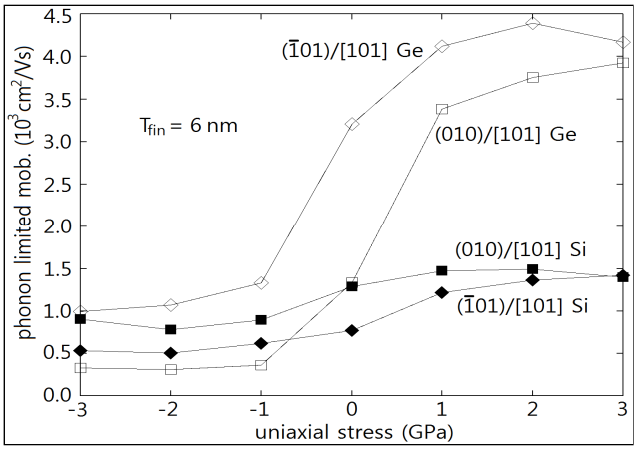

Fig. 3. Calculated electron mobility for Si- and Ge- nFinFETs under different uniaxial stress conditions along transport direction and sidewall orientations.

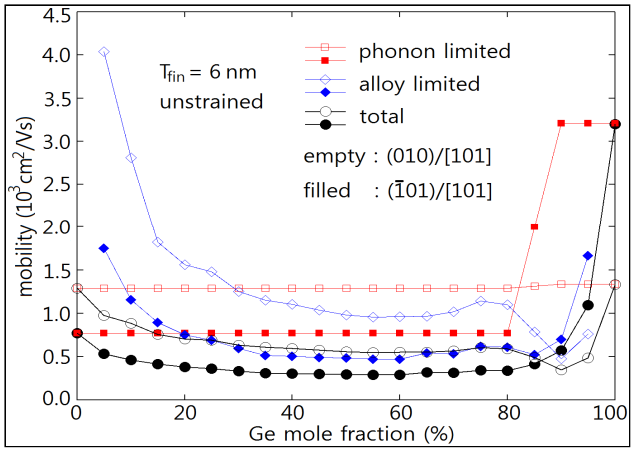

Fig. 4. Calculated electron mobility for unstrained SiGe-channel nFinFETs with different alloy mole fractions and sidewall orientations.

Figure 4 shows the calculated electron mobility for unstrained SiGe-channel nFinFETs with different alloy mole fractions and sidewall orientations. The phonon-limited mobility values for alloy-channel nFinFETs are assumed from those of Si- and Ge-nFinFETs, where a transition from Si- to Ge-like properties happens at about 85% of Ge mole fraction as the conduction band minimum changes from Δ-valley to L-valley. The reason of making the assumption is that the simulation of an alloy-channel requires a large size of atomistic random alloy structure to avoid artificial atom couplings due to periodicity and it is very time consuming. For the alloy-scattering-limited mobility calculations, however, the ensemble of realistic SiGe random alloy is considered. It should be noted that the internal stress induced by alloy atom configurations is neglected.

IV. SUMMARY

Atomistic simulations based on the valence force field (VFF) and the empirical tight-binding (TB) methods have been performed for better understanding and more accurate estimation of electron mobility in SiGe nFinFETs. This approach treats the electron-phonon interactions rigorously within the deformation potential theory and does not require any explicit fitting parameters for mobility calculations. Some basic material parameters for VFF and TB methods are extracted using the genetic algorithm and show good agreement with corresponding bulk material properties. No additional parameters are introduced for the mobility simulations for FinFETs, and the effect of the fin thickness, crystal orientation, external stress, SiGe alloy mole fraction has been investigated.

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