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# Electron mobility calculations of free-standing Si-nanowires with atomistic electron-phonon interactions

Yoshihiro Yamada, Hideaki Tsuchiya and Matsuto Ogawa

Kobe Univ. 1-1, Rokko-dai, Nada-ku, Kobe, 657-8501, Japan
Phone: +81-3-5549-6909 E-mail: tsuchiya@eedept-.kobe-u.ac.jp

## 1. Introduction

Until now, phonon-limited mobility in Si-MOS inversion layers[1] and Si-nanowire MOSFETs[2] has been calculated by modeling electronic bandstructures based on effective mass approximation and assuming dispersionless bulk phonon bandstructures. However, atomistic bandstructure modeling for electrons and phonons is indispensable for quantum transport simulations in nanoscale Si nanowire transistors[3]. In this work, phonon-limited mobilities of free-standing Si nanowires with diameters less than 5nm under a linear transport regime are presented.

## 2. Methodology

We combined atomistic tight-binding method for electronic bandstructures[4] and Keating potential method[5] for phonon bandstructures to compute electron-phonon interaction Hamiltonian matrix elements. And we used Fermi's golden rule to calculate phonon scattering rate including Pauli's exclusion principle. Finally we calculated phonon-limited mobility using linearized Boltzmann transport equation under a linear transport regime. Phonons were assumed to be equilibrium Bose-Einstein distributions. Furthermore, we compared atomistic phonon-limited mobilies with continuous model[2] assuming electronic bandstructures of effective mass approximation and phonon bandstructures of dispersionless bulk phonon bands.

## 3. Results and Discussions

*Atomistic bandstructures of electrons and phonons*

Fig. 1 shows electronic bandstructures of 3nm diameter Si nanowires. Locations and degeneracies of conduction band minima in arbitrary orientations are explained from quantum confinement of six ellipsoidal valleys in Si[6]. Fig. 2 shows transport effective masses with various diameters and orientations extracted at conduction band minima. As the diameter decreases, transport masses of <100> and <111> Si nanowires increase due to quantum confinement. However, transport mass of <110> nanowire decreases less than bulk effective mass as the diameter decreases. Effective mass reduction of <110> nanowire should lead to significant improvement of electron mobility. Fig. 3 shows phonon bandstructures of 3nm diameter Si nanowires in low frequency regimes. Fig. 4 shows diameter dependences of sound velocities extracted at Γ points. LA and TA denote longitudinal and transverse sound velocities respectively. As diameter decreases, both sound velocities decrease. This is phonon confinement effect. On the other hand, as diameter increases, LA and TA velocities show convergence to bulk sound velocities. Fig. 5 shows phonon density of states of Si nanowires with the diameter 3nm. Sharp peaks around 60~70 meV in all transport orientations indicate optical phonons. These optical phonons should have significant influences on electron mobility. And the density of states around 10~40meV indicate mixed states of acoustic and optical phonons. Fig. 6 shows atomic vibration vectors of lowest four acoustic phonon bands at Γ points. Unlike bulk phonons, four acoustic phonon bands of Si nanowires can be divided into two flexural, one torsional, one longitudinal mode[7] in ascending order. In Fig. 3 (a) and (c), two flexural modes in <100> and <111> nanowires are degenerate due to rotational symmetry as shown Fig. 6 (c) and (d). On the other hand, two non-degenerate flexural modes of <110> nanowire in Fig. 3 (b) appear due to structural anti-symmetry. Therefore, Keating potential method is able to capture the confinement effect and anisotropic effect.

*Phonon-limited electron mobility*

Fig. 7 and Fig. 8 show phonon-limited mobilities of atomistic and continuous models respectively. In Fig. 7, <110> nanowires show about twice larger than <100> and <111> due to the smaller transport mass than bulk mass as shown in Fig. 2. However, electron mobilities of <100> nanowires is larger than those of <110> nanowires as shown in Fig. 8. There are reverses of magnitude relation in atomistic and continuous models. This is because continuous phonon scattering model ignores variations of effective masses, sound velocities and deformation potentials for all orientations. These results indicate considering atomistic effects of electron and phonon bandstructures will play increasingly significant roles in modeling electron mobility of Si nanowires as the diameter decreases.

## 4. Conclusions

Phonon-limited mobilities of free-standing Si nanowires in <100>, <110> and <111> transport orientations were simulated by combining atomistic electron and phonon bandstructures. As a result, <110> Si nanowire showed most highest mobility with smaller diameters.

## Acknowledgements

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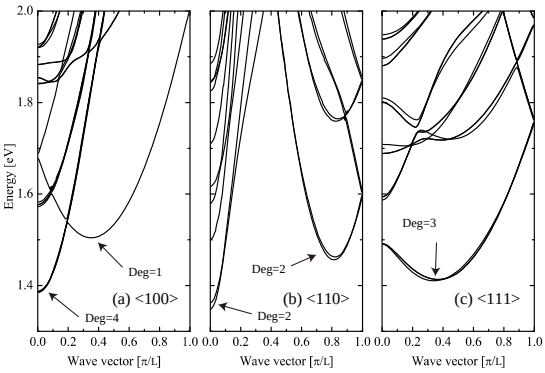


Fig. 1 Electronic bandstructures of Si nanowires of 3nm diameter with (a) <100>, (b) <110> and (c) <111> transport orientations. Deg denote degeneracies of conduction bands

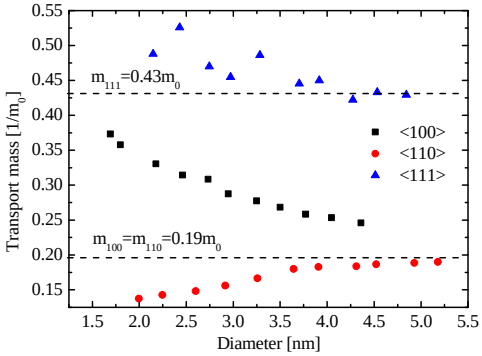


Fig. 2 Diameter dependences of effective masses at conduction band minima with <100>, <110> and <111> transport orientations. Dashed lines denote bulk effective masses.

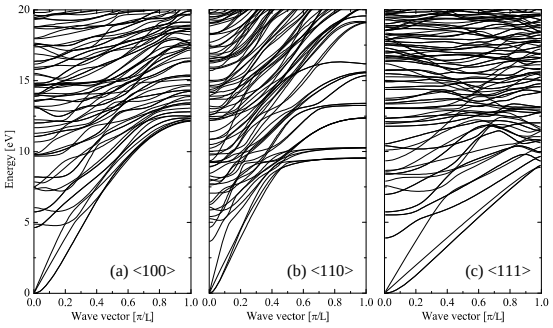


Fig. 3 Phonon bandstructures in low frequency regimes of Si nanowires in <100>, <110> and <111> transport orientations with the diameter 3nm.

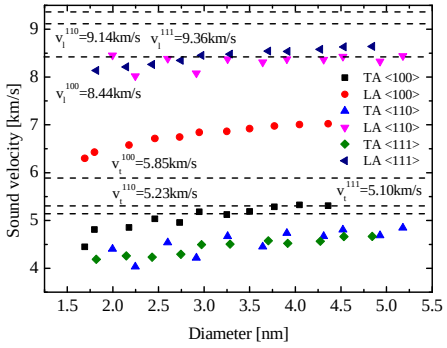


Fig. 4 Diameter dependences of sound velocities for acoustic phonons with <100>, <110> and <111> transport orientations. Dashed lines denote bulk sound velocities.

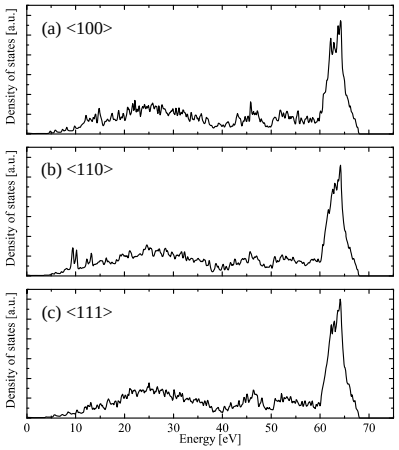


Fig. 5 Phonon density of states of Si nanowires in (a) <100>, (b) <110> and (c) <111> orientations.

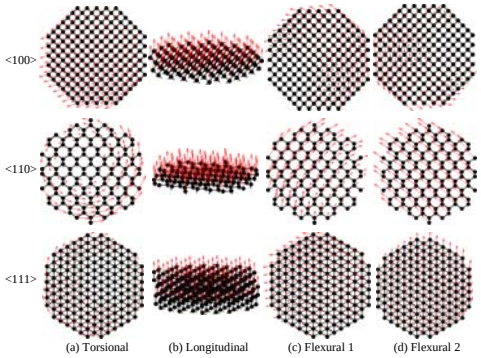


Fig. 6 Vector plots of atomic vibrations in <100>, <110>, <111> orientations with the diameter 3nm.

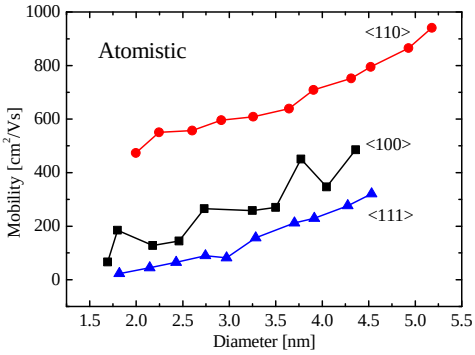


Fig .7 Atomistic phonon-limited mobility as a function of nanowire diameter.

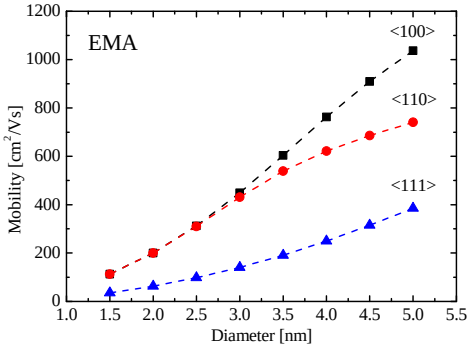


Fig .8 Phonon-limited mobility based on classical model as a function of nanowire diameter