Electron Energy Loss Behavior in Si Quantum Dots Interconnected with Tunnel Oxide Barriers

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Abstract

Electron and phonon wave functions are numerically calculated for 1D silicon/oxide heterostructure. The phonon emission rate is larger than the one calculated for Si quantum wire, while the energy loss rate at near the bottom of the minibands is much smaller, showing energy ranges at which energy loss is strongly suppressed.

Introduction

Recently, silicon/oxide heterostructures have attracted growing attention due to its optical applications, which stimulated the study of electron transport along silicon/oxide superlattices [1]. A possibility of energy loss suppression in Si dots interconnected with thin oxide layers has also been suggested [2][3]. In this work, electron energy loss behavior in such a 1D Si-dot/oxide system is studied. Electron and phonon wave functions are numerically calculated, and are used to evaluate electron-phonon scattering and energy loss rates.

Electron and Phonon States

Fig. 1 shows the illustration of the system under study. Electrons are confined in *y* and *z* direction, being delocalized only in the *x* direction. The Si dots are modeled as cubes of 4nm per side, and the thickness of the oxide layers is 1nm. For simplicity, electrons are assumed to be on the ground quantum states in the *y* and *z* direction. Fig. 2 shows the electron miniband structures produced by the periodic potential in the *x* direction. The barrier height of the oxides is set 1.0 eV. Fig. 3 shows the longitudinal phonon dispersion in the *x* direction, calculated by the 1D atomic linear chain model with harmonic approximation. Each Si region is composed of Si atoms, while each oxide layer contains Si and O atoms alternating each other. The Young's modulus of the bulk Si and SiO_2 determined the spring constants in Si and oxide region. Note that the energy gaps appear, and the optical phonons are dispersionless. These optical phonon waves are confined in Si regions, which is typically seen in superlattice structures and known as "confined optical phonons".

Phonon Emission and Energy Loss Rates

Fig. 4 shows the phonon emission rate calculated using the electron and phonon wave functions obtained above. The curve was obtained for the electrons on the 4th miniband. The broken line shows the result obtained for the system without oxide layers, that is, silicon quantum wire. Note that the introduction of the oxide layers increases phonon emission rate. Fig. 5 shows the energy loss rate, defined as the expectation value of energy loss at each phonon emission. Note that the energy loss rate at near the bottom of the miniband is less than the one calculated for silicon quantum wire, which was generally seen for other minibands. This indicates that the periodic insertion of the oxide layers generates the energy ranges at which electron energy loss is suppressed. The energy ranges are denoted as "Low Energy Loss Channel" in Fig. 6. This effect is caused by the modulation of electronic and phononic states due to superlattice structure. Details will be discussed in the presentation.

Conclusion

Periodic introduction of oxide layers in 1D silicon quantum wire may produce energy ranges at which electron energy loss is suppressed.

Acknowledgements

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References

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[2] Koshida *et al.*, Appl. Surf. Sci., 146, p. 371 (1999)
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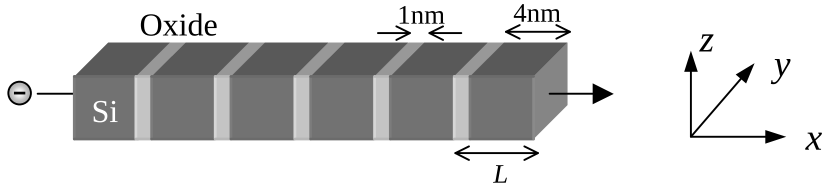

Fig.1 Schematic illustration of Si dots interconnected with thin oxide layers. *L* denotes the size of the unit cell in this periodic structure.

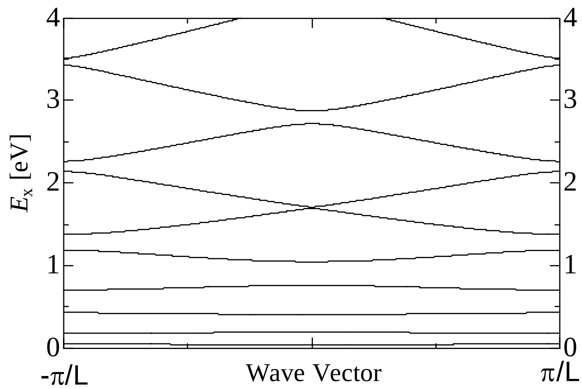

Fig.2 Electron miniband structure calculated for oxide barrier height of 1.0eV.

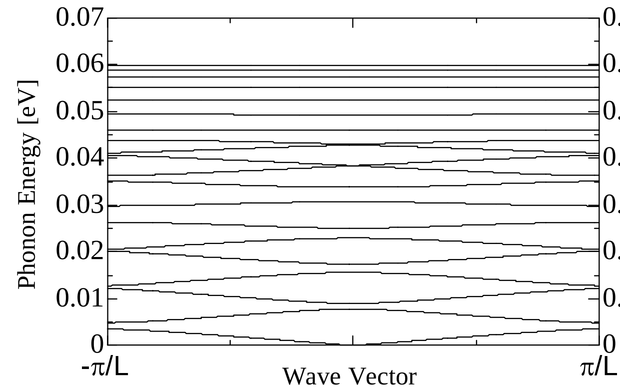

Fig.3 Longitudinal (along x-direction) phonon dispersion, showing energy gaps and confined optical phonon modes.

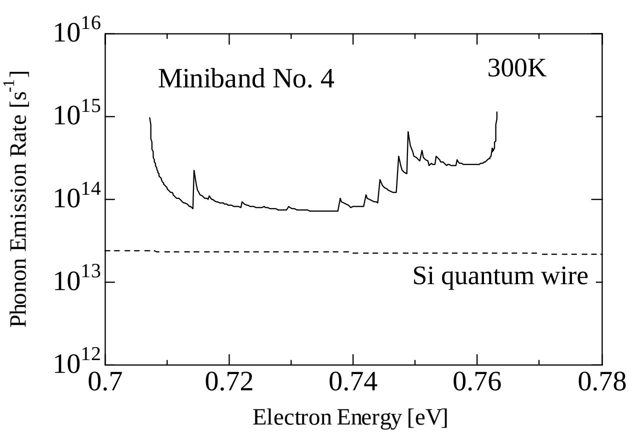

Fig.4 Scattering rate for phonon emission process calculated for electrons in the 4th miniband. Broken line shows the result calculated for the case without oxide barriers, i.e., Si quantum wire, showing that introduction of oxide barriers increases phonon emission rate.

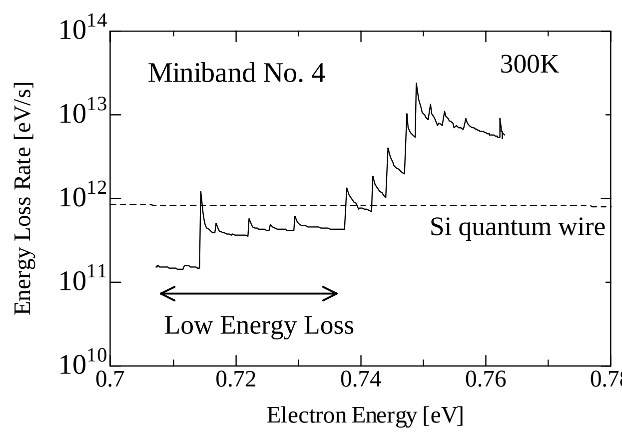

Fig.5 Energy loss rate calculated from the results shown in Fig. 4. Note that the energy loss rate at near the bottom of the miniband is less than the one calculated without the oxide layers, which was generally seen for other minibands.

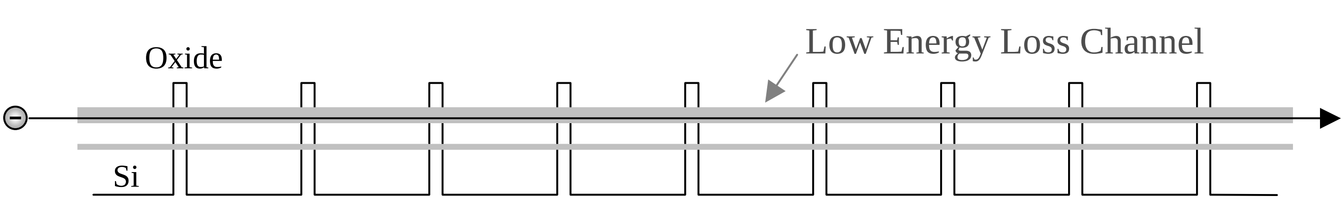

Fig.6 Schematic illustration of energy ranges at which electron energy loss is suppressed, denoted as “Low Energy Loss Channel” .