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A Theoretical Study of Electron Wave Function Penetration Effects on Electron–Modulated-Acoustic-Phonon Interactions in Silicon Nanowire MOSFETs

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1. Introduction

Silicon nanowire (SiNW) MOSFETs, illustrated in Fig. 1, have been attracting considerable attention as one of the promising device structures for further CMOS scaling due to their better electrostatic gate control [1, 2]. Acoustic phonons in nanostructures are modulated by interfaces between acoustically different materials, and therefore they differ from bulk phonons, which are usually used as substitute for actual acoustic phonons. Recent studies have reported that such acoustic phonon modulation (APM) has appreciable impacts on electron transport in free-standing SiNWs [4–7], as well as coated SiNWs [3, 8]. However, although the impacts also depend on electron states, it is not clear in operating SiNW MOSFETs how much effect the modification of electron states due to the gate voltage has on them. In this work, we theoretically investigate the interaction between modulated acoustic phonons and electrons in gate biased SiNWs.

2. Electron–Modulated-Acoustic-Phonon Interactions

Figure 2 shows the calculation model of acoustic phonons in a SiO_2-coated SiNW. Assuming the core and coating shell are isotropic continua, acoustic phonons can be derived from Navier's equation. Figure 3(a) shows their dispersion relation. Acoustic phonons scatter electrons through a deformation potential (DP), and the scattering rate is given by

$$\frac{1}{\tau_{mn}(k_z)} = \sum_{m',n'} \frac{D_{ac}^2 k_B T_L}{2\hbar v_l^2 \rho} \int_{-\infty}^{\infty} I_{mn,m'n'}(q_z)\delta(E - E')\left(1 - \frac{k_z'}{k_z}\right)\mathrm{d}k_z',$$

where (m, m') are the electron quantum numbers in the θ-direction before and after the scattering, respectively, (n, n') those in the r-direction, (k_z, k_z') the wavevectors along the z-axis, (E, E') the energies, and T_L the lattice temperature. Also, D_{ac}, v_l, and ρ are the acoustic DP constant, longitudinal sound velocity, and mass density in a SiNW, respectively. The form factor $I_{mn,m'n'}(q_z)$ is the wave function overlap between electrons and acoustic phonons, and describes all differences between modulated and bulk phonons. Figure 3(b) shows the form factor for the intra-lowest-subband scattering caused by modulated acoustic phonons in SiO_2-coated SiNWs of different t_{ox}'s. Note that the form factor at small $q_z a$ is larger than that for bulk phonons. This form factor increase enhances the electron scattering and degrades the mobility as shown in Fig. 4. The increase, however, becomes suppressed with thickening of the SiO_2 shell, because the shell strongly weakens the phonon vibration in the core. In addition, if the shell is acoustically harder than the core and sufficiently thick, the form factor would be smaller than that for bulk phonons, and hence the electron transport properties would improve [8]. As an example of such case, the results calculated for a HfO_2-coated SiNW are shown in Figs. 3(b) and 4.

3. Interactions in Gate Biased SiNWs

All calculations in the previous section were done under the assumption that electrons are confined to the core with an infinite potential well having a flat bottom. In SiNW MOSFETs, however, the potential is not flat due to the gate voltage, and therefore the electron states are different from those obtained in flat bottom potential well. The electron states in practical devices can be described by the Schrödinger–Poisson equation. We solved it for a cross section with/without taking into account wave function penetration (WFP) into the oxide shell in the same manner as that presented in Refs. [9] and [10]. The resulting electron states for a SiO_2-coated [001]-oriented SiNW are shown in Fig. 5. Figure 6 shows the modulated and bulk phonon form factors calculated for the intra-lowest-subband scattering in the 4-fold valley and for several gate voltages, V_G's. In the calculation, the interaction in the oxide shell was ignored or D_{ac} in the shell was set to zero, because the two form factors are insensitive to it, as can be seen from Fig. 7. The two form factors decrease with increasing V_G whether with or without WFP, which is clearly seen in Fig. 8(a). The figure shows the two form factors at $q_z a = 0$ as functions of V_G. As can be seen in Fig. 5(c), the electron wave function spreads throughout the cross section with increasing V_G, and accordingly it becomes narrower in the radial wavevector domain. The radial wavevector spectrum of the product of the initial and final wave functions for a scattering shows the contribution of individual acoustic phonon modes to the scattering. The spectrum for the intra-lowest-subband scattering is shown in Fig. 9, and as expected, it narrows toward small wavevector with increasing V_G, which indicates that phonons with a relatively large wavevector become less able to contribute to the scattering. Thus, the form factor decreases whether with or without APM. In addition, WFP reduces further the two form factors because it makes the wave function wider in the space domain and narrower in the wavevector domain. Figure 8(b) shows the ratio of the two form factors, and indicates that the APM effects become larger with increasing V_G or with taking WFP into account. This is because the wave function becomes closer to the interface between the core and shell which causes APM.

4. Conclusion

The interaction between modulated acoustic phonons and electrons in gate biased SiNWs was investigated theoretically. It was found that, although with increasing gate voltage

the form factor decreases whether with or without APM, the APM effects become larger. In addition, WFP reduces further the form factor and strengthens the APM effects.

References

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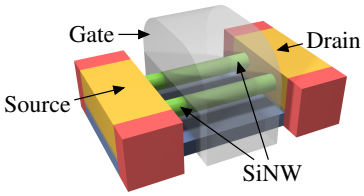

Fig. 1: Schematic view of a SiNW MOSFET.

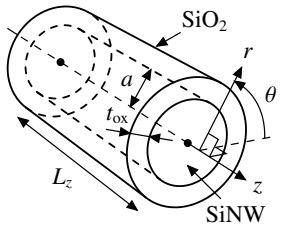

Fig. 2: SiNW model for acoustic phonons. A SiNW of length L_z and radius a is coated with a SiO_2 shell of thickness t_{ox}. We used the cylindrical coordinates, and assumed that L_z is infinite and the shell surface is free.

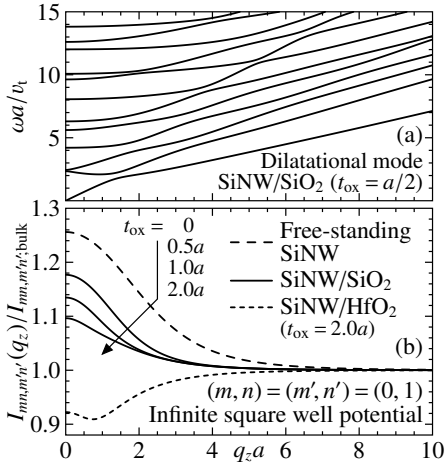

Fig. 3: (a) Acoustic phonon dispersion relation in a SiO_2-coated SiNW. The horizontal axis represents the phonon wavevector along the z-axis, q_z, and the vertical axis the frequency, ω. (b) Modulated phonon form factor calculated for the intra-lowest-subband scattering, plotted as a function of $q_z a$. The vertical axis is divided by the bulk phonon form factor.

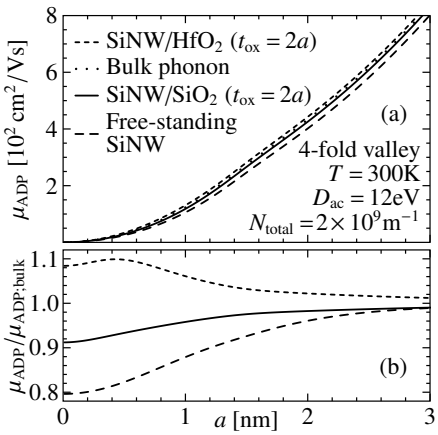

Fig. 4: (a) Values of electron mobility limited by the intra-lowest-subband scattering due to modulated acoustic phonons, calculated for 4-fold valley electrons in [001]-oriented SiNWs of different radii. (b) Their ratios to the bulk phonon limited mobility.

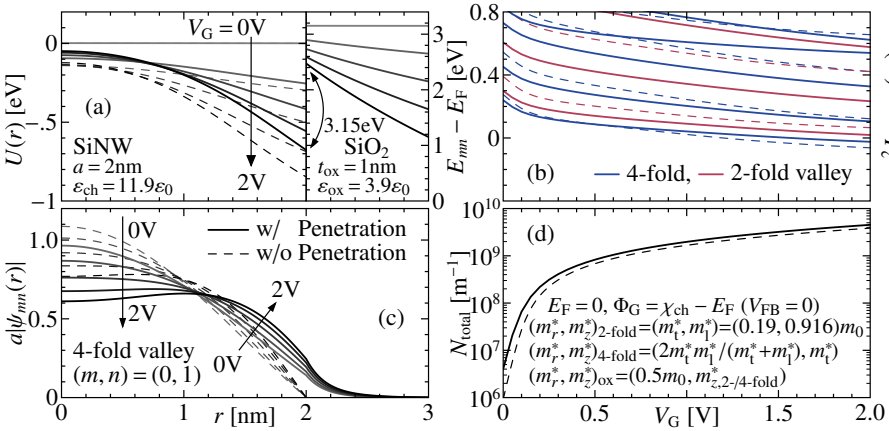

Fig. 5: Gate voltage dependence of the electron states in a cross section of a [001]-oriented SiNW with a SiO_2 shell: (a) potential profile, (b) energy levels mesured from the Fermi level, (c) wave function for the lowest subband in the 4-fold valley, and (d) total electron density.

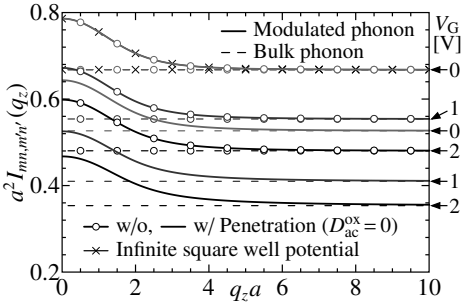

Fig. 6: Modulated (solid lines) and bulk phonon form factors (dashed lines) calculated for the intra-lowest-subband scattering, and for several V_G's. The horizontal axis represents $q_z a$. The calculation was performed for a [001]-oriented SiNW of $a = 2$ nm coated with a SiO_2 shell of $t_{ox} = 1$ nm, and with the electron wave functions shown in Fig. 5(c).

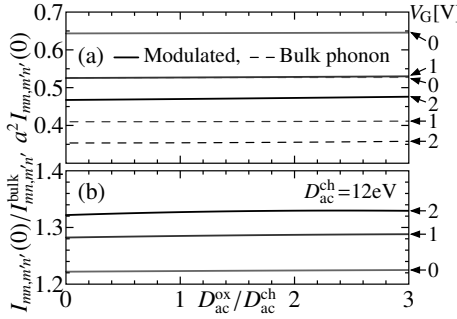

Fig. 7: (a) Modulated and bulk form factors at $q_z a = 0$ for several V_G's plotted as functions of D_{ac} in the shell divided by that in the core. (b) Their ratios.

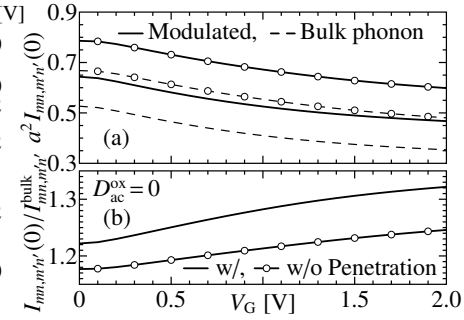

Fig. 8: (a) Modulated and bulk form factors at $q_z a = 0$ calculated for different V_G's with/without taking into account the electron wave function penetration, (b) Their ratios.

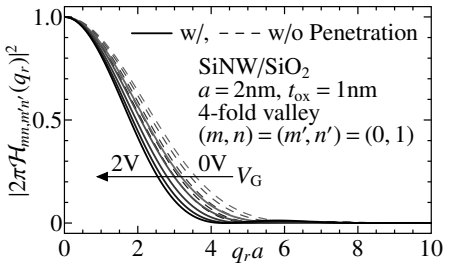

Fig. 9: Radial wavevector spectrum of the product of the initial and final wave functions for the intra-lowest-subband scattering, which can be obtained through the Hankel transform. The area of this spectrum gives the bulk phonon form factor for $D_{ac}^{ox} = D_{ac}^{ch}$.