Inelastic Acoustic Phonon Scattering in Ultra-thin SOI and Nanowire Structures

Nobuya Mori^{1,2}

 ¹Graduate School of Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan Phone: +81-6-6879-7698, E-mail: mori@physics.org
²CREST, JST, 5 Sanbancho, Chiyoda-ku, Tokyo 102-0075, Japan

Acoustic-phonon scattering is considered to play a dominant role in determining electron mobility in ultra-thin silicon-on-insulator and nanowrire structures, because in the elastic and equipartition approximation the scattering rate increases as a power function with decreasing the lateral dimension. The strong spatial confinement of electrons in ultra-thin structures, however, leads to an expansion in k-space, which makes the usual elastic approximation questionable. Here I present a theoretical calculation of acousticphonon scattering rate in ultra-thin structures without using the elastic approximation.

I consider two-dimensional electron gas (2DEG) in a Si slab of the thickness t and 1DEG in a Si nanowrire (Si NW) of the diameter D (= 2R). For ultra-thin structures, electrons mainly occupy the lowest subband. I thus calculate the acoustic-phonon scattering rate only within the lowest subband. Using the Fermi's golden rule, the scattering rate is given by

$$W_{\pm}(E_i) = \frac{2\pi}{\hbar} \sum_{q,f} D^2 \left(\frac{\hbar}{2\rho V \omega_g}\right) q^2 \{N_q + \frac{1}{2}(1 \mp 1)\} \\ \times |\langle f| e^{iq \cdot x} |i\rangle|^2 \delta(E_i \pm \hbar \omega_q - E_f), \quad (1)$$

where $W_+(E_i)$ ($W_-(E_i)$) is the absorption (emission) rate of an initial electron energy E_i , D the deformation potential constant, ρ the mass density, V the crystal volume, $\omega_q = s_l q$ the phonon frequency, s_l the longitudinal sound velocity, q the magnitude of the phonon wavevector, N_q the phonon occupation factor, and i (f) the initial (final) electronic state index. In the present study, I am interested in the impact of the elastic approximation on the acoustic-phonon scattering rate, and consider only electron–bulk-longitudinalacoustic-phonon scattering within an isotropic deformation potential approximation.

By using the elastic and equipartition approximation, the absorption rate becomes equal to the emission rate, and we have

$$W_0 = \frac{m_d k T D^2}{2\hbar^3 c_l} \int |\xi_0(z)|^4 dz = \frac{m_d k T D^2}{2\hbar^3 c_l} \frac{3}{2t}$$
(2)

for 2DEG, and

$$W_0(E_i) = \frac{kTD^2}{\hbar^2 c_l} \sqrt{\frac{m_d}{2E_i}} \iint |\xi_0(y,z)|^4 dy dz$$
$$= \frac{kTD^2}{\hbar^2 c_l} \sqrt{\frac{m_d}{2E_i}} \frac{f}{R^2}$$
(3)

for 1DEG. Here kT is the thermal energy, c_l the elastic constant, m_d the density-of-states mass, ξ_0 the lateral wavefuncion associated with the quantized motion, and f = 0.67. Effects of the elastic approximation are studied by comparing the scattering rates calculated through Eq. (1) with those through Eqs. (2) and (3).

Figure 1 shows normalized scattering rates as a function of the slab thickness t for $E_i = kT$ at T = 300 K. The normalized scattering rate is defined by the scattering rate of Eq. (1) normalized by the corresponding scattering rate of the elastic approximation. In the limit of vanishing thickness, all the phonon wavectors perpendicular to the slab equally participate the scattering in the elastic approximation. Phonons with larger wavectors, however, cannot contribute to the scattering when one include finite phonon energy because of large phonon energy. This results in the strong reduction in the normalized scattering rate for thinner regions. This reduction occurs when $t \leq 4\pi \hbar s_l/E_i$ (see Fig. 2). Therefore, one can safely use the elastic approximation only for thicker slab and higher electron energy. In the limit of $t \rightarrow 0$, I find that the scattering rate remains finite on the contrary to the elastic approximation (see Fig. 3).

Figures 4, 5, and 6 show the results for Si NWs. I find that resonant phonon emission occurs when $D \approx 2\pi\hbar s_l/E_i$ (see Fig. 5). It originates in the singular nature of the density-of-states at the bottom of the subband. Because of this resonance, the elastic approximation underestimates the scattering rate near the resonant condition. This is marked contrast to the 2DEG case where the elastic approximation overestimates the scattering rate. We see that the elastic approximation can be safely used only for thicker diameter and larger electron energy as in the 2DEG case (see Fig. 5).



Figure 1: Normalized scattering rates as a function of the slab thickness *t* for $E_i = kT$ at T = 300 K.



Figure 2: Normalized total scattering rates as a function of *t* for $E_i = kT/2$, kT, and 2kT. Vertical arrows show the condition of $t = 4\pi\hbar s_l/E_i$.



Figure 3: Slab-thickness dependence of the scattering rate normalized by W_0 of the elastic approximation at t = 10 nm.



Figure 4: Normalized scattering rates as a function of the NW diameter *D* for $E_i = kT$ at T = 300 K.



Figure 5: Normalized total scattering rates as a function of *D* for $E_i = kT/2$, kT, and 2kT. Vertical arrows show the condition of $D = 2\pi\hbar s_i/E_i$.



Figure 6: NW-diameter dependence of the scattering rate normalized by W_0 of the elastic approximation at D = 10 nm.