Size and Stress Effects in Ultraviolet Raman Spectra of Few-Nanometer-Thick SOI Nanofilms and Single Nanowires for Future CMOS Devices

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1. Introduction
Si on insulator (SOI) structure was introduced as a key building block for the next generation microelectronic devices. SOI nanofilms (NFs) with thickness \( H < 10 \text{ nm} \) are considered as important elements in the complementary metal-oxide-semiconductor technology for integrated circuits with enhanced performance such as reduced threshold and applied voltages, increased switching speed etc. Small cross-section nanowires (NWs) made of SOI attract especially high interest due to quantum confinement effects enhancing hole mobility and the NW field effect transistor. Phonon confinement and other phonon size effects are also becoming increasingly important in thin SOI NFs and NWs. Since the carrier mobility depends on stress, any information on the stress induced by an insulating oxide coating is also important.

In this work, we study SOI NF/NW Raman spectra (RS). In contrast to other works, where NF/NW Raman bands were artificially broadened due to size distribution, poor crystal quality etc., we obtain natural bandwidth and observe phonon boundary scattering (PBS) overlooked in other NF/NW Raman studies. We also study coating-induced stress in NWs and laser-induced stress in NFs.

2. Experimental
Commercially available initial SOI structures were received from SOITEC. [001]-oriented SOI were located on the top of a 145 nm BOX (\( H_{\text{BOX}} = 145 \text{ nm} \)) covering a Si substrate. Initial thickness of SOI (\( H \)) was 70 nm. Then \( H \) was decreased using thermal oxidation with the subsequent etching in HF. \( H \) was controlled by the electron microscopy, ellipsometry and optical reflection spectroscopy.

[110]-oriented Si NWs with the rectangular cross-sections were fabricated from the SOI layers with \( H \approx 7 \text{ nm} \) and \( \sim 12 \text{ nm} \) using electron beam lithography and electron cyclotron resonance plasma etching. One more set of 12 nm thick NWs was prepared, using \( \text{O}_2 \) etching at high temperature and low pressure. Then it was coated with a 2.4 nm \( \text{HfO}_2 \) layer, using atomic layer deposition, and with \( \sim 170 \text{ nm} \) thick \( \text{SiO}_2 \) layer using chemical vapour deposition. Fig. 1a schematically shows a sample with NWs while Fig. 1b shows TEM image of cross-sections of coated NWs.

RS were measured in the back-scattering geometry with the light directed along the [001] axis of SOI using a NanoFinder-30 confocal Raman microscope (Tokyo Instruments Inc.) equipped with a 364 nm wavelength laser corresponding to the resonant Raman enhancement and small (10-15 nm) penetration depth of light in Si. Most of the measurements were done at the liquid nitrogen temperature for the Raman band sharpening. High spectral resolution was achieved using Echelle grating working in the 65-th order. The lateral orientation of SOI was different from the orientation of Si substrate, namely, the [110] axis of SOI was parallel to the [100] axis of Si substrate (Fig. 1a). Therefore, the ZZ polarization configuration was correspondent to the allowed Raman signal from NWs and forbidden one from the Si substrate.

3. Phonon Confinement, Boundary Scattering and Stress Effects in SOI Nanofilms and Nanowires
Fig. 2 shows Raman intensity map of a \( \sim 12 \text{ nm} \times 20 \text{ nm} \) SOI NW and \( \sim 1 \mu\text{m} \) square piece of SOI NF. NF and NW Raman signals are allowed and enhanced by the Mie resonance [1] and interference in BOX [2], respectively.

Fig. 3 shows relationships between Raman band downshift (\( \Delta \omega \)) and broadening (\( \Delta \text{FWHM} \)) in NWs and NFs obtained in our experiment (scatters) and calculated using Richter-Campbell-Fauchet (RCF) model [3] describing phonon confinement through the relaxation of the wave
vector $q = 0$ selection rule. One can see deviations of both NW and NF experimental data from the theoretical curves. The experimental Raman band downshift is smaller than that suggested by the theory, band broadenings being equal.

Obviously, there is a band broadening mechanism that is not considered by the RCF theory. This is PBS that reduces the phonon lifetime in NFs/NWs. Thus, the full band width at half-maximum FWHM = $\Delta$FWHM$_{conf} + I_{bulk} + I_{bound}$ where $\Delta$FWHM$_{conf}$ is the asymmetric band broadening due to the phonon confinement, $I_{bulk} \sim 1.7$ cm$^{-1}$ is the natural bulk Si Raman band width at ~77K and $I_{bound}$ is the symmetric band broadening due to PBS. According to the Casimir limit in NFs, $I_{bound} = \frac{V}{2\pi c}$, where $V$ is the phonon group velocity and $c$ is the speed of light.

Fig. 4 shows 77 K RS of 3 nm thick SOI fitted with the RCF theoretical curve obtained using $I = I_{bulk} + I_{bound} = 2.85$ cm$^{-1}$, $\Delta$FWHM$_{conf} \sim 0.25$ cm$^{-1}$ is less than $I_{bound} = 1.15$ cm$^{-1}$ indicating a weak $q$ relaxation. Fig. 5 shows $\Gamma$ vs. $1/H$ dependence displaying a nice linearity with $V = 600$ m/sec. Phonon lifetime $\tau = \frac{1}{\Gamma} \Delta \Gamma$ and mean free path $\lambda = \frac{V}{\tau}$ vs. $H$ are shown in Fig. 6. Their decrease with the decrease in $H$ cause decrease in thermal conductivity and should be considered in the carrier mobility calculations.

3 nm thick SOI NF FWHM ~ 3.1 cm$^{-1}$ < FWHM ~15 cm$^{-1}$ of 4 nm thick NF [3]. This is why PBS was overlooked in Ref. [3] and some other works.

RS of SOI NWs with the 12 nm x 12 nm and 7 nm x 9 nm cross sections are shown in Fig. 7. Similar to SOI NFs, RCF fitting (green curves) was made not with $I_{bulk}$ but with $I_{bulk} + I_{bound}$ equal to 2.3 cm$^{-1}$ and 2.6 cm$^{-1}$, respectively.

Fig. 8 shows 77 K RS of 12 nm thick SiO$_2$-coated NWs with different W. The NW Raman shift increases and a tensile stress converts to a compression with decrease in $W$. This indicates stress non-uniformity, namely, compression at the edge while straining in the NW inner area. Assuming W-independence in the edge stress, we can expect a NW band upshift with decrease in $W$. It is confirmed theoretically and should influence the carrier mobility.

Fig. 9 shows dependencies of SOI NF Raman shifts on $H$ at two different laser excitation power densities. At the high excitation ~1mW/$\mu$m$^2$, SOI NFs with the thickness of 19 nm and 30 nm display strong Raman band upshift that can be explained only by compressive stress in the area heated by the laser light. We discuss the reason why this effect is taking place at specific SOI NF thicknesses.

3. Conclusions

We have fabricated SOI NFs and NWs for future CMOS devices and studied their RS. Phonon confinement effect ($q$ relaxation) is found to be weak, while PBS is strong. We take into account PBS for the NF/NW Raman band fitting using the RCF model. PBS shortens the phonon lifetime and mean free path and, therefore, influences thermal conductivity and carrier mobility. SiO$_2$ coating produces NW stress converting from tensile to compressive with the decrease in NW width. This should be considered in the carrier mobility calculations. High-power laser light causes compressive stress in SOI NFs at certain thickness.

References