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Probing Transverse-Optical Phonons in Strained Si Nanowire: Strain Profiles and Nanomechanical properties

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1. Introduction

Owing to the profound influence of strain on band structure and lattice symmetry of silicon, strain and stress nanoengineering has emerged as a powerful strategy to expand the capabilities of silicon-based nanoscale technologies [1]. For instance, strain was recently demonstrated to alleviate design difficulties and performance degredation faced in the emerging nanowire-based architectures such as tri-gate and gate-all-around nanowire MOSFETs. However, the exploitation of the full potential of strain-engineered silicon nanowire devices raises major challenges. One of them, is related to development of accurate, less invasive, and sensitive techniques to probe on the nanoscale the strain and the associated changes in the nanowire properties. A number of techniques have been proposed to measure the amount and distribution of strain in Si nanoscale systems. However, each of these techniques suffers a number of limitations such as being invasive or insensitive to all strain components, or having a limited spatial resolution. Raman spectroscopy has been found to be effective in mapping the strain fluctuations in Si despite its relatively limited spatial resolution. Recently, we improved the spatial resolution of ultra-violet micro-Raman imaging (backscattering configuration) by using Glycerin-immersed high numerical aperture (NA) objective lens [2]. Nevertheless, though imaging with only longitudinal-optical (LO) phonon is enough to map the average in-plane strain, Raman shift from transverse-optical phonons are required for a more accurate characterization of strain. This is because hole and electron relative mobilities are related to in-plane and out-of-plane stress distributions [3].

In this work, we demonstrate for the simultaneous observation of LO and TO phonons in single silicon nanowires. The nanowires were fabricated using ultrathin strained silicon-on-insulator (UT-SSOI) by combining electron beam lithography and reactive ion etching. The local strain and the involved free surface-induced strain redistribution during the formation of the ~15nm thick nanowire (30nm x 1000nm) is investigated using high-resolution polarized Raman spectroscopy. In-plane and out-of-plane strain profiles in single nanowires are obtained through the simultaneous excitations and detections of LO and TO phonons. The relaxation of strain associated with TO Raman shifts across individual strained nanowires is analyzed and compared to LO related shifts. The intensity of the measured Raman spectra is analyzed based on three-dimensional field distribution of linear polarizations focused by a high NA lens. The effects of sample geometry and collection efficiency of the lens on the sensitivity of TO measurement are considered. New insights into strain relaxation and its influence on the nanomechanical properties of nanowires are also discussed.

2. Experimental Configuration and Sample preparation

Polarized micro-Raman measurement was carried out in backscattering configuration using a modified inverted optical microscope with a PZT driven *xy* stage. This is based from our previous reports. The incident light was *x*-polarized parallel to the UT-SSOI nanowire and the scattered light was analyzed parallel and perpendicular to the SSOI nanowire axis. The nanowire affixed on the *xy* translation stage was scanned with a step size of 50nm. At each step, the scattered Raman spectrum was recorded at different analyzer orientation relative to a fixed UT-SSOI sample azimuth. A single Lorentz function was fitted to the Raman spectrum obtained using $z(x,y)\bar{z}$ setting (LO-active), to determine the peak frequency of LO phonons. On the other hand, a double Lorentz fit function was utilized for $z(x,x)\bar{z}$ setting (TO-active) to decompose and determine the peak frequency of TO phonons. This was because both LO and TO phonons exist in the obtained spectrum. It should be stressed that during double Lorentzian fitting, the LO peak position was fixed and assumed the value obtained from the single Lorentzian fit of $z(x,y)\bar{z}$ setting. This was done at each position in the nanowire simply because the LO phonons vary along the nanowire.

The cross-sectional transmission electron micrograph (TEM) of UT-SSOI film used in this study is shown Fig. 1(a). The ~15nm thick strained Si films were fabricated by epitaxial growth of Si on ~500nm thick $Si_{1-x}Ge_x$ buffer

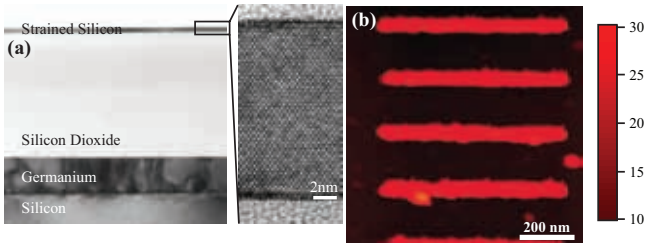

Figure 1. (a) TEM image of "background free" substrate UT-SSOI (b) AFM image of 30×1000nm nanowire.

layers on Si (001) substrate. Using the direct wafer bonding and ion-cut process, the strained layer was then transferred onto a handle substrate capped with oxide layer and ~120nm thick layer of Ge deposited by molecular beam epitaxy. The introduction of a highly absorptive Ge layer underneath the buried oxide was used to suppress substrate background during Raman analysis. Figure 1(b) displays the Atomic Force Microscope (AFM) image of an extended array of UT-SSOI nanowires. The patterned nanowires having dimensions of 30×1000nm are aligned along the <110> direction.

3. Discussion of Results

Figure 2a shows the shows the measured Raman spectra at the center of the ε-Si nanowire using $z(x,x)\bar{z}$ (TO-active) and $z(x,y)\bar{z}$ (LO-active). We can clearly see that the TO-active is broader than the LO-active condition. This is because the TO-active condition consists of contributions from both LO and TO phonons. The Si-Si LO mode peak position is centered at ~516.7 cm^{-1}, which is 2.4 cm^{-1} above the value in the initial film (~514.3 cm^{-1}). This strain relaxation is induced during patterning (RIE process). This is expected due to the formation of free surfaces. We found that the Si-Si TO peak position located at ~517.7 cm^{-1} is more relaxed compared to the Si-Si LO peak. Figure 2*b* shows the profiles of out-of-plane and in-plane stress calculated from the TO peak and LO peak positions using Eq. 1 and Eq. (2), respectively. The stress-induced Raman shift for doublet ($\Delta\omega_d$: TO phonons) and singlet ($\Delta\omega_s$: LO phonons) are obtained using[4]:

$$\Delta\omega_d = \left[p(S_{11}+S_{12}) + q(S_{11}+3S_{12})\right]\sigma / 2\omega_0 \qquad (1)$$

$$\Delta\omega_s = \left[pS_{12} + q(S_{11}+S_{12})\right]\sigma / \omega_0 \qquad (2)$$

where $\omega_0 = 520.5$ are the Raman frequency shift (cm^{-1}) of Si. The $S_{11} = 7.68$ and $S_{12} = -2.14$ (in GPa) are the elastic compliance tensor elements, while $p = -1.85\omega_0^2$ and $q = -2.31\omega_0^2$ are the phonon deformation potentials for bulk Si. The plotted data are the average from two scans on the same nanowire under the same experimental condition. We observed that both in-plane and out-of-plane stress relaxations become more pronounced away from the center of the nanowire. The stress behavior plateaus at $300 \le x \le 700$ nm, which means that the stress is insensitive to along the length of the wire in this region. The edges of the nanowire are more relaxed compared to the center and this can also be due to edge-induced stress. Based on Hu's generally acknowledge model of relaxing film stress, we can describe the distribution of stress $\sigma(x)$ along the wire using the equation below[5]:

$$\sigma(x) = A\left(1 - \exp\left[-\sqrt{\frac{2Kx}{d\pi}}\right] - \exp\left[-\sqrt{\frac{2K(L-x)}{d\pi}}\right]\right)$$

$$K = \frac{E_{SiO_2}(1-\nu_{\varepsilon Si}^2)}{E_{\varepsilon Si}(1-\nu_{SiO_2}^2)} \quad and \quad (S_{11}+S_{12}) = \frac{(1-\nu_{\varepsilon Si}^2)}{E_{\varepsilon Si}} \qquad (3)$$

where, A is proportionality constant which takes the maximum stress at the center and L is the length of the nanowire. The stress relaxation is dependent on the ratio of the thickness of the ε-Si layer ($d \approx 15nm$) and the relative rigidity K between the SiO_2 substrate and ε-Si. The relative rigidity defined in Eq (3) is a function of material mechanical property, where E and ν denotes the Young's modulus and the Poisson ratio, respectively. Using the Eq (3), the best-fit value for K is indicated in Fig. 2b. Result suggests that relative rigidity is different for in-plane (LO) and out-of-plane stress (TO). This is because the stress arises from the lattice parameter mismatch between the strained layer and oxide substrate. From Eq. (3), we can easily calculate the E and ν for strained silicon nanowire as shown in Fig. 2. The obtained values are consistent with the numerical calculations for Si (001). [6].

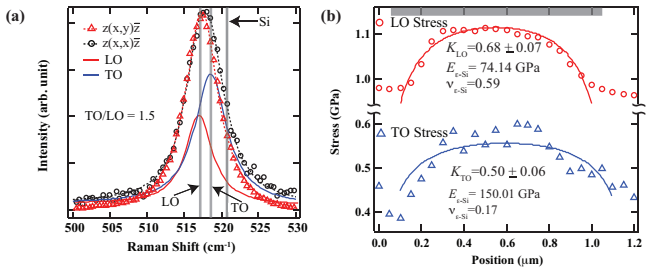

Figure 2. (a) Raman spectra of LO and TO phonon at the center of nanowire (b) Stress distribution along the UT-SSOI nanowire.

4. Conclusions

In summary, we have demonstrated a method to observe simultaneously the forbidden TO phonon and LO phonon mode in UT-SSOI with sufficient sensitivity and spatial resolution using polarized micro-Raman. The introduction of a Ge capping layer circumvented the issues associated with strong substrate background and thereby improving the sensitivity of TO measurement. Remarkable insights on the evolution of TO and LO phonons in SSOI nanostructures were obtained. The relaxation along the SSOI nanostructure is different due to the formation of edges. This heterogeneous LO and TO strain distribution and the coexistence of different strain relaxation originating along the SSOI nanostructures also provide the mechanical characteristic of strained nanowire that are also important on the study of stress and design of SSOI-based devices.

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