Optical Characterization of Ultrathin Ge-on-Insulator: Electron and Phonon Confinement, Raman Enhancement, Optical Phonon Lifetime Reduction, Acoustic Phonon Spectral Reconstruction and Drop in Thermal Conductivity

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Abstract

We fabricated Ge-on-insulator (GOI) monocrystal nanolayers with thickness H = 1 - 18 nm and studied their Raman and optical absorption spectra. Absorption spectra display L-point direct-band-gap peak blue shift due to electron quantum confinement. Raman spectra display longitudinal optical (LO) phonon and acoustic phonon bands. For H < 5 nm, additional bands due to amorphous-like inclusions appear in the spectra. In accordance with the wave vector quantization theory, observed confined-acoustic-phonon frequencies show $\sim 1/H$ dependence at H > 5 nm. However, for H < 5 nm, we observe deviation from this law. With a decrease in H, the LO phonon Raman band displays enhancement and downshift. Also as H decreases, the band homogeneously broadens proportionally to 1/H. We attribute these findings to a reduction in reflectance plus electron confinement, thickness-dependent stress and surface- disorder-induced phonon lifetime reduction. We also observe strong laser-induced GOI heating suggesting extremely low thermal conductivity.

1. Introduction

Ge is a promising material for high performance complementary metal-oxide-semiconductor (CMOS) transistors and optoelectronic devices since it offers much higher carrier mobility and smaller optical band gap than Si. Ge-on-insulator (GOI) can provide CMOS field-effect transistors with high-speed operation. A low junction leakage current in thin-body GOI is also a benefit for channel materials with small band gap. Another benefit of Ge is its compatibility with Si technology. Although its smaller band gap can often induce a higher junction leakage current, it has been reported that thinning Ge layers down to ~ 4 nm can suppress the off-state current. On the other hand, ultrathin GOI heating can be a problem. Therefore, fabrication and studying properties of ultrathin GOI is an important task. In this work, we fabricate ultrathin GOI nanolayers and study their electronic, phononic and thermal properties using Raman and optical absorption/reflection spectroscopy.

2. Experimental

We fabricated Ge-on-fused-SiO₂ monocrystalline nanolayers with the thickness H = 1 - 18 nm utilizing high

quality heteroepitaxial growth and Ge layer transfer with epitaxial lift-off technique on arbitrary substrate [1,2]. To evaluate Ge layer thickness, we selectively etched Ge by H_2O_2 -based solution down to the SiO₂ substrate and measured the depth of the formed trench by atomic force microscopy (AFM) (Fig. 1 inset).



Fig. 1. a) Raman spectra of \sim 6.5 nm and \sim 1.1 nm thick GOI in *XX* and *XY* polarization configurations. Arrows show a-Ge bands Inset schematically shows GOI thickness measurement using AFM.

b) Laser power dependencies of 6.5 nm thick GOI LO phonon band Raman shift and full width at half-maximum (FWHM).

Raman measurement was done using Nanofinder 30 Raman/AFM system (Tokyo Instruments Inc.) equipped with a 561 nm wavelength laser. Low-frequency measurement was done with a set of three volume-Bragg-grating notch-filters (OptiGrate Co). Additional Raman measurements were done using Renishaw spectrometer with 488 nm and 514.5 nm lasers. CRAIC micro-spectrophotometer was used for reflection/transmission measurement.

3.Results

Figure 1 shows Raman spectra of two GOI samples with H = 1.1 nm and 6.5 nm in two polarization configurations. In the *XX*-configuration with both polarizer and analyzer parallel to the [110] axis of GOI, one can see a strong longitudinal optical (LO) phonon Raman band at ~301 cm⁻¹. The 1.1 nm thick film spectrum displays additional broad bands of amorphous Ge (a-Ge) inclusions at 60-90 cm⁻¹, 180 cm⁻¹ and 280 cm⁻¹. These bands are pronounced in the *XY* configuration with analyzer parallel to the [1-10] axis suppressing LO-phonon band. Weaker a-Ge inclusion bands are displayed in other GOI samples with H < 5 nm. Fig. 1b shows laser power dependencies of LO phonon band Raman shift and FWHM revealing very strong laser-induced heating suggesting very low GOI thermal conductivity *k* reduc-

ing with a decrease in H.



Fig. 2.a) Theoretical (curves) and experimental (symbols) thickness dependencies of GOI Raman enhancement factor compared to bulk Ge at the 561 nm (black), 514.5 nm (green) and 488 nm (blue) excitation wavelengths.

b) Theoretical (red) and experimental (black) absorption spectra of ~2.4 nm thick GOI Arrows show peak positions.

Figure 2a shows thickness dependence of the LO-phonon Raman band enhancement factor compared to bulk Ge for 561 nm, 514.5 nm and 488 nm excitation wavelengths. Symbols stand for experimentwhile curves of corresponding colours show theoretical enhancement factors calculated with optical constants of bulk Ge. Theoretical GOI Raman enhancement is higher than the experimental one for the 561 nm excitation wavelength. Contrary, for 514.5 nm and, especially, for 488 nm wavelength, the experimental enhancement exceeds theoretical one. With a decrease in the excitation wavelength, experimental maximum shifts to smaller H while theoretical one remains unchanged. These findings are associated with the fact that the experimental Raman enhancement is influenced by both reflectivity reduction and electron confinement enlarging Ge L-point direct energy band gap and causing blue shift of the Raman resonance. Discrepancy between experiment and theory occurs because our theoretical calculations do not take into account the electron quantum confinement.

Figure 2b shows experimental (black) and theoretical (red) absorption spectra of ~2.4 nm thick GOI. Theoretical spectrum does not take into account quantum electron confinement. Therefore, we can determine confinement-induced blue shift of the L-point direct-band-gap absorption peak from the difference between the experimental and theoretical absorption peak positions shown in Fig. 2b. It is ~0.1 eV for $H \sim 2.4$ nm. For smaller H, the effect is stronger.

Figure 3a shows thickness dependence of the LO phonon Raman shift with excluded laser-induced heating. The band displays a downshift with reduction of GOI thickness. For H > 12 nm, GOI displays Raman upshift compared to bulk Ge. This can be explained only by compressive stress remaining after the fabrication process. Since the stress is involved, size-induced GOI Raman band downshift can be also explained by stress, tensile one in this case. Analysis of the LO phonon Raman band shape shows homogeneous band broadening proportional to 1/H (Fig. 3b). No noticeable band asymmetry associated with the wave vector relaxation is observed even for thinnest GOI. Linear fitting of FWHM(1/H) dependence reveals two values: 1) 2.56 cm⁻¹ is FWHM of infinitely thick GOI, which is larger than bulk Ge FWHM ~ 2.4 cm⁻¹, probably, due to stress and 2) 3.21 cm⁻¹nm describing impact of the oxide-induced surface disorder on the LO phonon lifetime.



Fig. 3.a) Thickness dependence of the GOI LO phonon band Raman shift. Horizontal line shows bulk Ge value \sim 301.1 cm⁻¹.

b) Dependence of GOI LO phonon Raman band FWHM on 1/H and its linear fitting. Red line shows bulk Ge value ~2.4 cm⁻¹.

Figure 4a shows low-frequency *XX*-configuration Raman spectra of several GOI samples. The spectra display confined acoustic phonon bands of four types marked with four different symbols in Fig. 4a,b. For H > 5 nm, acoustic phonon frequencies ω_{ac} show ~ 1/*H* dependence (Fig. 4b) in accordance with the wave vector quantization theory. However, for H < 5 nm graphs in Fig. 4b display deviation from ~1/*H* law due to change in GOI mechanical properties or change from discrete to continuum mode Raman activity.



Fig. 4.a) GOI acoustic phonon Raman spectra. *H* values are shown.b) Dependence of acoustic phonon frequencies on 1/*H*.

4.Conclusion

We fabricated few nanometer thick GOI layers and observed a number of size effects in their Raman and optical absorption spectra with a decrease in *H*: 1) Raman signal enhancement, 2) electron-confinement-induced L-point direct band gap enlargement, 3) LO phonon Raman band downshift and homogeneous broadening ~1/*H*, 4) acoustic phonon confinement with a) ω_{ac} ~1/*H* at *H* > 5 nm and b) deviation from ω_{ac} ~1/*H* law at *H* < 5 nm, 5) *k* reduction.

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