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OPTICAL STUDY OF MBE GROWN UNDOPED $Si-Si_{1-x}Ge_x/Si$ SUPERLATTICES

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Raman spectroscopy and spectroscopic ellipsometry have been used to characterize $Si/Si_{0.78}Ge_{0.22}$ superlattices grown by molecular beam epitaxy on (001)Si at different substrate temperatures. The results are interpreted to give information on material and interface quality, layer thicknesses, and state of strain. The observed frequencies of zone-folded longitudinal acoustic phonons in a high quality sample agree well with those calculated using Rytov's theory of acoustic vibrations in layered media.

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There is a current interest in $Si-Si_{1-x}Ge_x/Si$ multi quantum wells (MQW) and superlattices (SL) because of their potential application in optoelectronics: typically infrared photodetectors for thermal imaging devices with a photoresponse spectrum in the 8–13 μm wave band [1]. Such devices require a number of selectively p-type doped strained $Si-Si_{1-x}Ge_x/Si$ cal thicknesses of 3–10 nm, separated by wider Si barriers (30–50 nm) and capped with p-type doped Si for electrical contact.

Previously some results of Raman studies of acoustic phonons have been published for undoped Si–SiGe SLs with periods $N > 20$ and grown at substrate temperatures, T_s, below 500°C [2]. In this paper we report the results of Raman scattering and ellipsometry study of five-period $Si-Si_{1-x}Ge_x/(001)Si$ ($x = 0.22$) strained-layers SLs grown by solid source molecular beam epitaxy (MBE) (VG Semicon V90S) at different substrate temperatures T_s = 550, 650, 700, 750, and 810°C. The layer sequence, their thicknesses and corresponding conduction and valence-band edges [3] are shown in the inset of Fig. 1.

Raman scattering provides a rapid mean of characterizing a superlattice and also provides a technique for studying the vibrational and electronic properties,

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the strain within the superlattice layers, and ordering within the alloy layers. Spectroscopic ellipsometry was used to obtain the optical constants needed in the Raman studies. Light scattering measurements were carried out using the Brewster-angle quasiback scattering geometry with the angle of incidence set at 76.9° (Brewster's angle for the samples at 488 nm). The Raman spectrum was excited with 200 mW of 488 nm argon laser light, frequency analyzed with a U 1000 Jobin Yvon double monochromator, detected with a cooled RCA 31034A photomultiplier and recorded using a computer. All measurements were carried out at room temperature in a helium-gas atmosphere, which was used to eliminate air features from the spectrum. An analysis at the depth of about 345 nm allows for information about phonon modes in the multilayer structure and the Si-cap.

Low frequency Raman spectra are of special interest in semiconductor superlattices. The longer period d in the superlattices compared with the unit cell size results in a much smaller Brillouin zone (minizone) of maximum wave vector $q_{\max} = \pi/d$ compared to the original Brillouin zone $q_{\max} = 2\pi/a$, where a is the lattice constant. The existence of a reduced Brillouin zone in the SL substantially modifies the acoustic phonon spectrum through the "folding" of the original dispersion curves into the new minizone. According to the elastic continuum theory of Rytov [4] for layered media, the folded acoustic phonon dispersion can be described by

$$\omega = \omega_0(m \pm dq/2\pi), \qquad (1)$$

where q is the component of the light scattering wave vector perpendicular to the layers and is given by $q = [4\pi n_{\mathrm{SL}}(\lambda)/\lambda][1 - (1/4[n_{\mathrm{SL}}(\lambda)]^2)]$, $m = 0, 1, 2,...$ is the zone folding index, $m\omega_0$ is the minizone centre frequencies, λ is the incident laser light wavelength and $n_{\mathrm{SL}}(\lambda)$ is the refractive index of the superlattice at this wavelength.

In Raman experiments the semiconductor superlattices doublets of acoustic phonons (see Eq. (1)) can be observed. The number and the intensity of the observed doublets are mostly dependent on the crystalline and SL interface quality [5].

Low frequency Raman spectra obtained from two $Si/Si_{0.78}Ge_{0.22}$ superlattices grown at $T_s = 810$°C and 650°C are shown in Fig. 1. Sharp lines attributed to zone-folded longitudinal acoustic modes were observed only for the sample grown at $T_s = 810$°C and perhaps the non-ideal superlattice structure was responsible for the absence of folded acoustic modes for all another investigated samples.

The experimental and calculated Raman peak frequencies of the folded acoustics modes in the $Si/Si_{0.78}Ge_{0.22}$ ($T_s = 810$°C) superlattices are given in Table. The frequencies calculated with Rytov's theory and the observed peak positions are in good agreement. It should be noted that the Raman signal in the low-frequency region is extremely weak due to the cap layer absorption and the low number of periods ($N = 5$).

The optical phonons have been the most widely studied features in superlattices from both the theoretical and experimental points of view. The Raman spectrum of SLs at higher frequencies usually exhibits first order features characteristic of the two materials. In our $Si/Si_{1-x}Ge_x$ superlattices, the higher frequency Raman spectrum (Fig. 2) exhibits three main peaks attributed to scat-

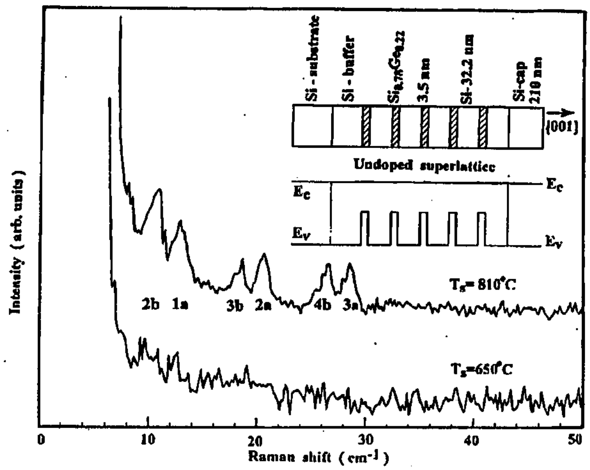

Fig. 1. Low frequency Raman spectra of two Si/$Si_{0.78}Ge_{0.22}$ superlattices with substrate growth temperature T_s = 810°C (upper curve) and T_s = 650°C (lower curve). Spectral resolution 1 cm^{-1}. Upper spectrum is shifted for clarity. The inset shows a schematic illustration of Si/$Si_{0.78}Ge_{0.22}$ strained-layer superlattice and the proposed real-space energy diagram.

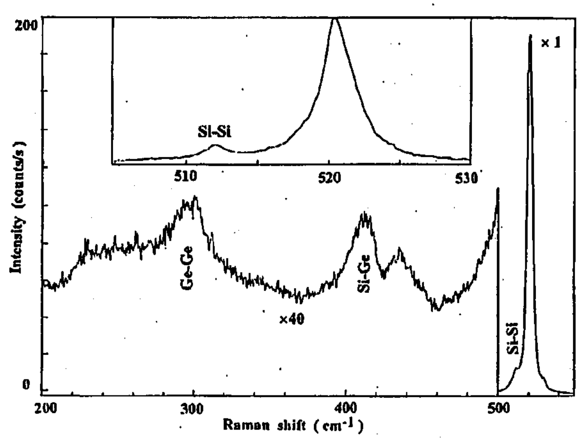

Fig. 2. Raman spectrum of Si/$Si_{0.78}Ge_{0.22}$ superlattice grown at 810°C substrate temperature. Spectral resolution 3 cm^{-1}. The inset shows the 500 cm^{-1} region of the spectrum recorded at a higher resolution of 0.5 cm^{-1}.

tering from longitudinal-optic phonons corresponding to vibrations of the Ge–Ge ($\approx$ 300 cm^{-1}), Si–Ge ($\approx$ 400 cm^{-1}) and Si–Si ($\approx$ 510 cm^{-1}) bonds in the strained alloy layers and a strong peak due to the optical lattice vibrations of the unstrained Si cap layer and the Si superlattice layers ($\approx$ 520 cm^{-1}). Weaker optic-phonon lines near 225 and 437 cm^{-1} have been attributed to a particular Si–Ge ordering within the alloy layers [6].

TABLE
Experimental and calculated Raman peaks for SL $Si/Si_{0.78}Ge_{0.22}$.

m	ν_{exp} [cm^{-1}]	ν_{calc} [cm^{-1}]
0	5.505	4.840
1a	12.906	12.639
1b	—	2.958
2a	20.547	20.439
2b	10.672	10.758
3a	28.581	28.238
3b	18.130	18.557
4a	—	36.037
4b	26.311	26.356

The shift to higher frequency of the Si–Si bond vibration in the superlattice alloy layers compared with the bulk alloy Si–Si bond vibration frequency is evidence of strain in the superlattice layers due to the difference in the lattice constants of Si and $Si_{1-x}Ge_x$. The following equation is deduced from the data of Ref. [7]:

$$\omega^{\text{bulk}}_{\text{Si-Si}} = -66.7\text{x} + 520 \ [\text{cm}^{-1}], \tag{2}$$

where x is the Ge concentration.

The in-plane mismatch strain $\varepsilon_{\parallel}$ is given by

$$\varepsilon_{\parallel} = (a_1 - a_2)/a_2, \tag{3}$$

where a_1 and a_2 are the lattice constants of Si and $Si_{1-x}Ge_x$, respectively.

Using the values $a_1 = 5.431 \times 10^{-8}$ cm and $a_2 = 5.476 \times 10^{-8}$ cm [8] for the germanium concentration $x = 0.22$, we obtain $\varepsilon_{\parallel} = -8.31955 \times 10^{-3}$. The lattice constant a_2 was deduced from the relationship [9]

$$a(x) = 0.5431 + 0.02x + 0.0026x^2 (\text{nm}). \tag{4}$$

The strain $\varepsilon_{\parallel}$ is related to the "biaxial" stress X by the elastic compliances S_{11} and S_{12} [10]

$$\varepsilon_{\parallel} = (S_{11} - S_{12})X. \tag{5}$$

Assuming a linear relationship between pure Si and Ge compliance constants in the alloy, we find a compressive stress $X = -12.29$ kbar.

The frequency shift of the phonon mode due to the stress is given by [2]

$$\Delta\omega = -b\varepsilon_{\parallel} = -\tau X, \tag{6}$$

where b is the strain-shift coefficient relating the displacement of the phonon frequency to the lattice distortion in the plane of growth, and τ is the stress factor, which is different for different phonon lines. Using the expression for the Si–Si mode stress factor [2]

$$\tau \approx 0.4 + 0.57x + 0.13x^2 \ [\text{cm}^{-1}/\text{kbar}] \tag{7}$$

and experimental value $\Delta\omega = 6.79$ cm^{-1} for the Si–Si phonon mode shift in the sample Si/$Si_{0.78}Ge_{0.22}$, it is possible to determine that $X = -12.83$ kbar, which is in good agreement with the above estimation.

In conclusion, strained-layer superlattices of Si/$Si_{0.78}Ge_{0.22}$ have been prepared by the technique of molecular beam epitaxy at different substrate temperatures and have been studied by Raman and ellipsometry spectroscopy. Raman spectroscopy have been shown to be useful for the characterization of Si/$Si_{1-x}Ge_x$ superlattices. The zone-folding effect on acoustic phonons in the high quality sample was observed. The measured acoustic phonon energies are in good agreement with calculations based on Rytov's theory of acoustic vibrations in layered media. The higher-frequency region of the Raman spectra consists of confined longitudinal optical phonons in the Si and $Si_{1-x}Ge_x$ layers. An analysis of the stress induced change in the frequency of the Si–Si bonds vibration mode in the alloy layer was performed.

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