Optical phonon localization in self-assembled Ge islands

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Abstract

We present a Raman scattering study for self-organized Ge islands on Si substrate carried out at 10 K. By means of difference Raman spectroscopy technique, we have separated the Raman signals from the Ge islands and Si substrate. The wetting layer thickness and strain were estimated from the line width and frequency peak. The estimated wetting layer thickness values are comparative with the Ge dot height obtained from microscopy measurements. The strain is decreased with an increase of the thickness.

Key words: Ge dots, optical phonons, Raman spectroscopy, localization

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Raman spectroscopy is a good tool to study strains and sizes of nanostructured islands [1]. However, there are problems concerning whether one can make unambiguous conclusions from the Raman spectra for Ge layers on Si substrates [2]. First problem lies in the presence of signals from Ge (one-phonon signal) and Si substrate (process involving two acoustic phonons) in the same frequency region. Second problem is caused by a delocalization of Ge-like LO phonons at high wavevector values [3]. It may be possible because Ge-like LO- and Si-like LA-phonon branches overlap. In this paper, we shall consider the problems analyzing obtained Raman spectra.

The experimental samples in the present study were prepared by solid source molecular beam epitaxy (MBE) system. It consists of a buffer layer of silicon with a thickness of about 50 nm, grown on Si(001) substrate, followed by the deposition of Ge. The self-organized Ge dots were characterized by atomic force microscopy (AFM). The dots show a shape of quasi-pyramidal. The size in the growth plane was 3050 nm. The average dot height was 0.8, 1.2, 1.5 and 4.2 nm for the samples N264, N265, N266 and N267, respectively. The dots overlap one another. Therefore, a minimum thickness of the Ge layer is not equal to zero.

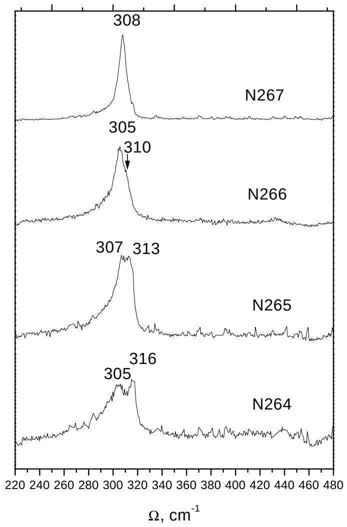

Fig. 1. The low temperature (10 K)Raman spectra of Ge islands on Si substrate

The Raman spectra were measured using a Dilor XY spectrometer and recorded in the $z(x,y)\overline{z}$ and $z(x,x)\overline{z}$ backscattering geometries. All the spectra studied were excited with the 514 nm line from an argon-ion laser.

A bulk Ge has a Raman peak at 304 cm^{-1} at 10 K.

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At the same time the Si substrate has a maximum at 305 $cm^{-1}(10K)$ caused by the scattering on two acoustic phonons. Therefore, for the thin Ge layer (for example, for the samples N 264 and 265) Raman spectra contain both signals in the same frequency region. Analyzing Raman spectra, one can separate this signals taking into account the following facts. Due to lattice mismatch of bulk Ge and Si, a Ge film and partly Si substrate are strained. The strain area in Si is compared with Ge dot size. On the other hand, the light penetration depth for a pure Si is about 600 nm at the wavelength of 514 nm [4]. Thus, the Si Raman signal is associated mainly with an unstrained Si region. Indeed, our experimental data show that the principal Si peak lying at 520 cm^{-1} does not change essentially from sample to sample, as compared to the pure Si. The intensity of the Si acoustic phonon peak is about the same with and without strains [5]. Therefore, to find out a signal from the Ge layer it is necessary to determine the difference between the complex spectra of the Ge/Si samples and those of Si. Certainly, before making the difference it is necessary to normalize all spectra on the amplitude of the principal Si peak. As result the spectra obtained by this operation do not contain the two acoustic phonon features at 229 cm^{-1} and 434 cm^{-1} that take place for the pure Si substrate (see, e.g., [2]). The Raman spectra measured at 10 K in the geometry $z(x,y)\overline{z}$ are presented in Figure 1. It should be noted that the Raman spectra were not observed in the geometry $z(x,x)\overline{z}$. According to selection rules it means that all spectra presented in Figure 1 are caused by Ge-like LO phonons. Supposing the appearence of the z-component of the electric field inside the Ge layer, one can conclude that the TO-phonons would be observed in both experimental geometries.

The spectra have different peak frequencies and line widths. The line is not symmetric and broadened to lower frequencies (especially one can see it for the sample N 264). Note that 2 TA-phonon Si line has a symmetric form and takes a place for the sample with the minimum thickness of the Ge layer (N 264). Broadening to lower frequencies indicates the presence in Raman scattering of localization optical phonon modes because of the dispersion curve of optical phonon in bulk Ge. To estimate the shift caused by the confinement effect we suggest that the strain-induced shift is the same for all the wave vector values. One can find the frequency of a localized phonon for a film, using the dispersion curve (see, e.g., [6]). Here we consider the first confined mode giving the maximum intensity in Raman scattering. The phonon confinement decreases phonon frequencies comparing to a bulk one. The bulk Ge has a Raman peak at 304 cm^{-1} at 10K. At the same time in the Fig. 1 one can see phonons at the frequencies higher than the bulk one. The reason of a blue shift is the presence of a strain in thin Ge layers. The phonon frequency of Ge islands and films on the Si substrate increases. The maximum shift of the Ge-like LO phonon at the zero wavevector corresponds to the 4th % strain and it is 16.5 cm^{-1} (see, e.g., [1]).

As it was mentioned above the Ge layer is a film with slowly changing thickness. For thin film one can consider that the Ge film contain of an integer number of lattice layers. These "islands" have still a lateral size bigger than their hight (this is valid especially for the samples N 264 and N 265). In this case one can consider as first approximation that phonons in the "islands" are independent. Any "island" selects the phonons with the wavevector that corresponds to the first confined mode. The maximum thickness of the Ge film gives the highest frequency value. The lower boundary of the line is correspondent to the minimum film thickness. For example, for the sample N 264 the lower boundary contains 270 cm^{-1} approximately. Using the dispersion curve graph (we took it in [4]), one can find the minimum film thickness. It is 5 Å about. The maximum thickness is 5+8=13 (Å). The phonon confinement at such thickness gives the frequency shift 3 - 4 cm^{-1}. The frequency peak is seen at 316-317 cm^{-1}. Therefore, the frequency in the point of the Brillouin zone is 320 cm^{-1}. It corresponds to the strain 3.8 - 4 % about. Analogously, one can find the minimum film thickness and the average strain in Ge for the sample N 265. They are 6 Å and 3.5 % about. It is not fully correct to apply this methodic to the samples N 266 and N 267 because of their "islands" have no more bigger lateral sizes than a hight. Nevertheless, one can evaluate a strain. It is 1.5 % - 1.7 % for these samples. One can see that the strain in the Ge layer decreasses with the layer thickness. Also we have concluded that the Ge-like LO phonons at high value of the wavevector gives a contribution in the Raman signal. This conclusion corresponds to a dependence of Raman scattering on a excitation wavelenght [7].

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