COMPOSITION AND ELASTIC STRAIN IN CAPPED SELF-INDUCED SiGe NANOISLANDS

M.YA. VALAKH, V.M. DZHAGAN, Z.F. KRASIL'NIK[1]**, O.S. LYTVYN, A.V. NOVIKOV**[1]**, V.O. YUKHYMCHUK**

Lashkarev Institute of Semiconductor Physics, Nat. Acad. Sci. of Ukraine
(45, Nauky Ave., Kyiv 03028, Ukraine; e-mail: valakh@isp.kiev.ua),

[1]**Institute for Physics of Microstructures, Russian Acad. Sci.**
(Nizhny Novgorod 603950, Russia)

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Self-induced SiGe nanoislands grown on a Si substrate by molecular-beam epitaxy MBE have been investigated by Raman spectroscopy and atomic force microscopy AFM. It is established that the capping of islands with a layer of silicon results in an increase of the Si content and elastic strain in them. It is shown that a variation of the Ge deposition rate within the range 0.12 – 0.5 Å/s does not affect the composition of islands and mechanical stresses in them. This phenomenon is explained by a dominating influence of interdiffusion, which is primarily caused by non-uniform stresses in islands and in the substrate around them, on stresses in islands and their composition.

1. Introduction

Recently, the self-induced SiGe nanoislands formed in the course of MBE of stressed Si/Ge heterostructures have been intensively studied [1–3]. A significant interest to such structures is caused by their interesting fundamental properties and their practical application in opto- and nanoelectronic devices.

In the majority of the works devoted to the study of properties of SiGe islands by Raman spectroscopy, the islands not covered with silicon were investigated [4—8]. It was conditioned by the fact that the morphology of such specimens can be studied with the help of the AFM method, the obtained data being compared with those derived by using Raman spectroscopy. Moreover, in this case, there was no problem concerning the contribution of a capping silicon layer to the Raman spectrum, as well as the problem of absorption of the exciting and scattered radiation. On the other hand, for developing opto- and nanoelectronic devices, it is necessary that the formed islands should be covered with a layer of silicon. It is caused by the necessity both to protect the islands from oxidation and to create Si/SiGe junctions. Capping the islands with silicon was shown in works [9, 10] to be able to change their form, dimensions, and surface density. The level of an influence of the capping of islands with silicon on their characteristics depends on the temperature, at which this process takes place. In work [10], it was shown that depositing a Si layer of only 6 Å in thickness at a temperature of 700°C resulted in such a variation of the form and the surface density of islands that practically a different ensemble of nanoislands was formed. To avoid significant morphological modifications of the formed islands, the initial stage of capping was fulfilled at relatively low temperatures of 300—400 °C. Then, after the silicon layer had covered the islands completely, the temperature was raised up to 500 °C, and the silicon layer was made grow further. This resulted in the formation of a necessary smooth silicon layer.

However, it turned out that the capping of islands even at relatively low temperatures (300—400 °C) resulted in a change of their parameters. Interdiffusion, which accompanies the specimen cooling from the temperature of growing to the temperature at which specimens will be capped with silicon, as well as the very capping of islands, changes their component composition. In addition, the formed SiGe islands, when being capped with a Si layer, are squeezed not only in the plane of growth but in the direction of growth too.

In this work, the variations of the island parameters that occurred in the course of their capping with silicon have been studied using Raman spectroscopy. Another goal of this work was to study the influence of deposition rate of Ge on the parameters of islands, which are being formed in the course of deposition.

2. Experimental Procedure

Two series of specimens with nanoislands formed during MBE, were used. The first series contained arrays of islands uncapped and capped by silicon, but the MBE conditions were identical in both cases: the deposition temperature was 600 °C, the nominal thickness of the

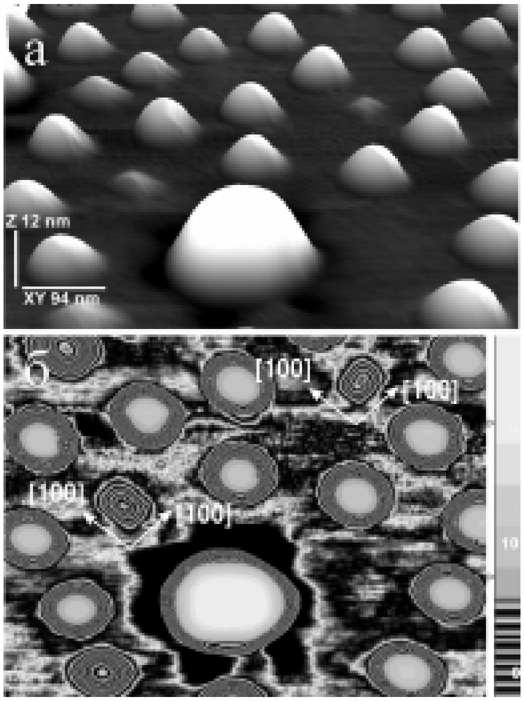

Fig. 1. AFM pattern of SiGe islands formed at a temperature of 600°C by depositing 9 ML of Ge: (*a*) view plan, (*b*) view from above

deposited layer was 9 monolayers (ML), and the deposition rate was 0.15 Å/s. The second series of specimens contained silicon-capped islands formed at a temperature of 600 °C and with the nominal thickness of deposited Ge layer of 8 ML, but the germanium deposition rate was varied from 0.12 to 0.5 Å/s.

Raman spectra were excited with the help of the Ar^+-laser radiation with a wavelength of 488 nm. The signal was registered by a cooled photoelectric multiplier operating in the photon counting mode. The experiment was carried out in a “back-scattering” geometry. The known values of plasma lines of an Ar^+-laser were used as reference points for the positions of the Raman bands to be determined more accurately. The surface morphology of the structures with nanoislands was studied making use of a Digital Instruments NanoScope IIIa atomic force microscope functioning in the tapping mode. Before and after measurements, the form of the apices of tips was tested. Measurements were carried out using tips with high symmetry, whose cross-section radius did not exceed 6 nm at a distance of 10 nm from the apex. This allowed us to neglect the convolution effect of the tip form and the researched surface when analyzing the form and volume of nanoislands.

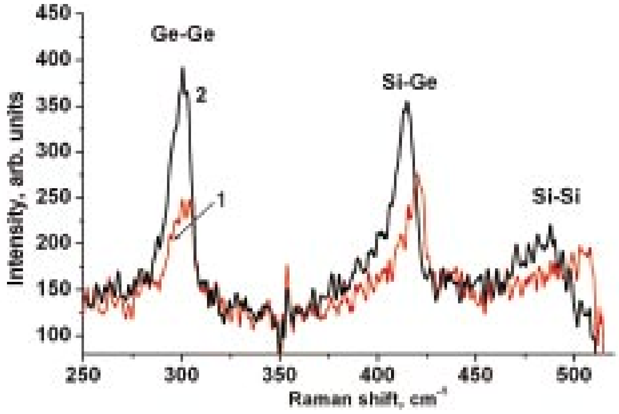

Fig. 2. Raman spectra of capped (*1*) and uncapped (*2*) SiGe nanoislands formed at a temperature of 600 °C by depositing 9 ML of Ge

3. Results and Discussion

It is known [1, 2, 5] that, at an epitaxy temperature of 600°C and at deposited 9 ML of Ge onto a silicon substrate, the formed islands have form of a dome or a pyramid (Fig. 1). Provided such conditions of MBE, the ratio domes/pyramids = 89/11. It is also known that the greater is the ratio between the heights and lateral dimensions of islands, the more substantial relaxation occurs in them. Provided identical component compositions, the dome-like islands become more relaxed than the pyramidal ones, because the ratio height/lateral dimension amounts to ∼1/5 for them, against ∼1/10 for pyramidal islands.

Fig. 2 exhibits the Raman spectra of capped (curve *1*) and uncapped (curve *2*) nanoislands. For the experimental spectra to be properly interpreted, the spectrum of a silicon buffer layer was subtracted from each of them [5]. It is known that the Raman spectra of a solid $Si_{1-x}Ge_x$ solution, of which the islands formed at a temperature of 600°C are made up, contains three basic bands corresponding to vibrations of the bonds Ge–Ge, Si–Ge, and Si–Si. We note that a thin (3–4 ML) wetting layer contributes practically nothing to the Raman spectrum, in accordance with the selection rules [11]. One can see from the presented spectra that, despite the availability of islands with two different forms, only one band for each type of vibrations (Ge–Ge, Si-Ge, Si–Si) manifests itself. It may stem from the fact that the total volume of dome-like islands is by at least one order as large as the volume of pyramidal ones [5], so that the dominant contribution to the spectrum is made by domes. Figure 2 (curve *1*) demonstrates that, after

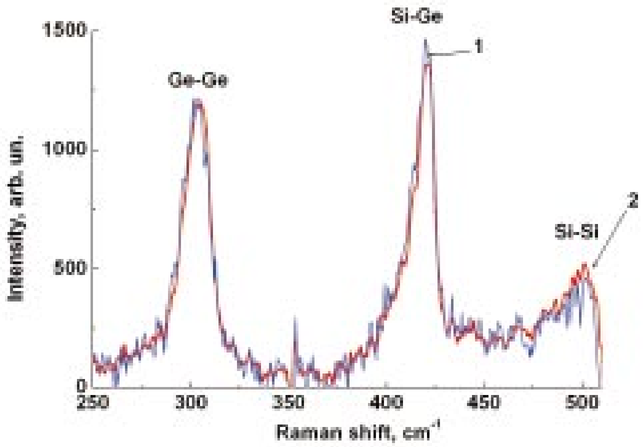

Fig. 3. Raman spectra of SiGe nanoislands formed at a temperature of 600 °C by depositing 8 ML of Ge with the deposition rates of 0.12 (*1*) and 0.5 Å/s (*2*)

capping the islands with silicon, the band frequencies change appreciably. For the islands composed of a solid $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ solution, the frequencies of the bands with component composition x and the elastic deformation ε are connected by the relations [4, 12]

$$\omega_{\mathrm{Si-Si}} = 520.5 - 68x - 815\varepsilon, \tag{1}$$

$$\omega_{\mathrm{Ge-Si}} = 387 + 81(1-x) - 78(1-x)^2 - 575\varepsilon, \tag{2}$$

$$\omega_{\mathrm{Ge-Ge}} = 282.5 + 16x - 385\varepsilon. \tag{3}$$

By using them, we found the corresponding values of x and ε quoted in the table.

As is seen, the islands capped with a Si layer contain more silicon. Owing to this circumstance, a mismatch between the lattice constants of the islands and the substrate reduces. Nonetheless, the elastic deformation of the islands grows. It is a result of the squeezing of the Si-capped islands by the Si matrix, which does not give them an opportunity to elastically relax. Moreover, the islands undergo the hydrostatic pressure from the surrounding Si matrix. Therefore, the process of capping the islands with silicon changes both the component composition and the elastic deformation, which is to be taken into account while growing the nanoisland structures for the purpose to develop opto- and nanoelectronic devices on their basis.

Now, let us proceed to the analysis of Si-capped nanoislands which were formed at the identical temperature and nominal thickness of the deposited Ge layer, but at different deposition rates. The previous AFM researches of islands uncapped with silicon showed that the surface density of islands grows from 7×10^9 to 2.5×10^{10} cm^{-2} as the deposition rate of Ge increases. In this case, the average size of islands decreases. It is caused by a reduction of the wetting layer sections around the islands, because those sections give away their own atoms for the islands to be formed by means of surface diffusion. The formation period of islands in the case of a low deposition rate of Ge (0.12 Å/s) is about four times as large as the relevant period at a high deposition rate (0.5 Å/s). So, one might have expected an increase of the Si content in the islands due to interdiffusion. However, the Raman spectra (Fig. 3) testify to that the frequency positions of the bands, as well as their intensities, are identical. Therefore, the estimation of the component composition x and the elastic deformation ε according to Eqs. (1)—(3) gives the following values for both specimens: $x = 0.65$ and $\varepsilon = -0.026$. This unexpected, at first glance, result can be regarded as the evidence for that non-uniform mechanical stresses in the islands and in the wetting layer around them are, in this case, the prevailing factor that governs the intensity of interdiffusion and, correspondently, the component composition of the islands. Really, diffusion in unstressed Si- and Ge-layers is not substantial at a temperature of 600 °C. At the same time, the concentration of Si reaches 30% in the SiGe islands formed at this temperature. Such a substantial effect of the mixing of components is possible only due to the abnormally intense diffusion enhanced by the fields of non-uniform stresses. This means that the diffusion in an island is maximal just at the first stage of the growth of islands, when the gradient of stresses is also maximal. As the Si concentration in the islands increases, the stresses in them decrease, which results in a reduction of the diffusion of Si in them. In such a case, a prolongation of the deposition time should not result in a significant increase of the Si content in islands.

The results obtained correlate with our results for nanoislands formed at a temperature of 700 °C and provided the identical deposition rate of Ge, but with various thicknesses (from 5.5 to 11 ML) of the deposited layer [5]. A prolongation of the deposition time by a

Parameters of SiGe nanoislands formed under various MBE conditions

T, °C	d_{Ge}, ML	V_{Ge}, Å/c	Thickness of capping Si-layer, nm	Content Ge, x	Elastic deformation, ε
600	9	0.15	100	0.62 ± 0.02	-0.023 ± 0.001
600	9	0.15	—	0.72 ± 0.02	-0.018 ± 0.001
600	8	0.12	80	0.65 ± 0.02	-0.026 ± 0.001
600	8	0.5	80	0.65 ± 0.02	-0.026 ± 0.001

factor of 2 did not result in a significant variation of the component composition ($x = 0.57$ at $d = 5.5$ ML and $x = 0.56$ at $d = 11$ ML) and the elastic deformation ($\varepsilon = -0.01 \pm 0.001$ at $d = 5.5$ ML and $\varepsilon = -0.012 \pm 0.002$ at $d = 11$ ML).

4. Conclusions

Thus, using Raman spectroscopy and AFM methods, we have shown that the capping of SiGe islands with silicon results in increasing both the Si concentration and the elastic deformation in them even at not high temperatures. It has been shown that a variation of the Ge deposition rate within the limits 0.12—0.5 Å/s changes the dimension and the surface density of islands, but their component composition and elastic deformation almost are not varied. We explain this phenomenon by interdiffusion which is primarily caused by the non-uniform stresses in islands and in the wetting layer around them and predominantly influences the process of formation of both the component composition and the stresses in islands.

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КОМПОНЕНТНИЙ СКЛАД ТА ПРУЖНА ДЕФОРМАЦІЯ В ЗАРОЩЕНИХ САМООРГАНІЗОВАНИХ SiGe-НАНООСТРІВЦЯХ

М.Я. Валах, В.М. Джаган, З.Ф. Красильник, О.С. Литвин, О.В. Новіков, В.О. Юхимчук

Резюме

Методами спектроскопії комбінаційного розсіяння світла та атомної силової мікроскопії досліджено самоорганізовані SiGe-наноострівці, сформовані в процесі молекулярно-променевої епітаксії Ge на кремнієву підкладку. Встановлено, що заращування сформованих острівців шаром кремнію, приводить до збільшення в них вмісту Si та величини пружної деформації. Показано, що варіювання швидкості осадження Ge в межах від 0,12 до 0,5 Å/с не змінює компонентний склад та механічні напруження в острівцях. Цей факт пояснений тим, що на компонентний склад та величини напружень в острівцях переважаючий вплив має інтердифузія, зумовлена, в першу чергу, неоднорідними напруженнями в острівцях та в підкладці навколо них.