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Structure and optical properties of periodic submonolayer insertions of Ge in Si grown by MBE

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Introduction

Silicon is the basis of almost the entire market of microelectronic devices, but it can practically not be used in light-emitting devices because of the indirect nature of its bandgap, which drastically limits the luminescence efficiency of this material. As silicon integration with optical interconnects is an urgent task of the industry, different ideas are under discussion to overcome this significant disadvantage. We propose to incorporate dense arrays of submonolayer (SML) narrow gap Ge insertions into a Si matrix. The incorporation of SML insertions in other material systens was previously demonstrated in resulting in very small islands having a very high density (for a review see *e.g.* [1]). In the case of Si–Ge structures SML islands, or quantum dots (QDs) can, on the one side, provide a partial lifting of the k-selection rule for radiative recombination. On the other side, electron attraction to the confined holes may result in confined excitons, assuming that the potential spike in the conduction band due to Ge SML is small. This, taken together with potentially very high density of SML QDs, the resulting efficiency of luminescence and gain may be , probably, sufficient for optical applications. Photoluminescence from SML Ge embedded in silicon was investigated by Sunamura *et al.* [2]. The PL energy was shown to decrease with increasing Ge coverage. The effect was explained by quantum confinement caused by the formation of quantum wires at surface steps and the emission was attributed to a biexciton process. At the same time no structural characterization of these features has been performed.

More traditionally SiGe QDs are fabricated by relatively thick SiGe deposits, resulting in transition to Stranski–Krastanow (SK) growth (see *e.g.* [3]). In [3] SK QDs were grown by low-pressure chemical vapor deposition and their PL properties were investigated. The authors observed that the localization of excitons in the dots leads to an increase of the luminescence efficiency as compared to the smooth SiGe layers. The disadvantage of SK QDs is the low in-plane density and the relatively large size, which defines only weak lifting of the k selection rule on one side, and a small e–h wavefunction overlap due to the type-II band alignment on the other.

The goal of this work is to study structural and optical properties submonolayer Ge insertions in a Si matrix with an aim of developing a better approach for QDs in this system.

Experiment

To investigate the influence of the nominal Ge thickness matrix on the structural properties, two samples with were grown by MBE (Fig. 1(a)). Both structures were grown using Riber SIVA 45 setup on a Si(100) n-type substrates (conductivity 3 Ω cm). Five-inch Si substrates (OKMETIC) were used. After chemical treatment the substrates were transferred to the MBE setup. During the growth process the rotation of the samples was used, the temperature inhomogenity along sample was about ~5%. Structures consist of a 100 nm-thick Si buffer layer, Ge(0.7 Å or 1.4 Å)/Si(44 Å) superlattice (20 pairs) and a 20 nm-thick Si cap layer. The substrate temperature was 750°C for the superlattice growth. For all other layers it was 600°C. The growth rates for Si and Ge were 0.5 Å/s and 0.05 Å/s, respectively.

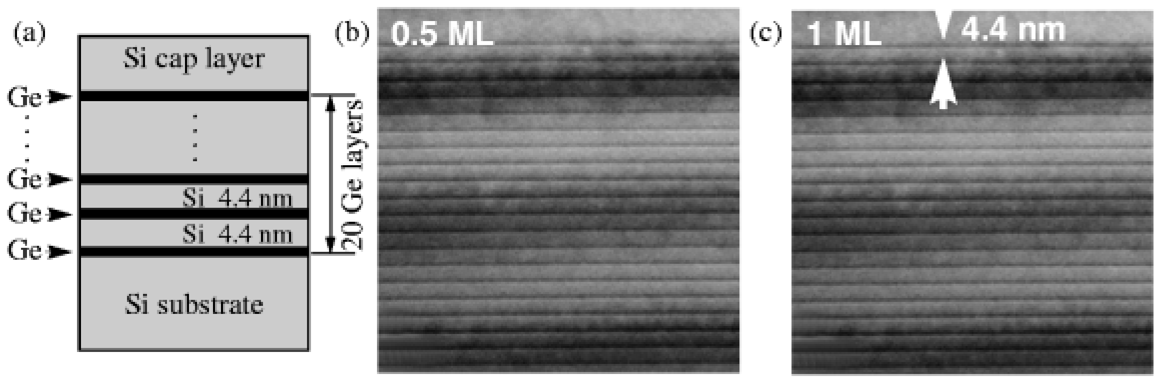

Fig 1. (a) Sequence of the layers in the grown structures. The thickness of the Ge layers was 0.5 ML (0.07 nm) or 1 ML (0.14 nm) in two different samples. Cross section diffraction contrast images of specimen with 0.5 ML Ge (b) and 1 ML Ge (c). The periodicity in the [001] direction is equal to 4.4 nm in both cases.

The growth rates were controlled by 2 mass-spectrometers with feedback, the spectrometers were set to 28 (Si) and 74 (Ge) masses. The total gas pressure during the growth was better than $5 \cdot 10^{-9}$ Torr. The surface was *in situ* controlled using reflection high-energy electron diffraction.

Photoluminescence (PL) was excited by Ar^{+}-laser $\lambda = 514.5$ nm, maximal excitation density ~500 W/cm^2. PL was detected by Ge cooled photodiode. The samples were investigated by different electron microscopic techniques and Selected Area Electron Diffraction (SAED).

Results

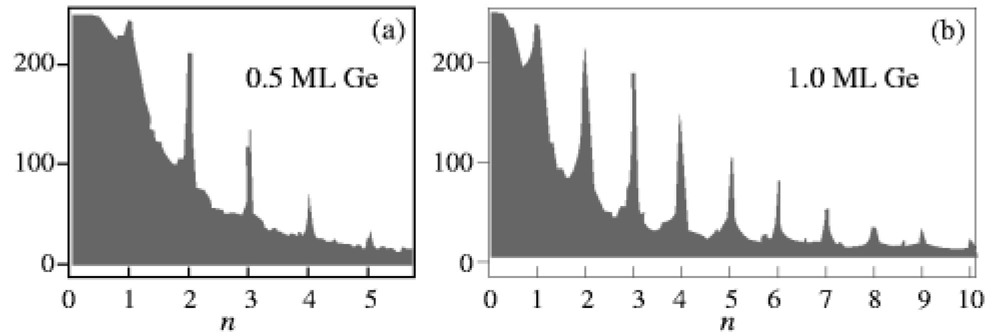

Fig 2. Line scans in [001] growth direction of zero beam spot in diffraction patterns from multilayer structures A (a) and B (b). In the case of sample B the number of satellites n is twice as large as in sample A.

The cross section images of the grown structures taken in a diffraction contrast mode at relatively low resolution are shown in Fig. 1(b,c). The periodicity in growth [001] direction is 4.4 nm in both cases. It should be noticed that the images of both structures A and B look almost identical at these imaging conditions. However diffraction patterns show a distinct difference (Fig. 2(a,b)). In the diffraction pattern from super lattice formed by 0.5 ML Ge layers (specimen A) the number of Fourier harmonic n is twice less than in the case of 1 ML one (specimen B). This means that the thickness of the incorporated Ge layers in the second case is practically one or/and two mono atomic layers while in the first case it amounts to several mono layers.

Compositional nonuniformities of different contrast and very high density are clearly resolved in plan-view TEM image (Fig. 3(a)) of the SML sample, as opposite to the smooth TEM image of the 1ML structure.

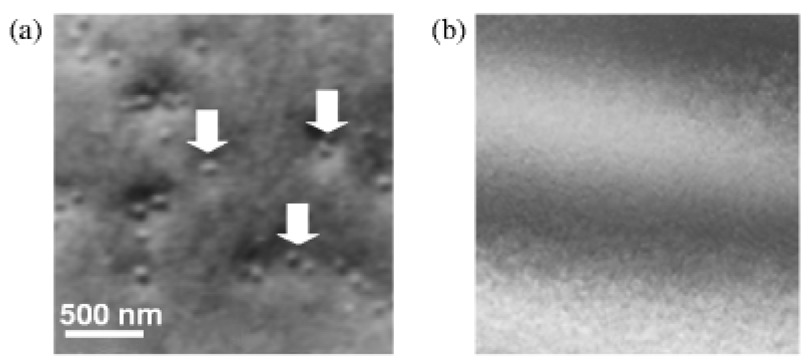

Fig 3. Plan view images of sample A (a) and B (b). The compositional fluctuations can be clearly seen in sample with 0.5 ML Ge, while the sample B (1 ML Ge) is very homogeneous.

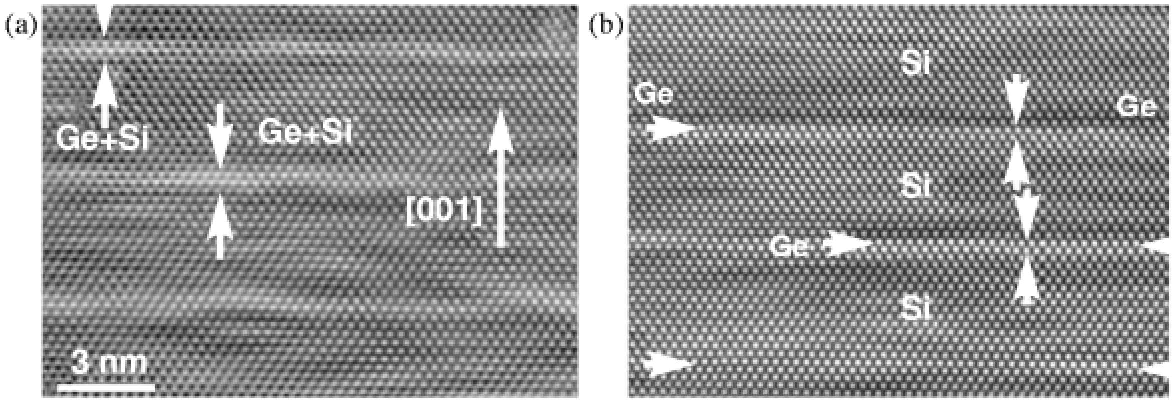

Fig 4. HRTEM cross-section images of samples A (a) and B (b). The thickness of compositional fluctuations measured along [001] growth direction are marked. It is equal about ~1 nm and ~0.27 nm in specimens A and B respectively.

The single layers of Ge are clearly seen in high resolution cross-section image (Fig. 4(b)) taken from very thin crystal region ($t \approx 20$ nm) where the kinematical approximation still works well enough. According to this approximation concentration of Ge $x = (k-1)/(f_{Ge}/f_{Si}-1)$, where f_{Ge}, f_{Si} — atomic scattering amplitudes for Ge and Si respectively,

$$k = \frac{I_x}{I_{Si}} = \frac{I_{x,max} - I_{x,min}}{I_{Si,max} - I_{Si,min}}.$$

It gives $x = 0.9 \pm 0.1$ what indicates that these layers are practically pure Ge. In the case of sample A (Ge submonolayers) the compositional fluctuations are observed in (Fig. 4(a)). The thickness of these fluctuations in the growth direction [001] is about 0.8 nm being in a good agreement with the diffraction data in Fig. 2(a). Besides, in the plane view images of sample A one can observe larger domains ($N = 1.7 \times 10^{10}$ 1/cm^2) which look like very small quantum dots. They are completely absent in the sample B (Fig. 3(a,b)). The lateral size and the width of these QD estimated in cross-section HRTEM image (Fig. 5) are equal 7 nm and 3.5 nm respectively. These larger Ge domains may be responsible for high-contrast features revealed in the plan-view image, while the weaker contrast plan-view perculiarities may be associated with flatter islands revealed in Fig. 4(a). PL spectra from specimens A and B are shown in Fig. 6. One can notice an appearance of a peak at 1.064 eV in sample A. At the same time, the Ge-related emission in this range is very weak in sample B with 1 Ge ML due to small localization energy of carriers in the 1 ML sample [4].

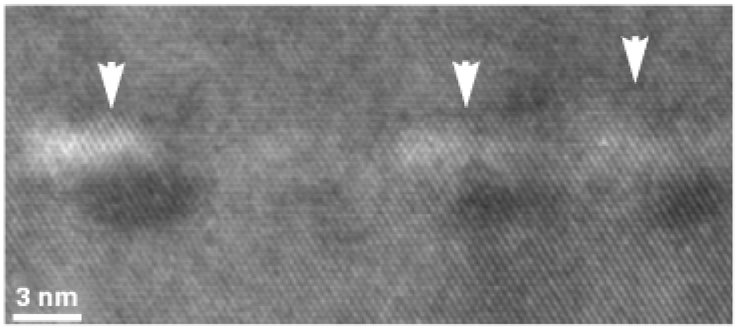

Fig 5. Cross-section HRTEM image of the Ge-rich domains in sample A. The lateral size and the thickness of the domains are about 7 nm and 3.5 nm respectively.

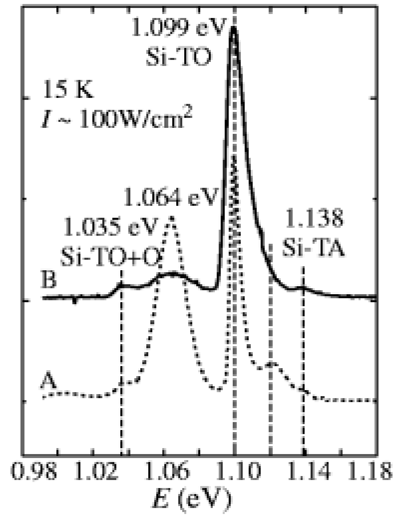

Fig 6. PL spectra from samples A and B (0.5 and 1 ML Ge respectively).

Discussion

One should point out that the appearance of intense PL peak at 1.064 eV in the SML sample is related to the Ge compositional fluctuations. These fluctuations appear only in sample A with 0.5 ML insertion. Sample B with 1 ML shows rather uniform distribution of Ge in the layer plane. Almost no intermixing in perpendicular direction is revealed. This is a strong indication of morphological stability of one monolayer structure. Strong compositional fluctuations in sample A (Figs. 3(a), 5) can be treated as QDs which can result in the charge carriers localization. In the case of SML QDs the ir size (<8 nm — in-plane, <3.5 nm-thickness) is much smaller than for SK QDs [2] (~150 nm-diameter, ~9 nm thickness). This is possibly a reason for shift of PL peak at approximately 100 meV into high energy region. It occurs due to increasing confinement energy with decreasing QDs thickness. In the case of sample B the thickness of Ge insertions is too small (1–2 ML) for charge carrier localization.

Acknowledgements

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