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Optical transitions in quantum wells and quantum dots based on SiGe heterostructures

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Abstract. The growth of GeSi nanoislands and potoluminescence features in structures with localized states of electrons and holes are discussed.

Introduction

Silicon and germanium are known to be indirect band semiconductors with a low photoluminence efficiency, especially at room temperature. The conduction and the valence bands of low-dimensional strained SiGe heterostructures largely differ from bulk materials, this difference depending on size quantization and deformation effects. The advances made in the past few years in the technologies for nanostructure growth on the basis of Si, Ge and their solid solution open new possibilities in terms of electron state engineering, including upgrading of photoluminescence effectiveness as one such target. The latter is what a potential application of these structures in the near-IR optoelectronic devices relies upon [1].

In this paper the photoluminescence features in SiGe structures with localized states of electrons and holes are discussed. A radiative recombination of electrons and holes in an indirect gap semiconductor is a three-particle process involving an electron, a photon and a third particle responsible for conservation of momentum in a recombination procedure. If an electron involved in recombination is well localized in space, its momentum is uncertain. The electron here may have the momentum value corresponding to a direct optical transition from the conduction to valence band. As a rule, the momentum-space-direct recombination transitions in SiGe heterostructures prove possible for electrons and holes that are located on different sides of a heterointerface [2]. The probability of such transitions is higher with a greater overlap of the electron/hole wave functions.

1 Energy band structure

Analysis of the energy bands for Si/Ge_xSi_{1-x} and Ge/Si_xGe_{1-x} heterojunctions shows that the potential well for holes is located on the heterointerface side with a smaller Si content [2]. The potential well for electrons may be on either side of the heterointerface, which depends on the character of elastic deformation, a alloy composition, etc. There are six electron valleys in the conduction band. It is important for modeling of structures

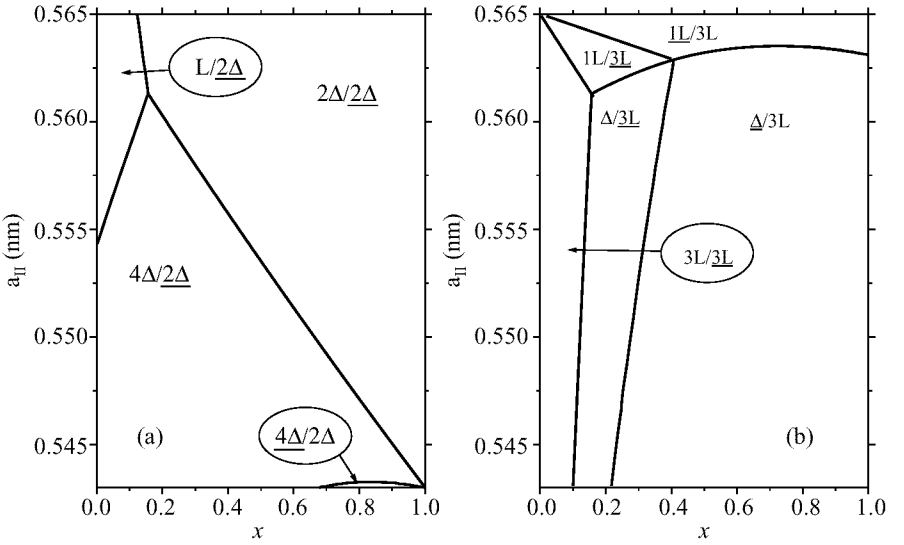

Fig 1. Regions of specific relative energy positions of the conduction-band-edge states in elementary semiconductors (Si or Ge) and in their alloys for (001) $Ge_{1-x}Si_x$/Si (Fig. 1(a)) and (111) $Ge_{1-x}Si_x$/Ge (Fig. 1(b)) heterostructures [2].

with allowed direct optical transitions which of the valleys form the conduction band bottom. A favourable situation is when the conduction band bottom is formed by a valley whose minimum in the momentum space is shifted relative to the valence band top in the direction perpendicular to the heterointerface. An electron confinement motion in this direction, i.e., near-heterointerface, which is quite likely for a number of reasons, leads to an uncertainty of the corresponding component of the electrons' momentum, so the direct transitions become allowed.

In Fig. 1 the calculation results are provided for two types of a heterointerface. The parameter regions corresponding to the above situation are such as to ensure that 2Δ-valleys will lie lowest in the conduction band for a Si/Ge_xSi_{1-x} heterostructure grown on a Si(100) substrate and L-valleys for a Ge/Si_xGe_{1-x} heterostructure grown on a Ge(111) substrate. The electron can be confined by forming a quantum well in the appropriate layer [3]. A detailed analysis of, for example, a Si/Ge_xSi_{1-x} heterostructure on a Si substrate shows that the thickness of a 2D layer of solid solution towards this effect has to be tens of Angstrom and the Ge fraction in the alloy must exceed 30–40%. It is known that the growth process of such structures may facilitate self-organization of nanometer-scale GeSi islands, which are a major issue of the present work.

2 Technology

Basic features of self-organization of Ge islands in silicon in the MBE [4, 5] and CVD [6] growth of heterostructures have been established by now. The sizes and surface density of the islands largely depend on the growth conditions (substrate temperature, growth rate and Ge fraction in the deposited layer [4]).

The structures under investigation were grown on the "KATUN" and "BALZERS"

MBE systems. The residual gas pressure was of at 3×10^{-10} Torr. The systems were equipment with e-gun for evaporation for Si and Ge. The growth process was controlled *in situ* by a spatial/temporal analysis of variations in the patterns of reflected high-energy electron diffraction (RHEED). Variations in the intensity profiles versus time were measured along the (00) streak in the [110] azimuth. The growth rate of Ge films was 0.005–0.1 nm/s, the substrate temperature varying in a $100 \div 700$°C range. Silicon films were grown at $550 \div 950$°C at the rate of 0.02–0.5 nm/s. For

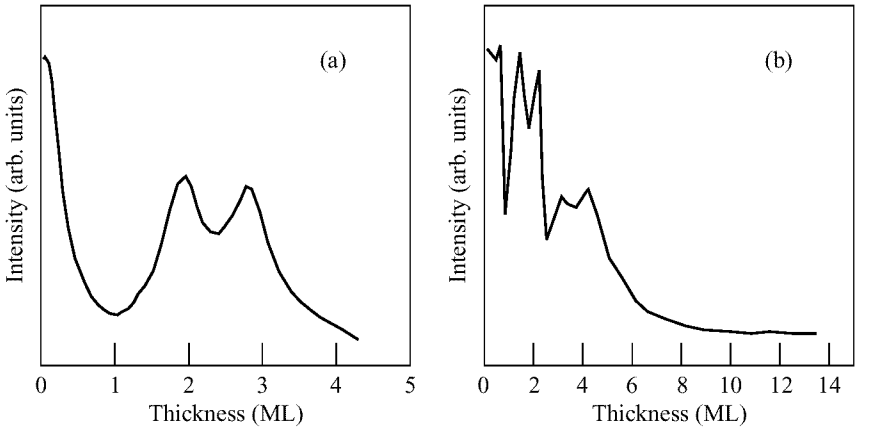

Fig 2. RHEED intensity oscillations of specular-beam observed from the surface of Ge films on Si (111) (a) and Si (100) (b).

the RHEED study of Ge islands formation it is important that this effect is associated with a 2D to 3D transition of the growth mode. This allows to precisely control the onset of a self-organization process. Figs. 2a and 2b demonstrate the typical intensity oscillations of a specular beam from the (111) and (001) surfaces of a Ge/Si film, respectively. It is clearly seen that the oscillation amplitude and average intensity start decreasing right after the onset of Ge growth. This decrease is caused by clustering and islands formation inherent in the growth by the Stranskii-Krastanov mode. The critical thickness for the 2D layer-by-layer mechanism to 3D mode transition (h_c) was found by measuring thickness values at which the oscillations vanish. In the Stranskii-Krastanov growth method, the less the elastic strain on a growing film, the larger h_c. In our case, elastic strains is reduced with a smaller Ge content in a Ge_xSi_{1-x} alloy. We observed two oscillation periods throughout growth of a Ge film on Si at $T = 650$°C (Fig. 1a) and six periods for a $Ge_{0.5}Si_{0.5}$ film. Another factor affecting growth of Ge islands is crystallographic orientation of substrate. One can see in Fig. 1 that the critical thickness for Ge growing on Si(111) and (001) surfaces is 2 monolayers (ML) and 5 ML, respectively.

3 Experimental results

Microprobe studies were carried out at room temperature on a Park Scientific Instrument atomic force microscope (AFM). The photoluminescence (PL) spectra from Ge/Si(001) structures excited by a Kr^+ laser ($\lambda = 647$ nm) were measured at 4.2 K with BOMEM

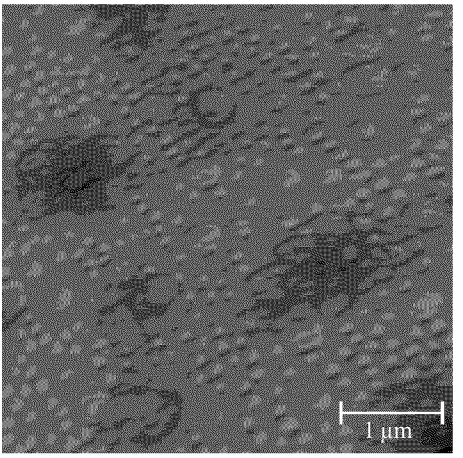

Fig. 3. AFM images of Ge film with a nominal thickness of 10 ML.

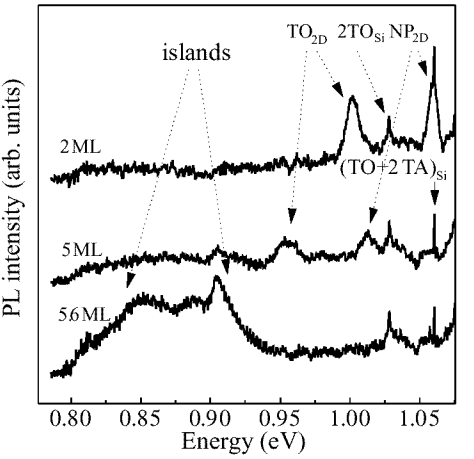

Fig. 4. PL spectra of Ge layers grown at 700°C with different thicknesses. The nominal thickness of Ge layers is given.

DA3-36 Fourier-transform spectrometer incorporating an InGaAs cooled photodetector.

Fig. 3 shows an AFM image of a sample comprising a Ge layer of thickness $d =$ 10 ML, grown on Si(100) at $T = 700°C$. According to the microprobe analysis data, the value of h_c at our growth conditions was 5 ML, which is in good agreement with the RHEED results. As the Ge content was, the sizes and density of the islands increased. By their transverse sizes D, the islands can be divided into three groups: $D \leq 190$ nm, $200 \leq D \leq 300$ nm, and $D > 350$ nm. The sizes and shape of the islands in groups I and II suggest that they must be dislocation-free outgrowths in which partial relaxation of the elastic strain was caused by local deformation of the nearsurface layer of Si [5] and by relaxation of strain on the islands free surface. Group III includes the islands that have experienced relaxation of the elastic strain through plastic deformation and formation of misfit dislocations in them. The size of the islands in the growth plane, that allows formation of misfit dislocations is close to the critical size of the elastic-strained islands $D > 300$ nm, as measured in [6].

The surface density of islands, N_s, depends on a Ge layer thickness and varies for different contents of deposited Ge from $8 \times 10^7\,cm^{-2}$ to $2 \times 10^9\,cm^{-2}$ [7]. As the growth temperature goes down to 550°C, the distribution of islands becomes more homogeneous in size, the average size is getting smaller ($D \approx 190$ nm), and the surface density increases. The size and surface density data for self-assembled islands agree with the results in [4].

Fig. 4 is the PL spectra for Ge/Si(001) heterostructures. Besides the luminescence lines of a Si substrate (TO- and TA-phonons-assisted replicas (see Fig. 4)), the spectra observed from samples with an effective Ge layer less than 5 ML exhibit luminescence lines from the Ge (2D) wetting layer (TO_{2D} for the TO-phonon-assisted replica and a no-phonon NP_{2D} line). For the sample with $d_{Ge} = 2$ ML, the NP_{2D} line falls within the phonon lines range $(TO + 2TA)_{Si}$ of substrate luminescence. With an increasing Ge

content the PL lines from the Ge layer are shifted to lower-frequencies due to a size quantization effect.

When a Ge layer thickness is above some critical value, there appears a wide peak in the region $0.8 \div 0.925$ eV, attributed to formation of Ge nanoislands.

4 Discussion

Typical sizes of islands in the growth plane are above 100 nm. Their height is by about an order smaller. Given such sizes the energy of the size quantization of holes in Ge islands would not exceed 20 meV, which leads us to a conclusion that the marked shift of the PL line $(80 \div 925)$ meV energies relative to Si cannot be treated unambiguously as being related to pure Ge islands on silicon. One may assume that the islands are a Ge-Si alloy [4] and then evaluate the molar fraction of Si in them. In Fig. 5 we provide

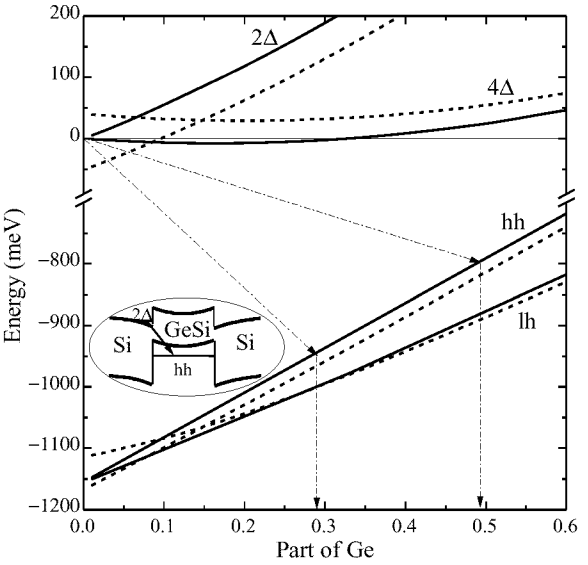

Fig 5. Conduction and valence bands of SiGe alloy, grown pseudomorphicaly on Si substrate (the lattice constant is equal to 5.43 Å– solid lines, the lattice constant is equal to 5.46 Å– dashed lines).

the band edge positions for a thin pseudomorphicaly alloy of $Si_{1-x}Ge_x$ on Si, calculated by the model in [2]. The symbols hh and lh are used to designate the heavy and the light hole subbands, respectively; 2Δ– is for two delta-valleys of the conduction band, in which the electron mass is maximum along the growth direction; 4Δ – label the other four delta-valleys of the conduction band; L is the L-valley. The calculations testify to a possibility of photoluminescence in a $800 \div 925$ meV range for a pseudomorphicaly alloy grown on a Si substrate, provided the Ge fraction in the islands is 30–50%. The solution seems to form in the islands through segregation of Ge.

The structures feature a p-type conductivity, and the islands are potential wells for the holes which accumulate in the islands, giving them a positive charge. The surface density of holes in the islands given $\sim 10^{15}\,\mathrm{cm}^{-3}$ concentration of holes in Si, can be

evaluated as for a quantum well with the same energy level of the ground state for heavy holes: $\sim 4 \times 10^{10}\,\mathrm{cm}^{-2}$. Due to the Coulomb repulsion the holes inside the islands are expected to concentrate along the heterointerfaces. The positive charge of the island creates a quantum well for the photoelectrons in Si near the heterojunction (see the insert in Fig. 5). When the conduction band bottom in Si lies lower than in the islands (Fig.5 shows that this occurs at $x > 0.32$, the PL energy $E_{pl} < 960$ meV), the quantum confinement result in the fall of 2Δ–valleys energy with respect to 4Δ ones, because of the larger electron masses along the (001) direction than in 4Δ–valleys. The focus here is on the electrons concentrated near the base and the tip of the islands, since it is them that provide the major contribution in photoluminescence because of a large difference in the areas of the lateral sides and the bases. Size quantization terminates the momentum conservation law (the Brillouin zone is two-dimensional), and the electron states of the 2Δ–valleys shift towards the center of 2D Brillouin zone. In this case, the interband optical transitions become direct in the momentum space ($p_{\mathrm{final}} - p_{\mathrm{initial}} = 0$), but in the real space the transitions are indirect, as the electrons and holes are localized on different sides of the heterointerface.

Assuming a partial relaxation of elastic strain in a solid solution through deformation of the surrounding silicon, the Ge fraction in islands whose PL lines fall within the $0.8 \div 0.925$ eV energy range must decrease, as follows from the calculations, compared to the islands that had no such relaxation. We can arrive at this conclusion by examining Fig. 5 in which the dotted lines show the positions of the band edges in a solid solution surrounded by deformed layers of silicon.

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References

[1] R. People, J. C. Bean, et al., *Appl. Phys. Lett.* **61** 1122 (1992).
[2] V. Aleshkin, N. A. Bekin, J. Phys.: *Condens. Matter.* **9** 4841 (1997).
[3] C. G. van de Walle, R. M. Martin, *Phys. Rev. B* **34** (8), 5622 (1986).
[4] G. Abstreiter, P. Schittenhelm, et al, *Semicon. Sci. Technol.* **11** 1525 (1996).
[5] D.J. Eaglesham and M. Cerullo, *Phys. Rev. Lett.* **64** 1944 (1990).
[6] G. Capellini, L. Di Gaspare et al., *Appl. Phys. Lett.* **70** 494 (1997).
[7] V. Aleshkin, N. Bekin, N. Kalugin et al., *Pis'ma ZhETF* **67(1)** 48 (1998).