

Local Trapping and Recombination of Charge Carriers in Heterostructures with Ge Nanoclusters

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To investigate the recombination processes, we study the spectral and time dependences of lateral photoconductivity of Si/Ge heterostructures with SiGe nanoclusters, obtained by molecular beam epitaxy. Photoconductivity at low temperatures, in the spectral region where Si is transparent, is conditioned by transitions involving localized states of SiGe nanoclusters. When the temperature decreases the most significant decrease in the photoconductivity is due to fundamental absorption in nanoclusters. This shows the high efficiency of electron-hole recombination centers in SiGe nanoclusters.

1. Introduction

Semiconductor heterostructures with nanoscale objects attract significant attention due to the size quantization effects that lead to changes in the electron spectrum. The investigation of SiGe/Si heterostructures offers wide opportunities to develop new principles of nano- and optoelectronic devices such as medium and far infrared detectors, photodiodes, memory systems, lasers, etc. [1-3]. The transport properties of a lattice mismatched system are largely governed by the presence of quantum states, strain fields, and interface defects created during epitaxial growth. The strain field modulation, size, and composition distribution [4,5] which are influenced by processes such as segregation and diffusion play a key role in the formation of a disordered ensemble of quantum dots (nanoclusters), where the structure and transport properties of the individual dot are inhomogeneous as well [6].

In Si/Ge heterostructures with SiGe nanoclusters (NCs) the spatial separation of nonequilibrium charge carriers takes place - holes in the valence band states are captured by SiGe, and electrons are accumulated in the potential well of Si surrounding. As a result, the SiGe quantum dots (QDs) at low temperatures can accumulate positive charge. These features can cause nanometer scale variations in the electrostatic potential, which have a significant impact on the recombination processes in the generation and transport of charge carriers.

2. Experimental Technique

Si/Ge heterostructures with SiGe NCs were grown by molecular beam epitaxy [7,8] on the substrates of Si (100) of p-type, doped with boron atoms (B), with resistivity $7.5 \Omega \cdot \text{cm}$. At first, on the Si substrate the Si buffer layer was grown with the thickness of 100 nm, which was doped by B with concentration of 10^{16}cm^{-3} . The impurities of the same concentration were located in Si substrate. To create a p-i-n structure the QDs of Ge were grown at 500°C with the height of 2 nm. Figure 1a shows AFM images of different SiGe nanoclusters grown on Si (001). The deposition rate was 1.0 nm/min for Si and 0.6 nm/min for Ge. After the QD layer growth the spacer layer of Si

was growing until the observation of high contrast Si(100) 2×1 electron diffraction pattern, which is typical for Si. The period of structure with the layer of QDs and Si spacer layer was varied in the range from 5 to 40 (see Figure 1b). The last layer of QDs was closed by the layer of Si of thickness 20 nm, which was doped by antimony atoms (Sb) with concentration 10^{16} cm^{-3} . Therefore, the n-p structure with QDs was grown in the potential barrier area.

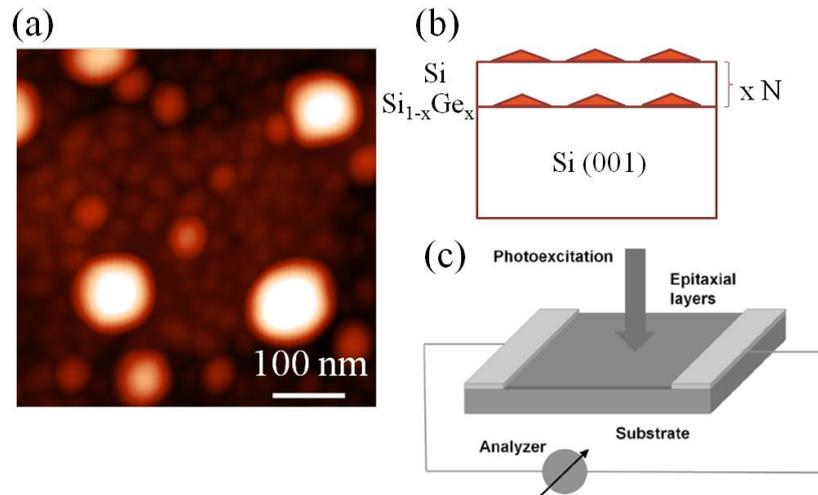


Fig.1. (a) AFM images of different SiGe nanoclusters grown on Si (001); (b) schematic image of heterostructure with QD layers and spacer Si layers between them; (c) experimental setup.

The measurements of the spectral dependence of photoconductivity were carried out on the basis of a standard infrared spectrometer in the spectral range 0.6-1.4 eV using radiation halogen lamps of 250 watts. The frequency modulation of the excitation radiation was 80 Hz. The spectral dependences were normalized to a constant number of photons using a non-selective pyroelectric receiver.

3. Results and Discussion

The spectral dependences of longitudinal photoconductivity of Si/Ge structure with 19 layers of NCs are shown in Figure 2.

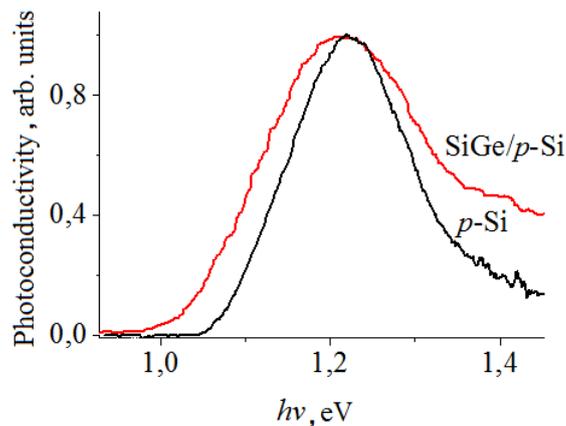


Fig. 2. Longitudinal photoconductivity spectra of multi-layer heterostructure with 19 layers of SiGe NCs of 2 nm height and without NCs at the temperature 290 K.

The spectra were measured at room temperature and modulation of excitation radiation with the frequency of 80 Hz. Photocurrent with the marginal energy of quanta of excitation radiation $h\nu_{\text{mar}} > 1.0$ eV is caused by the interband transitions in Si. For comparison, the measurements of longitudinal photoconductivity of the p-Si sample, which did not contain SiGe NCs, were carried out under similar conditions.

The shape of photoconductivity spectrum of a multilayer structure with SiGe NCs indicates a low surface recombination velocity at 290 K ($\sim 10^3$ cm/s). This signal was absent in the measurement of photoconductivity of p-Si structures without layers of SiGe NCs. It is well-known, that the photoconductivity signal near the long-wavelength edge is proportional to the optical absorption coefficient. Therefore, the difference between the photoconductivity spectra is primarily due to its change. It can be caused by non-uniform strain in Si/Ge heterostructure, which reach their maximal value in the SiGe NCs and their Si surrounding. In the work [9] the authors found that inhomogeneous deformation can cause significant changes in the optical properties due to the shift of the electron spectrum on the order of 100 meV.

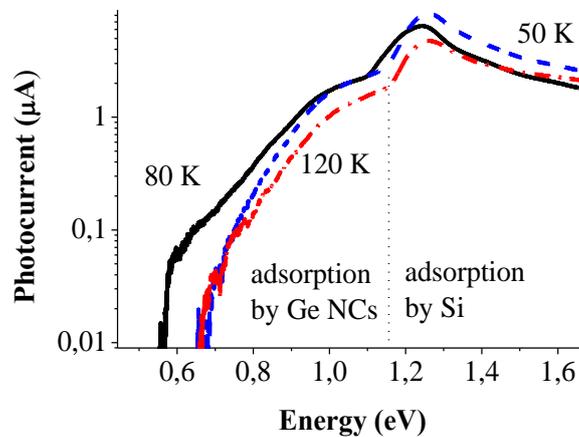


Fig. 3. Longitudinal photoconductivity spectra of the Si/Ge heterostructure with $\text{Si}_{1-x}\text{Ge}_x$ NCs on the p-Si (001) substrate.

The calculations of mechanical strain fields in Si/Ge structures with quantum dots of Ge [10] showed that the most stressed area is located under the NC basis, and the value of the silicon lattice deformation along the plane of the structure decreases with the distance to NC. As a result, the band structure of NC silicon surrounding is characterized by the presence of band gap variations in the plane of the structure, so it is a graded band gap structure. The region of Si with the minimal value of band gap, which is also less than the band gap of the deformed c-Si, is located near the base of NC. Photoresponse in the infrared range 1.0 - 1.05 eV can be explained by the fact that the compressed regions of Si near the NCs have smaller band gap (ϵ_g) in comparison with unstrained Si matrix. In addition, the local electric field caused by the heterogeneity of the NCs surrounding, may be rather strong, therefore the fundamental absorption edge of c-Si undergoes additional blurring due to the Franz-Keldysh effect.

The spatial separation of electron-hole pairs by local fields may affect the rate of recombination of carriers photogenerated in the Si substrate. The smaller value of decline in shortwave region of photoconductivity spectrum for the structure with NCs is the proof of this fact (see Figure 2).

Let's consider the basic properties of photoconductivity in the case of the simplest Si/Ge heterosystem with $\text{Si}_{1-x}\text{Ge}_x$ NCs on the substrate of p-Si (001). Photoconductivity spectra (see Figure 3) measured at stationary excitation and temperatures 50-80-120 K contained two components. When $h\nu > \epsilon_{g,\text{Si}}$ (1.16 eV at 50 K), the main contribution to the photoconductivity is given by the electron-hole pairs, photoexcited due to the interband transitions in the p-Si substrate. In the spectral region where Si is transparent, photoconductivity is caused by the electronic

transitions involving localized states in $\text{Si}_{1-x}\text{Ge}_x$ NCs. When the temperature decreases to 120 K the long-term relaxation of the photocurrent is observed.

Figure 4(a) shows the time dependencies of photocurrent, measured after the photoexcitation by the quanta with the energy $h\nu = 0.9$ eV at different temperatures: 50, 80 and 120 K. After the cessation of lighting, the current decreased under the law:

$$I = I_0 + I_{\text{PC}} \exp\left(-\frac{t}{\tau}\right),$$

where I_0 and I_{PC} are the values of dark current and stationary photocurrent, respectively, and τ is the relaxation time of the photoexcitation. The inset on Figure 4 (a) shows the dependence of $\ln \tau$ on $1/(kT)$ and its linear fit. From the slope of the line we determined the photoconductivity activation energy $\varepsilon_a=12\text{meV}$. The spectral dependence of the relaxation time is shown in Figure 4 (b). We found that the decay constant increases with the increasing of the energy of excitation quanta. The relatively faster relaxation after the excitation of $\text{Si}_{1-x}\text{Ge}_x$ NCs only by the quanta with the energy $h\nu=0.8$ eV is the evidence of the fact, that the recombination through the states of NCs is more effective in comparison with the recombination in the surface layer of depletion of the p-Si substrate.

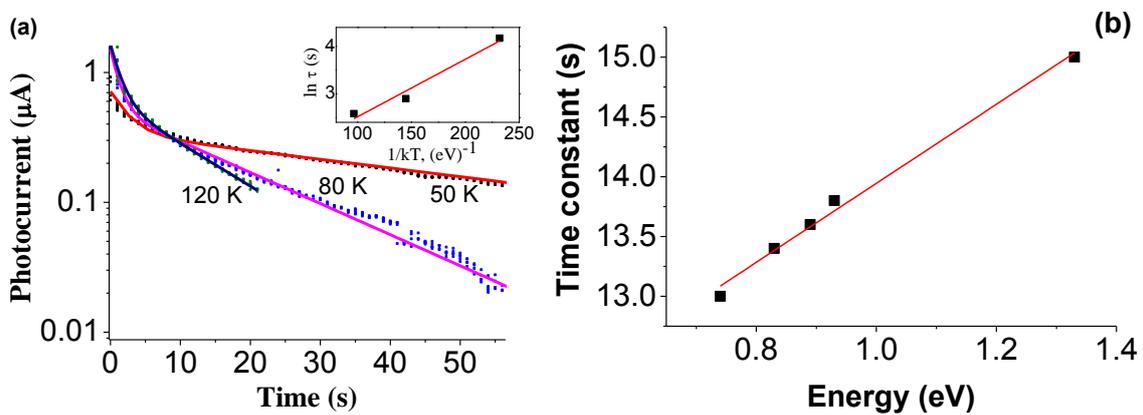


Fig. 4. (a) Time dependencies of photocurrent, measured after the photoexcitation by the quanta with the energy $h\nu = 0.9$ eV at different temperatures: 50, 80 and 120 K; inset – the dependence of relaxation time of the photoexcitation on inverse temperature and its linear fit. (b) Spectral dependence of photocurrent decay constant of the sample at the temperature $T = 120\text{K}$.

The decrease of the rate of recombination of nonequilibrium electrons and holes photogenerated in the Si substrate, is promoted by the uniform electric field of the surface layer of depletion of the p-Si substrate. This field has a direction that facilitates the drift of nonequilibrium holes, which are photoexcited due to band-to-band transitions in Si, towards the illuminated surface. At the same time, nonequilibrium electrons fill the potential well near the surface. Spatial separation of nonequilibrium charge carriers, thus, reduces the probability of recombination and slows the kinetics of the photocurrent at low temperatures. As shown in Figure 3, the decline in the shortwave region of the photoconductivity spectrum at $h\nu > 1.3$ eV is greater at higher temperature. Usually, the decreasing of the photoconductivity in this region of spectrum is explained by the fact, that with increasing $h\nu$ more and more excitation radiation is absorbed in the surface region of Si, where the rate of recombination of charge carriers is higher in comparison with the volume regions of the substrate. The observed changes in the shape of the spectra indicate that the recombination rate in the surface layer of the Si substrate decreased during cooling when the spatial separation became effective.

If photoexcitation of nonequilibrium electron-hole pairs is caused by the indirect electron transitions from localized states in the valence band of $\text{Si}_{1-x}\text{Ge}_x$ to the conduction band of Si

surrounding, photoexcited holes are localized in NCs. Photoexcited electrons, thus, accumulate in the potential well in the immediate vicinity of NCs.

The capture of the holes will be more effective, the greater is the depth of the potential well for holes. This is implemented in practice in heterostructures with $\text{Si}_{1-x}\text{Ge}_x$ NCs, enriched by Ge. Photoexcited holes could be shifted into the volume of substrate by the electric field of depletion layer, thereby avoiding the recombination with electrons from NC surroundings, only after the thermal discharge from the potential well into delocalized states of silicon surroundings. Lowering of the temperature obviously reduces the probability of the process of emission of localized holes, which contributes to their accumulation in NCs and increases the probability of recombination.

The surface charge of captured redundant holes affect the value of the band bending in p-Si substrate. In particular, the growth of positive surface charge leads to further depletion of space charge in the surface region.

4. Conclusion

Long-term decay of the photocurrent in Si/Ge heterostructures was observed at temperatures below 120 K after excitation by quanta with different energy. We showed that SiGe NCs, built-in into the multi-layer structures based on silicon, become the centers of recombination of electron-hole pairs photogenerated in Si and, in general, determine the surface recombination velocity in this heterostructures. It was found that during the selective photoexcitation of NCs the recombination of electron-hole pairs in SiGe is determined by the spatial separation of nonequilibrium charge carriers, when holes are trapped in the valence band states of SiGe, and electrons are in their silicon surroundings.

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