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Multilayer strained Si/SiGe structures: fabrication problems, interface characteristics, and physical properties

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The objectives of this investigation are structural and physical characteristics of the n-$Si_{1-x}Ge_x$/n(p)-Si heterojunction under strong elastic deformation of $Si_{1-x}Ge_x$ layers which gives rise to misfit dislocations in the heteroboundary region; the factors playing the main role in formation of the band structure of the system; the use of transmission electron microscopy and optical methods for determination of the phenomena connected with misfit dislocations in the grown epitaxial structure; the electrical characteristics of diode structures and the process of electron-hole recombination via dislocation states in a heterojunction.

Keywords: heterojunction, silicon, solid solution, misfit dislocation, photoluminescence, electrical properties.

1. Introduction

In the last decade, the properties of silicon-germanium heterostructures that are of active interest for opto-, micro- and nanoelectronics as one way of advancing silicon into a higher-frequency area, have been widely discussed in the literature. Fabrication of effective light emitting Si structures is the challenge taken up by many investigators. The most attractive objects to this effect today are Er doped Si, porous Si:Er systems, dislocations in strained Si layers, short period Si-Ge superlattices and quantum Ge/$Si_{1-x}Ge_x$ multilayer heterostructures. Possibilities of inducing light emission in the frequency range relevant to optoelectronics, both for epitaxial Si:Er layers and heteroepitaxial Si-Ge structures have been demonstrated in different works. Yet, the radiation efficiency in these systems is not sufficient, that is why searching for new ways to solve this problem and exploring other mechanisms of light emission in Si-Ge solid solutions is very important today. One approach proposed to date, is to modify the band structure of Si in order to make Δp for electrons about zero. Theoretical considerations show that this should in principle be possible by using, as an example, Si_nGe_m heterocompositions. Another possibility is to employ electrons in a crystal which are localised with the localisation length, at least in one direction, less or comparable with $h/\Delta p$. A typical example of silicon nano-size systems with the characteristic sizes comparable with $h/\Delta p$ is porous Si. It is well known that porous Si exhibits high photoluminescence (PL) efficiencies at room temperature, but the long-term stability of porous silicon LEDs is very poor.

Recently, rare earth-doped Si (in particular, Er doped Si) gained credibility as a potential candidate for optoelectronic applications. Alternatively, one can use impurities or extended defects, which behave as efficient radiative recombination centers. It is known that an increase in the dislocation density leads to a rapid decrease in the free exciton luminescence in Si, with a simultaneous appearance of new dislocation-related luminescence (DL) lines. Moreover, the integral intensity of DL can be larger than that of free excitons. The dislocation lines in Si and Si-Ge structures have been investigated rather extensively. Four bands (D1-D4) were found, of which D1 (0.804 eV) is most interesting for optoelectronic applications. However, the dislocation photoluminescence mechanisms and the nature of these PL bands are still not fully understood to this day. Solving the problem of increasing radiation efficiency in the dislocation Si (SiGe structures) may be very problematic, though, because it is very difficult to make highly competitive diode structures having high dislocation density and good injection characteristics. At the same time we address these issues in this paper with a view to increasing SiGe radiation efficiency towards creation of Si light sources for optoelectronics. The objectives of this investigation were to study the crystal structure, the optical and electrical properties of n-SiGe/n(p)-Si(100) heterostructu-

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res, and the efficiency of electron-hole recombination via dislocation states in a heterojunction.

2. Structural and light emitting properties of $Si_{1-x}Ge_x$/Si heterocompositions

We used a modification of the molecular beam epitaxy method (Si-GeH_4 MBE) to grow relaxed $Si_{1-x}Ge_x$ layers on n- or p-Si (100) substrates [1,2]. Penetration of Ge atoms into $Si_{1-x}Ge_x$ layers depends in this case on the proceeding of chemical reactions of GeH_4 decomposition on the growth surface. The Si component of a solid solution is built in by condensing a silicon atomic flow arising via sublimation of the Si monocrystal. The kinetics of layer growth by this method has been discussed in Refs. 3 and 4. The Ge content in the $Si_{1-x}Ge_x$ layers determined by the XR-diffractometry and Raman spectroscopy methods varied from 5 to 20 at. %. The $Si_{1-x}Ge_x$ solid solution layers had thicknesses from 0.1 to 1 μm. The thickness of the Si epitaxial film in most cases was in the 0.3 to 1 μm range. Si and $Si_{1-x}Ge_x$ epitaxial layers were doped with the electron impurity of $(1–5)\times10^{15}$ cm^{-3} and had the n-type conductivity. For all samples the thickness of $Si_{1-x}Ge_x$ layer exceeded its critical value which favoured formation of the misfit dislocation network in a heterojunction. Misfit dislocations are powerful sources of recombination centres.

The cross-section of two of such structures, obtained by the transmission electron microscopy (TEM) method is shown in Fig. 1. A rather thick (up to 0.5 μm) plastic deformation layer containing misfit dislocations with the density of extended defects of about 10^7–10^9 cm^{-2} was formed mainly in the silicon part of the structure. The density of the threading dislocations in the $Si_{1-x}Ge_x$ layer was estimated at 1×10^4 to 3×10^5 cm^{-2} by the metallography method.

The photoluminescence (PL) spectra of these samples exhibit additional D1-D4 lines besides the traditional PL lines connected with the free TO excitons both in a solid solution layer and in a Si substrate. The D1 and D2 lines which are more interesting for optoelectronics are absent in the structures with a small degree of plastic deformation when a solid solution film thickness does not exceed its critical value. For thick layers with a thickness exceeding their critical value these lines were pronounced, but the intensities of the D1(2) lines and the TO line in Si differed strongly for various structures. The intensity of the D1 line surpassed the intensity of the TO line for the structures with a high content of Ge component in the $Si_{1-x}Ge_x$ ($x > 0.1$) layers and a layer thickness of about 1 μm. Distinctive PL spectra from the structures considered above are presented in Fig. 2. PL spectra at 5 K temperature have been obtained on a standard graded spectrometer with a coolled Ge light recorder and by Ar-laser excitation. The nature of D1(2) PL bands is, however, still unknown. Possible candidates for D1(2) centres assumingly are some dislocation configurations that have not been practically investigated so far. One cannot exclude other reasons, for example, some common impurities (like oxygen) can be responsible for this luminescence, being incorporated in the dislocation core. Dislocations are, in fact, deep sinks for impurities owing to the gettering effect. That is why one can assume that these lines are most likely to be related with radiation transitions in the region of a "doping atmosphere" localised close to both threading dislocations in the layers and misfit dislocations on the "$Si_{1-x}Ge_x$ layer – Si substrate" heteroboundary. This could be ascertain, if dislocations could be prepared in really clean conditions.

Fig. 3 demonstrates the position of the indicated lines versus plastic deformation in the system, which we characterise by the $h = xd$ parameter. When the value of x increases, the total elastic energy accumulated in the structure will remain constant due to the dislocations generation. The local elastic energy of a silicon matrix in a $Si_{1-x}Ge_x$ layer will increase both with a higher Ge content and with a

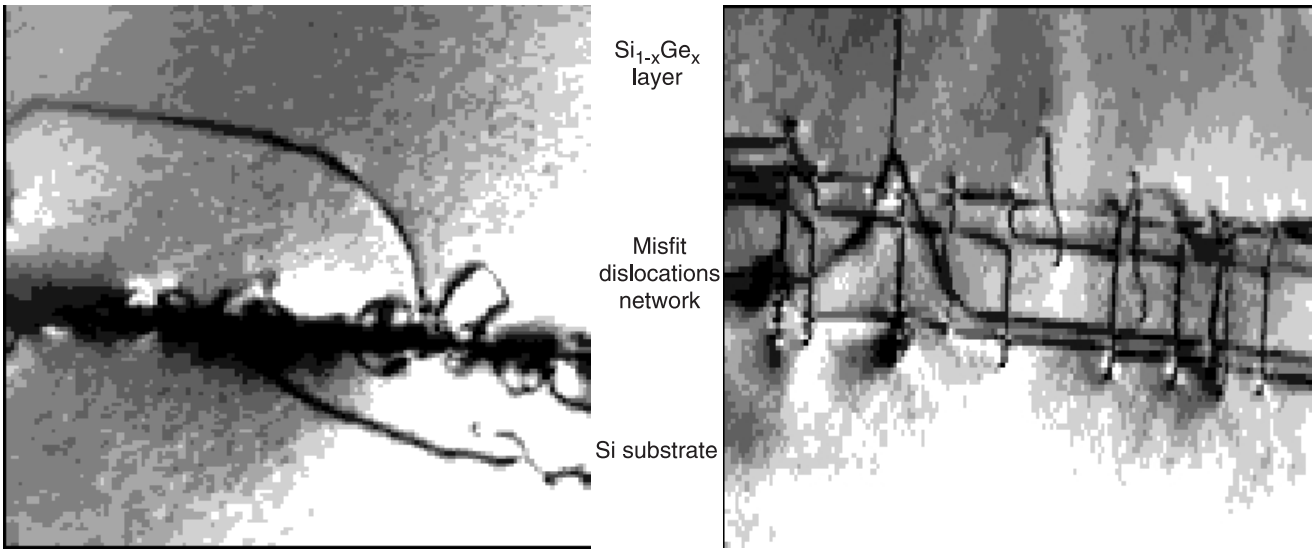

Fig. 1. TEM image of stressed $Si_{1-x}Ge_x$/Si heterocompositions with the dislocation network in the region of the heteroboundary.

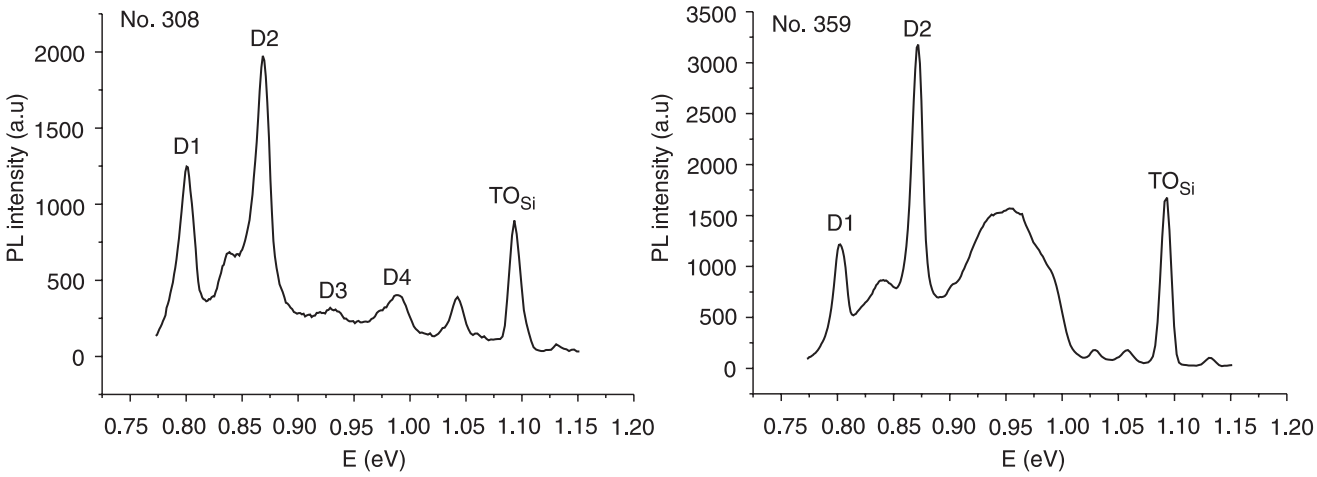

Fig. 2. PL spectra ($T = 5$ K) from $Si_{1-x}Ge_x$ structures with $Si_{1-x}Ge_x$ ($x \approx 0.1$) layer thickness $d = 1.2$ μm (No. 308) and $d = 0.6$ μm (No. 359).

higher thickness d of a growing $Si_{1-x}Ge_x$ layer. In the latter case it happens through reduction of the influence of the silicon substrate on the $Si_{1-x}Ge_x$ layer. It is clearly seen that a larger h (or x) does not provide substantial shift of the D1 (D2) line position, which once again confirms their connection with electron transitions via the states of the centres nearest to dislocation.

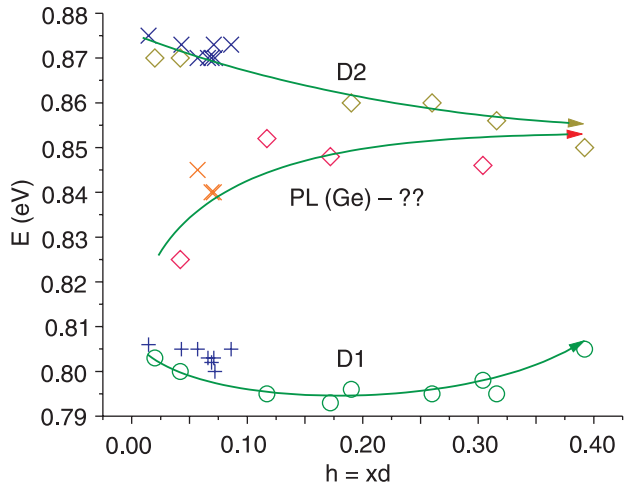

Fig. 3. D1 and D2 PL line positions in PL spectra of $Si_{1-x}Ge_x$ layers versus h parameter.

3. Injection properties of the n-SiGe/n-Si heterojunctions

To have efficient electroluminescence in diodes fabricated on the basis of strained heterostructures takes heterojunctions with good injection characteristics and high recombination currents via light emission centers. For relaxed heterostructures with a high dislocation density this is very problematic because of the non radiation electron transition. Therefore a study of the potential barrier characteristics in a heterojunction and of the properties of the recombination centers in this region is an urgent problem today.

Investigation of the electrophysical properties of our structures by the Hall method along with the CV-profiling of the charge carriers concentration (Fig. 4), shows, with a high degree of certainty, the presence of localised space charge in the region of the misfit dislocation network. This part of the structure has a p-type conductivity. The activation energy of these centers, according to our measurements, is about 0.017 eV.

The light absorption band edge in the photovoltaic spectra of the most investigated $Si_{1-x}Ge_x$/Si structures is rather rough (Fig. 5). The centres localised in the vicinity of misfit dislocation in Si, which create a "doping atmosphere" through the gettering effect do not show up because their absorption band lies inside the absorption band of the $Si_{1-x}Ge_x$ layers with the gradient content (x is increasing towards the outer surface of the $Si_{1-x}Ge_x$ layer [4]) due to the Ge segregation effect.

In Fig. 6 we schematically show the bands structure in the n-n$^+$ i n-p – heterojunctions at T > 200 K when some dipole layer connected with the charged centers inside the dislocation network is present. The charge localised on these centers ensures both an effective barier for electrons

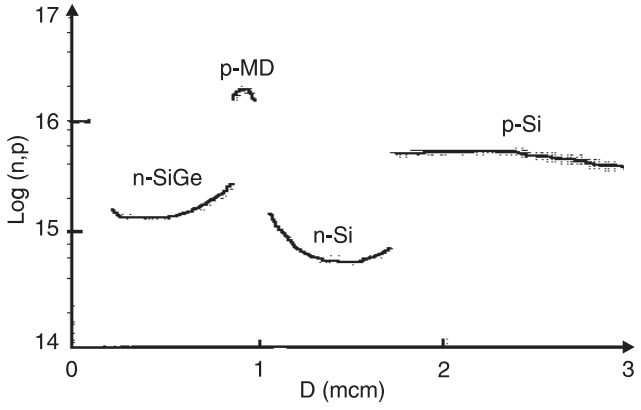

Fig. 4. CV – profiling of the n-$Si_{1-x}Ge_x$/n-Si/p-Si(100) sample (No. 358) with $x = 0.08$.

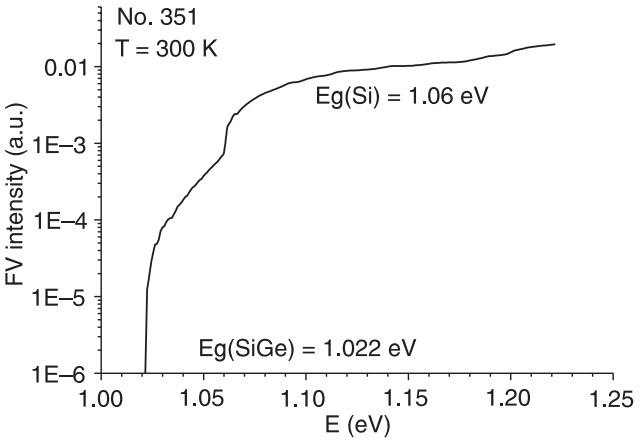

Fig. 5. Photovoltaic characteristic of the sample (No. 351) with n-$Si_{1-x}Ge_x$/n-Si (x = 0.2) heterostructures.

and an additional channel for the electron-hole recombination.

In accordance with Fig. 6, one can assume that the barrier connected with the localized states in the plane of misfit dislocation will play the main role in transverse electron transport. Below we discuss the peculiarities of the current – voltage (I-V) characteristics of these structures measured at room temperatures. For these measurements the omic Al contacts with the area 0.8×0.8 mm^2 on the top surface of the samples have been prepared.

Current-voltage characteristics (I-V) of different n-$Si_{1-x}Ge_x$/n-Si samples are presented in Fig. 7. For comparison we also show one I-V characteristics [curve 2 in Fig. 7(b)] of the Schottki barrier fabricated on one of the grown structures. Theoretical curves have been calculated by two methods. A faierly good agreement between theory and experiment take place when the simplest formula $J = J_0\{exp(eU/n^*kT) - 1\}$ for the current density through n-n^+ heterojunction is used for evaluation. Thus, heterojunction is considered to be a simple Schottky diode with incorporated factor n^* which reflects the presence of recombination currents in the heterojunction. The corresponding curve calculated for J_0 = 0.002 A and n^* = 5 is presented in Fig. 7(a) (solid line 2). A significant value of factor n^* in the n-n $Si_{1-x}Ge_x$/Si heterodiodes and a higher value of the density of the reverse current J_0 as compared to the I-V characteristic of the Schottky diode fabricated on the same structure [Fig. 7(b)] show an essential contribution of the recombination current in the total current through the n-n heterojunction.

The dot line (3) in Fig. 7(a) corresponds to the Opdorp's model of the n-n heterojunction with two Schottky diodes connected in series opposition. The current through the diodes in this case is expressed by the formula:

$$J = \frac{2J_{S1}J_{S2}sh\left(\frac{eU}{2kT}\right)}{J_{S1}\exp\left(\frac{eU}{2kT}\right) + J_{S2}\exp\left(-\frac{eU}{2kT}\right)}$$

where $J_{S1(2)}$ is the saturation current throus diode 1(2), U is the voltage on the potential barrier in the heterojunction. It is possible to determine saturation currents from the experiment. The use of the method in Refs. 5 and 6 which consists in finding of the inflection point on the I-V curve (in our case for sample No. 347 this point corresponds to voltage U = 0.6 V) does not, however, give a satisfactory agreement of the theoretical and experimental dependencies. A more satisfactory agreement [Fig. 7(a), curve 3] is achieved by using the following values of parameters: J_{S1} = 0.002 A; J_{S2} = 0.02 A, which correspond to the voltage U = 0.06 V on the heterojunction. Diode 1 corresponds

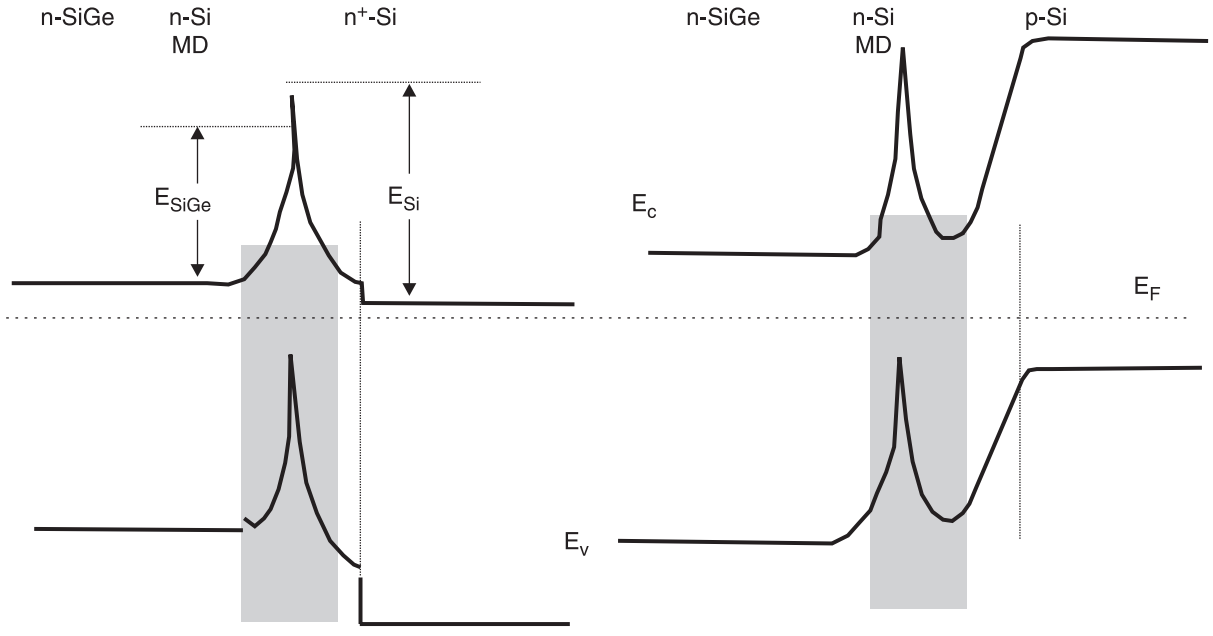

Fig. 6. Diagram of the energy bands in n-n- and n-p heterojunctions at T > 200 K.

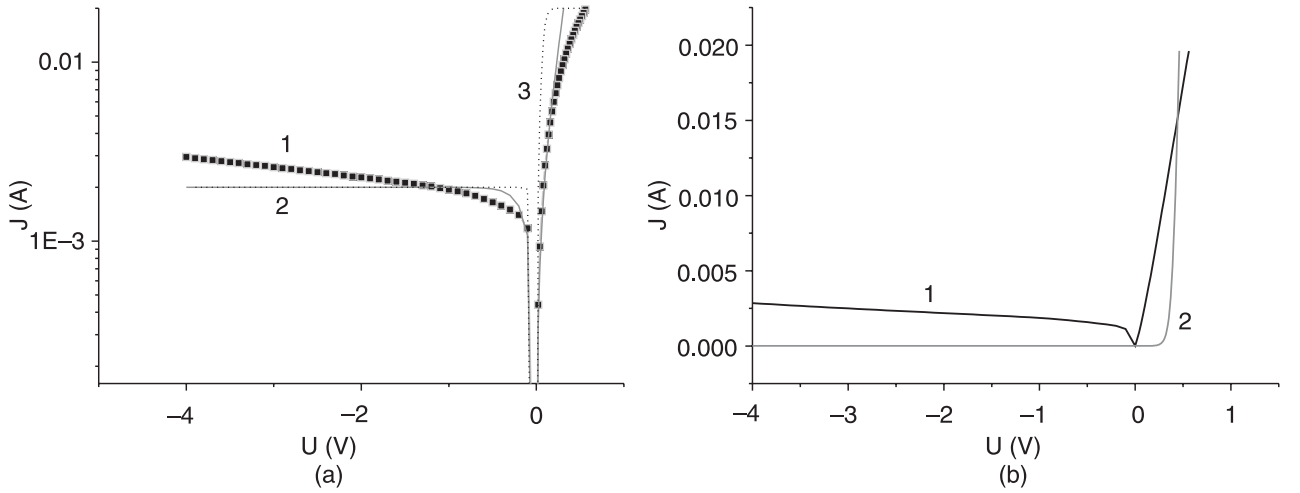

Fig. 7. I-V curves of the n-$Si_{1-x}Ge_x$/n-Si heterocompositions grown on n^+ – Si substrates (a,b – line 1); Schottky barrier (b – line 2) fabricated on this structure and the theoretical curves (a – lines 2,3) calculated for two models – one (2) and two (3) Schottky diodes.

to Schottky barrier in the heterojunction from the silicon side. Forward current flows through diode 1 when positive voltage is applied- to the upper omic contact on the surface of a solid solution layer.

Knowing (even aproximately) values of saturation currents allows one to calculate the height of the energy barriers from both sides of the heteroboundary. According to the emission model, the expression for J_S has the following form: $J_{SI} = 4\pi me(kT)^2h^{-3}S\ exp(-E_I/kT)$, where m is the efficient mass of conductivity (for silicon m = 0.26 m_0), S is the area of the contact. Assuming $m = m_{Si} \approx m_{SiGe}$ for $J_{S1(2)}$ we find, accordingly: $E_{Si(SiGe)}$ = 0.42 (0.36) eV. These data agree very well with the Opdorp's results obtained for the n-Ge/n-Si system [5,6]. The difference in the barrier energy: $\Delta E_c = (E_{Si} - E_{SiGe})$, when the charge states in the heteroboundary are absent, correspond to the energy of the conductivity band offset on the $Si_{1-x}Ge_x$/Si interface. According to Refs. 5 and 6 this energy is equal to 0.15 eV for the Si – Ge system. In our structures the dipole layer in the region of the misfit dislocation increases this value, that is why the calculated energy ΔE_c = 0.06 eV does not correspond to the real conductivity band offset. The conductivity band offset on the $Si_{1-x}Ge_x$ /Si heteroboundary due to the deformation effects is close to zero (ΔE_c = –0.02 eV) [7].

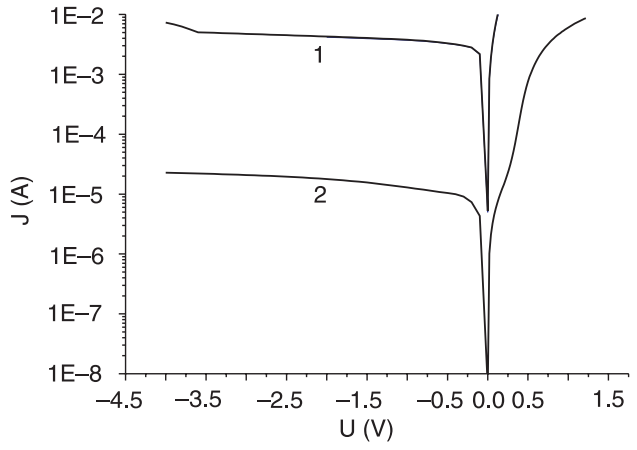

Fig. 8. I-V curves of the n-$Si_{1-x}Ge_x$/n-Si heterocompositions (1 – No. 351; 2 – No. 358) grown on p – Si substrates. (T = 300 K).

To observe a more effective light emitting recombination in the heteroboundary region we have to made an electron-hole injector in the form of an n-p junction. The band diagram of this n-p – diode is presented in Fig. 6. The I-V-characteristics measurements for two n-p – structures (samples No. 351 and 358) are shown in Fig. 8.

The level of the reverse current in this system depends very strongly on the density of localized states in the heteroboundary. The plastic deformation and the density of misfit dislocations in structure No. 351 (x = 0.2, D_{SiGe} = 0.3 μm) are higher than in structure No. 358 (x = 0.08, D_{SiGe} = 0.8 μm). In these structures the n-SiGe/n-Si heteroboundary is near the injecting n-Si/p-Si junction (Fig. 6). This geometry allows to inject both electron and hole into the region of the misfit dislocation, which increases the probability of light emitting recombination. The existence in the structure of two barriers, however, (one barrier connected with the localized states on the boundary, the other – with the n-p – junction) can influence the form of the I-V curves resulting in, for instance, appearance of regions differing in the steppness of the I-V characteristics of the structures due to the breakdown one of the barrier.

4. Conclusions

We considered the structural and physical properties of the n-SiGe/n-Si heterojunction for possible application in optoelectronics. The energy of the potential barrier in the conductivity band nearest to the heteroboundary, connected with the recombination centers in the region of misfit dislocation network, has been estimated on the basis of electrical measurements of the structures and the theoretical Schottky model.

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