

SURFACE RECOMBINATION OF CHARGE CARRIERS IN STRUCTURES “SILICON NANOCRYSTALS ON SILICON”

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The possibility to suppress the surface recombination of charge carriers in monocrystalline silicon (c-Si) has been studied at low temperatures, and the band-edge luminescence in c-Si has been observed. The increase of the effective lifetime of minority charge carriers and its correlation with the intensity growth of the edge photoluminescence have been revealed in c-Si covered, making use of pulsed laser deposition, with SiO_x films ($x \rightarrow 2$) which contain Si nanocrystals.

1. Introduction

The article is devoted to the consideration of nanocrystalline silicon (nc-Si)—c-Si nanostructures (“silicon-on-silicon”) with band-edge photoluminescence (PL). They constitute the subject of a new direction of researches which deal with suppressing the surface recombination in c-Si at low temperatures and aim, in particular, at creating the emitters based on silicon with edge electroluminescence at a wavelength of $1.1 \mu\text{m}$. The reduction of the surface recombination in such emitters remains a challenging problem from the viewpoint of improving the properties of silicon-based transistors and solar cells, fabricating microelectronic elements with extremely small dimensions, and so on.

In 1976, in work [1], semi-insulating polycrystalline silicon (SIPOS) was suggested and successfully used for the passivation of the surface of high-voltage transistors. SIPOS was a Si layer doped with oxygen and nitrogen. In essence, it was a nanocomposite, which included Si nanoparticles as one phase and an insulator — SiO_2 or SiN_2 — as the other phase. Such layers were deposited onto the c-Si surface by the chemical vapor deposition (the CVD method). According to the estimations made, the rate of surface recombination in diodes that were passivated by SIPOS layers was about 200 cm/s . The roles of Si nanoparticles and the CVD technology, which was used for their formation, in the reduction of recombination losses on the c-Si surface have not been clarified.

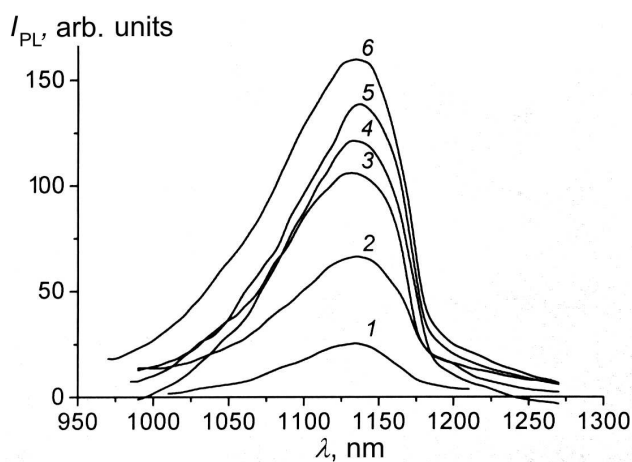
In 2004, in work [2], photoelectrochemical processes in GaAs and InP, with CdS nanoparticles having been deposited onto their surface from the aqueous solution, were studied. It has been shown that the enhancement of the photosensitivity of those semiconductors is connected with a decrease of recombination losses on their surface. CdS nanoparticles were considered as being deposited onto the active centers on the surface, which were created by defects, to neutralize them. These centers were assumed to be the centers of radiationless recombination of charge carriers, and the catalytic activity of nanoparticles was considered higher for smaller particles.

This work aimed at studying the possibility to reduce the surface recombination in c-Si by modifying its surface. The modification consisted in depositing Si nanoparticles onto the c-Si surface at room temperature making use of the pulsed laser deposition method.

2. Experimental Part and Discussion of Results

Having examined the literature data on the issue of modifying the c-Si surface with Si nanoparticles in order to reduce the surface recombination and to observe the band-edge luminescence in c-Si, we came to the conclusion that our researches reported below are among the pioneer ones.

We studied the structures obtained by the pulse laser deposition of nanocrystalline silicon (nc-Si) films onto the (100) face of single-crystalline silicon (*p*-Si, $10 \Omega \times \text{cm}$). The films comprised biphasic systems which contained quantum-sized Si nanocrystals in a SiO_x matrix ($x \rightarrow 2$) [3, 4]. Hence, the investigated structures were the heterojunctions between a wide-gap low-dimensional silicon (nc-Si) and a single-crystalline silicon (c-Si). The films of two types were fabricated. The films of the first type were deposited using the high-energy stream of particles from an erosion plume, in the oxygen atmosphere, and onto a c-Si substrate, remote in



Band-edge photoluminescence spectra of *p*-Si covered with a SiO_x film ($x \rightarrow 2$), which includes Si nanocrystals and is either undoped (1) or doped with various impurities: In (2), Er (3), Fe (4), Au (5), and Al (6). The corresponding lifetimes τ_{eff} of the minority charge carriers are 9 (1), 11 (2), 15 (3), 17 (4), 20 (5), and 27 μs (6)

the normal direction from the *c*-Si target. The films of the second type were deposited using the low-energy particles from the inverse stream, in the inert gas atmosphere, and onto the substrate located in the target plane. The beam emitted by a YAG:Nd³⁺ laser operating in the modulated *Q*-factor mode (the wavelength of 1.06 μm , the energy density of 20 J/cm², the pulse duration of 10 ns, and the repetition frequency of 25 Hz) was used to scan either the *c*-Si target or the *c*-Si target with a metal film (Au, Ag, Cu, Al, In, and others) deposited above.

The rate of surface recombination S was evaluated from the value of the effective lifetime of nonequilibrium charge carriers τ_{eff} in specimens with the thickness of the order of the charge carrier diffusion length. In its turn, the value of τ_{eff} was determined by analyzing the kinetics of the thermal emission decay beyond the edge of intrinsic absorption at laser excitation of the specimen [5].

We also investigated the correlations between the conditions of the *c*-Si surface passivation by nc-Si films, the rate of surface recombination in *c*-Si, the intensity of edge PL in *c*-Si [6], and the density of boundary electron states (BESs) at the nc-Si/*c*-Si boundary of these structures [7–9]. The BES spectra were determined by analyzing the measured temperature dependence of the condenser (surface) photovoltage.

The uncovered *c*-Si surfaces and *c*-Si surfaces covered with nc-Si films of the first type were characterized by

the highest values of S , $S > 10^3$ cm/s. The highest BES densities, $N_{\text{BES}} > 10^{12}$ cm⁻² eV⁻¹, and the highest densities of nonequilibrium charge carrier traps were inherent to them. Edge PL in *c*-Si was not observed for such specimens.

At the same time, the edge PL signal with the maximum at 1.09 eV, provided room temperature, appeared in the structures of the second type. The reference experiments, where nc-Si films were deposited onto mica substrates, proved that PL did not result from the emission of large-size Si nanocrystals in the film, but stemmed from the emission of the *c*-Si substrate. Doping films with metals led to the enhancement of the PL signal (see the figure). These structures manifested a distinct correlation between the PL intensity and τ_{eff} ; the values of the latter fell into the range 9–27 μs . The rate of surface recombination S was equal to $5 \times 10^2 \div 2 \times 10^3$ cm/s at that. The density of defects in these structures was lowered. The most substantial reduction of N_{BES} (down to 10^{11} cm⁻² eV⁻¹) occurred when the films were doped with gold atoms.

The structures with the copper-doped films also did not manifest edge PL, and the values of τ_{eff} were small for them. As a rule, the contamination of silicon with transition 3*d*-metals, such as copper, leads to the degradation of the charge carrier lifetime. The acceptor (Al, In) doping of the films deposited onto *p*-Si, led to an increase of the PL signal, because the highest rate of surface recombination may be inherent to the surface of an intrinsic semiconductor. A promoting influence of Au atoms, which have a large electron affinity, with respect to the PL enhancement is connected with their passivation of the silicon broken bonds – the main centers of radiationless recombination. On the other hand, Au atoms reveal catalytic properties during their oxidation and assist in the formation of stoichiometric oxide SiO₂ with a lower defect density. The passivation of the *c*-Si surface by depositing Si nanocrystals onto it can be explained by the fact that Si nanocrystals become deposited onto the active centers on the *c*-Si surface which are formed by surface defects. Since small particles are more active catalytically, it is the deposition of quantum-sized Si nanocrystals that assists the passivation of the *c*-Si surface.

3. Conclusions

The correlations between the increase of the effective lifetime of minority charge carriers in *c*-Si, the reduction of the BES density at the nc-Si/*c*-Si boundary, and the increase of the edge PL intensity in *c*-Si at the pulsed

laser deposition of SiO_x films ($x \rightarrow 2$) that contain Si nanocrystals on the c-Si surface have been found.

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ПОВЕРХНЕВА РЕКОМБІНАЦІЯ
НОСІЇВ ЗАРЯДУ В СТРУКТУРАХ
“НАНОКРИСТАЛИ КРЕМНІЮ НА КРЕМНІЇ”

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Резюме

Досліджено можливість зменшення низькотемпературним способом поверхневої рекомбінації носіїв заряду в монокристалічному кремнії, а також його крайову люмінесценцію. Виявлено збільшення ефективного часу життя неосновних носіїв заряду та його кореляцію зі збільшенням інтенсивності крайової фотолюмінесценції при кімнатній температурі в монокристалічному кремнії після імпульсного лазерного осадження на його поверхню плівок SiO_x ($x \rightarrow 2$), що містять Si-нанокристали.