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Enhancement of the luminescence of nc-Si/SiO$_2$ Structures due to radiation-thermal treatment

I.P. Lisovskyy[1], M.V. Voitovych[1], V.G. Litovchenko[1], V.Ya. Bratus[1], V.V. Voitovych[2]

[1]*Laskarev Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, 03028 Kyev, prosp. Nauki 41, Ukraine, E-mail:* m.v.voitovych@ukr.net

[2]*Institute of Physics, National Academy of Sciences of Ukraine,03028 Kyiv, prosp. Nauki 46, Ukraine*

Optimization of the emission characteristics (intensity enhancement and widening the emission spectral range) of the nc-Si/SiO$_2$ systems remains an actual task yet. A large number of investigations have shown that heat treatments in the ambient atmosphere, which includes hydrogen, are the most powerful for luminescence intensity enhancement. Recently [1] we have shown that efficiency of hydrogen annealing may be significantly (some times) increased if nc-Si/SiO$_2$ systems were preliminary exposed by high dose of ionizing radiation. This effect is connected with the formation of light emitting centers at the ncSi-SiO$_2$ interface. However, the mechanism of such defects creation process remains uncertain. To clarify it the influence of the heat treatments in the inert atmosphere on the luminescent properties of the irradiated nc-Si/SiO$_2$ systems was investigated in the present study.

The structures of nc-Si/SiO$_2$ were produced by high-temperature (T=1100 ^{o}C) heat treatment of SiO$_x$ (x≈1.3) layers. These structures have been irradiated by electrons (1 MeV) or γ-quanta (^{60}Co), the dose of exposure being 2×10^7 rad. Initial and irradiated samples were subjected to isothermal and isochronal anneals in Ar atmosphere within the temperature range of 50–500 ^{o}C. Infrared (IR) transmission, electron spin resonance (ESR) and photoluminescence (PL) spectra have been measured. In the latter case the dependence of the PL band intensity on the excitation level has been also analyzed.

Heat treatments of the initial nc-Si/SiO$_2$ samples within the whole temperature range did not influence on the PL intensity (I_{PL}). Irradiation decreased about two times the original value of the PL intensity. Subsequent annealing at the temperatures of 200 – 300 ^{o}C only replaced I_{PL} magnitude, what was expected and was evidently connected with elimination of recombination defects introduced by radiation at ncSi–SiO$_2$ interface [2].

Heat treatments of the irradiated nc-Si/SiO$_2$ samples within the temperature range of 300 – 500 ^{o}C resulted in a new effect: rise of the intensity (up to 5 times) and red shift (~40 nm) of the maximum position of the PL band (peak at ~ 800 nm). Analysis of dependence of the PL intensity on the excitation level made it possible to conclude that these events are connected with appearance of new PL band (peak position near 850 nm); intensity of this band being dependent on the conditions of post-radiation anneals. At the same time, the ESR peak (g=2.0058) related to silicon broken bonds decreased only slightly. Intensity, peak position (~1085 cm^{-1}) and the shape of the absorption band connected with Si–O stretching vibrations did not change, in other words concentration of Si–O–Si bonds in the sample did not varied in the result of radiation-thermal treatment.

Conditions of the post-radiation anneals are principal for the effect observed. At least two-stage heat treatment is necessary for appearance of a new PL band; first stage being carried out at less temperature. Subsequent increase of the temperature leads to rise of the PL intensity.

The effects are very similar to those which have been seen earlier after anneals of irradiated structures in the hydrogen ambient [1]. However, two main distinctions exist. The first one is associated with the specific regime of the post-radiation anneal. The second distinction is connected with the behavior of the ESR peak with g=2.0058: it was completely removed after heat treatments of irradiated structures in hydrogen. The latter fact seems to be natural and is obviously related to passivation of the silicon broken bonds with hydrogen. This effect should be absent for the samples heat treated in the inert atmosphere. Thus the nature of the revealed new PL band is most likely identical in both cases and may be explained as a result of creation of the light-emitting centers in the vicinity of ncSi – SiO$_2$ interface due to combined action of radiation and subsequent heat treatment.

The details of the process of the light-emitting defects generation and their possible nature are discussed.

1. Lisovskyy I., Voitovych M., Litovchenko V., Voitovych V., Nasieka Iu., Bratus V. Radiation Induced Enhancement of Hydrogen Influence on Luminescent Properties of nc-Si/SiO2 Structures // Nanoscale Research Letters – **2016** 11:545, DOI**:** 10.1186/s11671-016-1744-7
2. I.P. Lisovskyy, M.V. Voitovych, V.V. Voitovych, I.M. Khacevich. Influence of Radiation on the Luminescence of Silicon Nanocrystals Embedded in SiO$_2$ Film // Journal of Nanomaterials Volume **2016**, Article ID 9674741, 7 pages