Nanocomposites and nanomaterials

Photoluminescent properties of nc-Si–SiO$_x$ nanosystems

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Heterogeneous systems based on silicon nanocrystals (nc-Si) attract attention of researchers due to the wide range of possible applications, in particular memory elements [1] and single electron transistors [2]. Silicon oxide is the most natural dielectric material for silicon technology. The study of optical and photoluminescent properties of the silicon–silicon oxide nanosystems expands prospects of creating a new generation of optoelectronic devices.

The nc-Si–SiO$_x$ composites were obtained by evaporation of silicon powder using a vacuum system with residual air pressure ~10^{-3} mm Hg and deposition on the Si wafer. A film of amorphous nonstoichiometric SiO$_x$ (x<2) condensed on the substrates as a result of the reaction of vaporized silicon with residual oxygen. Then deposited SiO$_x$ films were irradiated from ^{226}Ra source and were annealed at 1000°C to grow nc-Si. Optical parameters of nc-Si–SiO$_x$ films were determined by the ellipsometric technique. In this work, the influence of annealing duration and radiation on the photoluminescence intensity of obtained nanosystem is shown.

A theoretical model of nc-Si–SiO$_x$ nanosystems photoluminescence was proposed. The *ab-initio* methods based on pseudopotentials and atomic-like base sets as well as all-electrons methods for calculation of electronic structure of model clusters were used. The results of calculations electronic structure of silicon quantum dots in dielectric matrix from first principles shows that the change passivation of dangling bonds with oxygen atoms leads to changes in band gap of silicon nanocrystals. The size dependencies of the electronic structure parameters and physical properties of the studied objects were obtained.

1. *Yano K., Ishii T., Hashimoto T., Kobayashi T., Murai F., Seki K.* Room-temperature single-electron memory // IEEE Trans. Electron. Dev.-1994.-**41**.-1628.
2. *Dutta A., Oda S., Fu Y., Willander M.* Electron transport in nano-crystalline Si based single electron transistors // Jpn. J. Appl. Phys.-2000.-**39**.-4647.