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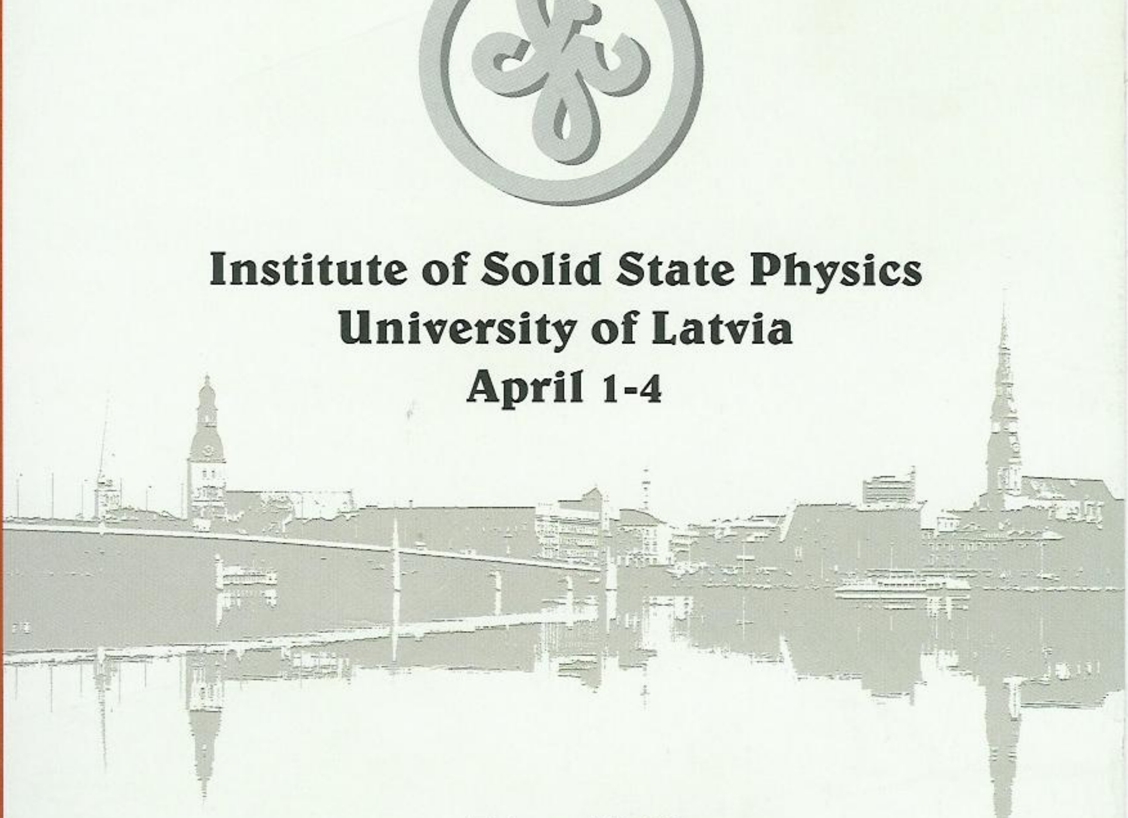

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REMARKS ON PHOTOLUMINESCENCE OF Si NANOCRYSTALS

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It is a widely accepted opinion that the intense photoluminescence (PL) of Si nanocrystals (Si-nc) is caused by electron-hole recombination. It is also widely believed that the Auger recombination in Si-nc occurs only at collisions of one electron and two holes (e-h-h process) whereas e-e-h Auger process (occurs at collisions of two electrons and one hole) in Si-nc cannot exist in analogy with bulk silicon. e-h-h Auger recombination process is non-radiative. – A lot of studies has appeared where decay of PL after excitation by a laser pulse has been examined. It was expected that the decay function is an exponent which is represented by a straight line in the half-logarithmic scale. In reality the PL decay curve is nonlinear and can be approximated by a stretched exponential function. This stretched exponential decay law is explained theoretically [1] by exciton transfer from the smaller to the bigger Si-nc.

Our analyses of available theoretical and experimental data show that Si-nc has an indirect band structure and, therefore, it is doubtful that electron-hole recombination is the main mechanism of intense PL [2, 3]. Due to quantum confinement effect the band gap of Si-nc widens and the second conduction sub-band moves away from the first one. It makes the e-e-h Auger recombination process possible. We propose a model, according to which a fraction of electrons reaches the second conduction sub-band by e-e-h Auger process, the main part of the intense radiation being caused by direct electron transitions from the second conduction sub-band to the first one [2, 3]. We construct continuity equations for the electron transport in the first and the second conduction sub-bands. The system of equations is solved numerically. At suitable adjustable parameter values the calculated PL decay curve coincides well with the experimental results [3]. Some properties discovered experimentally are explained on the bases of this mechanism.

Recently very intensive investigations in this area are performed. In this poster we analyze the relation of our PL model to the latest achievements in literature. – If the reason of the stretched exponential decay is the interaction between Si-nc, such decay should be observed only at sufficiently large densities of Si-nc. However, careful experiments [4] showed that even in the case where Si-nc is completely isolated from each other, the decay kinetics corresponds to the stretched exponential law. This means that the stretched exponential decay does not result from an interparticle interaction. – The carrier tunneling rate calculated in [5] is on the picosecond time scale for the typical range of confined carrier energies and Si-nc separations in silicon nanocomposites. The tunneling time is much faster than the characteristic PL decay time which is about 0,1ms for Si-nc. It means that PL occurs only in the largest Si-nc and the carrier tunneling cannot explain the stretched exponential decay. Hence, now only our model provides a basis for its explanation. – Investigation of PL quantum efficiency of Si-nc has showed that only some percents of Si-nc are radiative [6].

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