**Transport mechanism and high-field electroluminescence of silicon nanocrystals/$SiO_2$ superlattices**

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## Abstract

The size-dependent electronic and optical properties of silicon nanocrystals (Si-NCs) embedded in $SiO_2$ matrix have been extensively studied during the last years, as they are fundamental to exploit this system for light-emission or photovoltaic applications.[1,2] Besides, to guarantee a good control of the NC size, the superlattice (SL) approach has demonstrated to be an excellent method for obtaining Si-NCs with controlled size.[3] Although the transport within these nanostructured and ordered systems have been studied in the recent past,[4] some aspects of their electro-optical properties and its correlation with the charge transport mechanisms have not been fully studied.

In the present work, $SiO_xN_{0.23}/SiO_2$ SLs have been deposited on *p*-type c-Si substrate by means of plasma-enhanced chemical-vapor deposition (PECVD). Different structural parameters were varied from sample to sample, namely, the thickness of the $SiO_xN_{0.23}$ ($t_{SRON}$) and oxide barrier ($t_{SiO2}$) layers, and the Si excess within the Si-rich ones. A post-deposition annealing treatment was carried out at 1150 °C for 1 h in $N_2$ ambient, to precipitate and crystallize the Si excess in the form of NCs. To investigate the electrical and electro-optical properties of the Si NC superlattices, a MOS device structure was fabricated by sputtering ITO on top and Al on the bottom (see Fig. 1). Further details on the sample and device fabrication can be found elsewhere.[5,6]

From an electrical point of view (see Fig. 2), a notorious increase in conductivity of the SL systems is found when $t_{SRON}$ and the Si excess increase, and $t_{SiO2}$ decreases. In addition, the dependence of the electrical properties on voltage and temperature confirmed Poole-Frenkel (PF) as the main transport mechanism in our SL system. An electroluminescence (EL) study was carried out on the devices, showing a clear emission peak attributed to radiative recombination of electron-hole pairs within the NCs (see Fig. 3). On one hand, a blue-shifted emission is observed in devices containing thinner $t_{SRON}$ (i.e. with smaller NCs) and lower Si excess, attributed to the quantum confinement effect. On the other hand, the EL peak position remains unchanged at thinner $t_{SiO2}$, indicating that the nanostructure morphology is held constant. Finally, the correlation between all our experimental observations support an EL excitation mechanism consisting of electron impact ionization on the Si NCs, which can be correlated to the PF transport through NCs (see Fig. 3).

## References

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## Figures

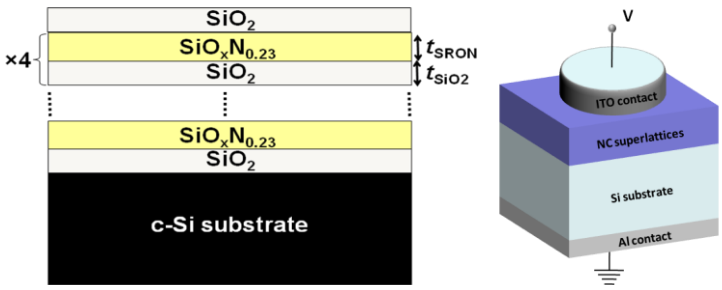


**Fig. 1.** (Left) Cross-section scheme of the PECVD-deposited $SiO_xN_{0.23}/SiO_2$ superlattiices for the present study. The sketch indicates the parameters that were varied, namely, the Si-rich oxynitride and oxide barrier layer thicknesses, $t_{SRON}$ and $t_{SiO2}$, respectively, and the Si excess ($x$ in $SiO_xN_{0.23}$). (Right) Device structure where the superlattices were embedded.

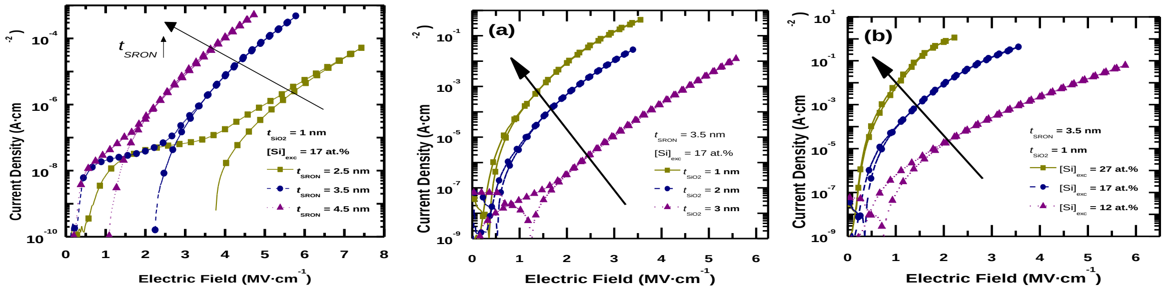


**Fig. 2.** Current density versus electric field characteristics of $SiO_xN_{0.23}/SiO_2$ superlattices consisting of different Si-rich oxynitride layer thickness (left), different barrier thickness (middle) and different Si excess within the Si-rich layer (right).

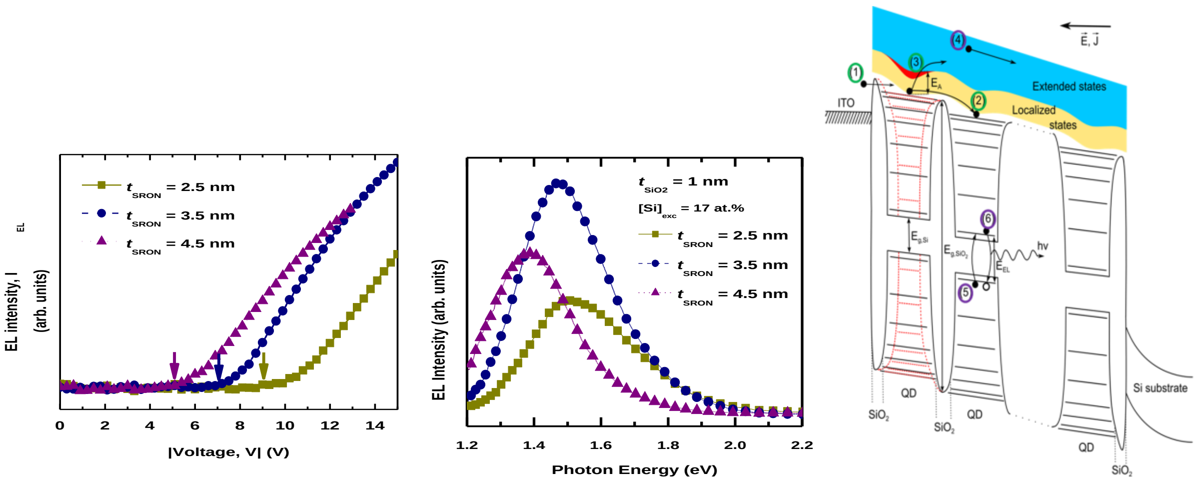


**Fig. 3.** (Left) Electroluminescence integrated intensity as a function of the applied voltage, showing an EL onset that depends on the Si-rich oxynitride layer thickness. (Middle) EL spectra corresponding to samples with different Si-rich oxynitride layer thickness, i.e. different NC sizes. (Right) Schematic energy band diagram of the studied superlattice under the presence of an external electric field, which shows the electron transport process and the EL mechanism. The changes in the band structure induced by the QD size reduction appear in red. Numbers indicate the different processes that take place: (1) electron injection through the ITO electrode; (2) trap-to-trap electron hopping; (3) thermally-activated electron jump towards the extended conduction band states; (4) high kinetic energy electrons that take part in the impact ionization process; (5) promotion of the bound electrons within the QD valence band states to the QD conduction band (electron-hole pair generation); (6) radiative recombination of the electron-hole pair, yielding a photon (EL emission). Energies are not to scale. Image taken from Ref. [6].