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Origin of Photoluminescence of Samarium-Doped Strontium Titanate Nanostrucutre under UV Light

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Abstract – $SrSm_{0.01}Ti_{0.99}O_3$ (ST_Sm) and $SrTiO_3$ (ST) has been investigated by a combined experimental and theoretical approach. The nanocrystalline powders were prepared by the polymeric precursor method (PPM). Order and disorder has been investigated by means of X-ray diffraction (XRD), Transmission Electron Microscopy (TEM) images, Electron Paramagnetic Resonance (EPR) and photoluminescence (PL) emission experimental techniques. The broad PL band and the Sm emission spectrum measured at room temperature indicate the increase of structural order with annealing temperature.

Within this class of perovskite compounds, $SrTiO_3$ (ST), in its crystalline form, displays a semiconductor behavior and when pure ST is excited by radiation above its energy band gap, which usually ranges from 3.2 to 3.4 eV, a broad greenish luminescent band appears whose intensity decreases rapidly when the temperature is above 50 K [2]. There are in the literature different approaches to explain the radiative decay taking place in perovskite-like structures. But, it is well established that impurities, surface states, and defects play an important role in the photoluminescence (PL) properties of perovskite-type oxides [3].

From the experimental side of this work, $SrTiO_3$ and $SrSm_{0.01}Ti_{0.99}O_3$ (ST_Sm) nanostructured powders were prepared by the polymeric precursor method (PPM). Order and disorder has been investigated by means of X-ray diffraction (XRD), Transmission Electron Microscopy (TEM) images, Electron Paramagnetic Resonance (EPR) and photoluminescence (PL) emission experimental techniques.

From the theoretical side, first principles quantum mechanical techniques, based on density functional theory at B3LYP level, have been used in sense to give a theoretical approach to the experimental PL results. It was simulated three disorder-type in the crystalline (ordered) cubic 1x 1 x 2 supercell, as fallow: in the network former (Ti), in the network modifier (Sr) and in the network former-modifier (Ti/Sr).

The experimental results, in the disordered powders, indicated that defects in the lattice are linked to inherent defects formed by complex clusters. First principle calculations indicate that generate localized states, in the band gap reduce the gap energies. As the structural order increases, the gap energy increases. These observations confirmed the fact that PL is directly associated with the localized states existing in the band gap and that the degree of order-disorder changes these localized states.

The complex clusters already existing in the ground state facilitate the emission process leading to PL, i.e, the radiative recombination. In our model, the Wild Band Model, the most important events occur before excitation, that is, before the photon arrival. The deep and shallow complex clusters generate localized states in the band gap and inhomogeneous charge distribution in the cell, thus allowing the trapping of electrons. The localized levels are energetically distributed, so that various energies are able to excite the trapped electrons.

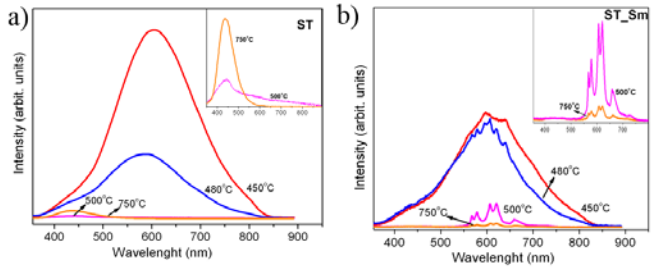

Figure 7. a) Room-temperature photoluminescence spectra of: a) ST powder samples annealed; and b) ST_Sm powders samples; annealed at 450, 480, 500 and 750 °C for 2 h in an oxygen flow. The exciting wavelength was the 350.7 nm line of a krypton ion laser.

References

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