A joint theoretical and experimental study of the relation photoluminescence - structural disorder in barium and strontium titanate thin films

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Abstract

Thin films of barium and strontium titanate (BST), synthesized by the polymeric precursor solution and spin coated on [Pt (140nm)/Ti (10nm)/SiO_2(1000nm)/Si] substrates were found to be photoluminescent at room temperature when heat treated below 973K, *i.e.* before their crystallization. First principles quantum mechanical techniques, based on density functional theory were employed to study the electronic structure of two periodic models : one standing for the crystalline BST thin film, regular model, and the other one for the structurally disordered thin film, deformed model. The aim is to compare the photoluminescence spectra of the crystalline and disordered thin films with their UV-vis spectra and with their computed electronic structures. With this study, we do not pretend to explain **how** the photoluminescence appears in this type of perovskite structure because many authors have already proposed satisfactory mechanisms like radiative recombination, self trapped excitons, etc…. We attempt to explain **why** photoluminescence exists in those particular thin films. The calculations show that new localized states are created inside the band gap of the crystalline model, as predicted by the UV-vis spectra. The study of the charge repartition in the structure before and after deformation of the periodic model shows that a charge gradient appears among the titanate clusters. This charge gradient, together with the new localized levels, gives favorable conditions for the trapping of holes and electrons in the structure, and thus to a radiative recombination process. Our models are not only consistent with the experimental data, they also allow to explain the relations between structural disorder and photoluminescence at room temperature.

Keywords : Films, Precursors-organic, Microstructure-prefiring, Optical properties, $BaTi0_3$ and titanates