CONFINEMENT EFFECT IN CdTe NANOCRYSTALS EMBEDDED IN SILICA THIN FILMS

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Nanostructures based on II–VI materials have attracted much attention for their great fundamental, experimental and applied interests. Extensive investigations of the optical properties of films containing semiconductor nanocrystals (NCs) have demonstrated their potential applications in optoelectronics [1]. These NCs have the properties of narrow size distribution, good crystallinity, and high PL efficiency [2]. However, their wider application has been restricted due to their liquid form. Embedding these NCs in a rigid matrix is a solution to this as well as photostability. As a rigid support, glass has several good properties such as transparency, robustness against atmospheric attack and UV irradiation. Semiconductor nanoparticles dispersed in optically transparent glass matrix have many applications in optical switching, optical filters, optical sensors, and wave guides. In this work SiO\textsubscript{2} matrix grown by the rf magnetron co-sputtering technique with subsequent annealing in vacuum. Absorption spectroscopy, Raman scattering, grazing incidence X-ray diffraction (GIXRD), X-ray photoemission spectra (XPS) and photoluminescence (PL) were used to study the grown samples.

GIXRD indicates that the as-grown samples have an amorphous nature, in agreement with earlier observations [3]. Fig. 1 shows the GIXRD spectra of the annealed CdTe doped silica films grown at different conditions. The comparison of these spectra with the JCPDS database (card 15-770) allows us to conclude that CdTe NCs in the cubic phase were grown inside the silica matrix. We can estimate the NCs sizes from the GIXRD results using the well known Scherrer equation. Depending on the grown conditions, different NCs average size was obtained ranging from 3 to 10 nm. Raman spectroscopy applied to annealed samples show a slightly asymmetric and broad peak centred at 169 cm\textsuperscript{-1}, corresponding to LO phonons in the CdTe.

The post-grown annealed samples show shoulders on the absorption spectrum in the range of 650 – 700 nm, clearly shifted from the bulk CdTe energy band gap (825 nm). These shoulders could be attributed to NCs exciton line, clearly indicating the effect of quantum confinement. A typical PL spectrum (Fig. 2) obtained from these samples display two peaks. A narrow one centered at 709 nm that we attribute to carriers recombination in the ground states of CdTe NCs. The broader one centered at 478 nm could be attributed to radiative recombination at defects in the interface NC/matrix.

The chemical and phase composition was determined using XPS technique taking into account the coefficients of elemental sensitivity (photoelectrons output cross section). We observed the size-dependent shift of the CdTe nanocrystal component of the Cd3d and Te3d photoelectron lines that was described in [4]: when a crystal reduces its size down to a nanometer scale, its electronic structure is changed and the entire core-level features moves simultaneously toward to high binding energy. The theoretically predicted value of this shift is size-dependent. The binding energy of Cd and Te core levels increases on +0.7 eV in comparison with the bulk standard. This shift is connected to the nanocrystallinity of the
chemical compound. The Te 3d\textsubscript{5/2} component at 576.6 eV binding energy is connected with oxidized Te atoms located on the nanocrystal/matrix interfaces. The relative number of these atoms is 23 at.%. Analyzing of this concentration, and assuming the spherical shape of the nanocrystals, we can calculate the diameter of CdTe nanoparticles. The size of CdTe NCs is 4.5 nm on base of XPS data. This value is in a good agreement with the one, evaluated from GIXRD data (5.2 nm).

Acknowledgements:
This work was partially supported by the European Commission through project called SEMINANO under the contract NMP4-CT-2004-505285 and by the project POCTI/FIS/56930/2004 financed by Portuguese Foundation for Science and Technology (FCT). SL thanks FCT for the financial support (grants SFRH/BPD/26532/).

References:

Figures:

Fig. 1. GIXRD spectra of the CdTe NCs doped SiO\textsubscript{2} glass films. The peak position of cubic CdTe are shown as vertical lines (from JCPDS database 15-770).

Fig. 2. PL spectrum of CdTe doped glass obtained at room temperature, with an excitation wavelength of 400nm.

Fig. 2. Cd 3d and Te 3d photoelectron spectra of S31.