# Elaboration and Study of Optical Properties of CdSe Nanocrystals Dispersed in a KBr Monocrystalline Crystalline Matrix and in a Thin Film of $SiO_2$ Amorphous Matrix

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**ABSTRACT**
In this work, we firstly present the elaboration of CdSe nanocrystals (NCs) dispersed in a KBr crystalline matrix in order to build nanostructured composed materials showing monocrystalline structure, and also using another technique, to deposit thin film of amorphous silica ($SiO_2$) containing CdSe quantum dots. These elaborated guest-host systems were investigated for potential applications in optoelectronic field. In the second part of this work, we present the structural and optical properties of these composite materials using several techniques: X-ray-diffraction (XRD), UV-visible absorption. Crystallites size estimated from XRD is equal 27 nm. Optical absorption shows size quantization effect marked by a blue shift by 0.308 eV from its standard bulk band gap value 1.7 eV. Comparing size determined by XRD crystallites size estimated from the blue shift was found to be smaller.

## 1. INTRODUCTION

Within the latest there is an increasing interest on wide gap semiconductor nanocrystals, especially II-VI binary semiconductors due to their electronic, magnetic, mechanical and over all original optical properties caused by the quantum confinement induced by the small size of the crystallites [1]. The strong electrons confinement is allowed by the quantum dots (QDs) of II-VI semiconducting nanocrystals.

When the crystallites size is in the same order of magnitude of the Bohr radius of the bulk crystal exciton, the binary semiconductor CdSe exhibit both linear and nonlinear optical properties that can be applied in optoelectronic devices [2, 3]. In order to compare and comfort our results, two different and complementary experiments were used to elaborate our samples. First technique of elaboration of QDs dispersed in a transparent KBr crystalline matrix was a fusion method using a monocrystalline growing heater according the so-called "Czochralski's growing technique". The transparency of the KBr host system is in UV-visible range. The second method is to synthesize thin films of amorphous $SiO_2$ matrix doped by CdSe crystallites using sol-gel technique and deposited on glass substrate.

The composed materials achieved by this ways were investigated structurally by XRD, and optically by UV-visible absorption.

## 2. EXPERIMENTAL

Monocrystals showing a good crystallographic quality with noticeable size were obtained by the fusion method according to the Czochralski principle. The crystal growth was performed in a homemade heater. Solid KBr crystals were melted at the melting point temperature of 850°C. As starting germ for the crystal growth, we used a good crystallographic quality and a polished sample to allow the material adhesion. This initial sample was dipped in the melting solution by a sample holder.

The temperature of the melting solution was slowly cooled down with a careful control of the appearance on the surface of the solution and around the germ, a brilliant ring corresponding to the meniscus. At this moment, the germ is slowly upward with 1cm/hour speed. The monocrystal growth starts in the three direction of the space. Two motors were used for this effect. First one for the vertical moves and the second one for the rotation of the sample (1 rotation per minute). Monocrystals prepared by this way present a good transparency and crystallographic quality. In order to synthesize a KBr doped CdSe NCs, the powder of CdSe NCs was regularly introduced in the melting solution during the withdrawal process. It result a transparent bulk that has a carrot aspect. With such technique, one can make crystal growth presenting several centimeters (figure 3)

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*Figure 1. Homemade heater used for monocrystalline synthesis.*

*Figure 2. Monocrystallines growth.*

*Figure 3. KBr Monocrystal doped CdSe.*

## 3. RESULTS AND DISCUSSION

### 3.1 Structural analysis by XRD

X ray diffraction analyses were performed at room temperature with a diffractometer D8 Siemens equipped with a rotating anode CuKα (λ=1.540Å). Figure 4 shows XRD pattern of CdSe semiconductor powder obtained by mechanical shredding and used as dopant in the KBr crystalline matrix. The obtained XRD pattern exhibits the same peaks as those of the CdSe hexagonal wurtzite structure belonging to the $P6_3mc$ space group reported by American society for testing material (ASTM) sheets.

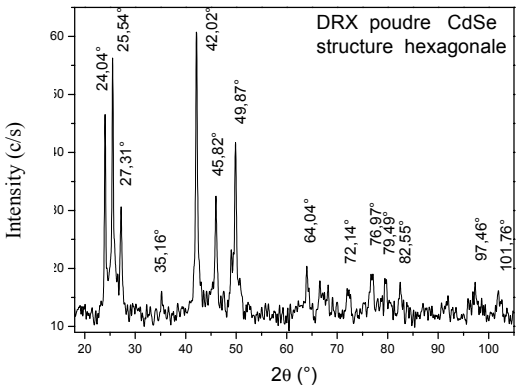


*Figure 4. CdSe nanocrystals X ray diffraction pattern.*

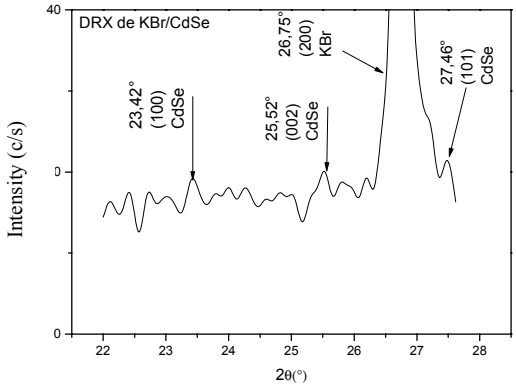


*Figure 5. CdSe nanocrystals pattern dispersed in a KBr crystalline matrix.*

Figure 5 shows the XRD pattern of a KBr monocrystalline pellet doped by CdSe nanocrystals. The pellet was cut according the (100) cleavage plan perpendicular to the (001) growing axis. One can see peaks belonging to the KBr crystalline matrix and additional peaks corresponding to the (100), (002), (200) and (101) diffracting plans of CdSe nanoparticles. Thus evidence the nanocrystals incorporation in the KBr matrix.

The average radius of the dispersed nanoparticules in the KBr crystalline matrix was estimated using Sherrer formula in which the crystallites have a spherical shape.

$$2R = 0.9\frac{\lambda}{W}\cos(\theta), \tag{1}$$

where $R$ is the crystallite average size; $\lambda$ is X ray excitation wavelength. Our measurement were performed at $\lambda$ = 1.540 Å that corresponds to CuKα tube emission. $\theta$ is the diffracted angle and $W$ the full width at half maximum (FWHW) of the intensive peak.

The calculated value of the nanocrystals was about 27.5 nm.

### 3.2. Optical analysis

Optical absorption spectra were measured at room temperature with UV-PC 3101 Shumatsu spectrophotometer in the range of 800 nm to 190 nm. Absorption spectrum of a pure KBr crystalline matrix in the UV-Visible

spectrum is shown on figure 6. The pure KBr structure appears to be transparent in this range. Only two weak peaks of absorption at the wavelength 250 nm and 200 nm appear due to the presence of defects in the KBr structure.

By contrast, figure 7 shows the optical absorption of a cut pellet of KBr monocrystal doped by CdSe NCs. Three peaks can be observed in the wavelength range [400 nm, 650 nm]. First one at 625nm, the second at 582 and the third one at 460 nm, respectively. These additional results confirm once more the incorporation of the CdSe NCs in the KBr host matrix.

Moreover, same results were obtained on thin layers of $SiO_2$ host system doped by CdSe NCs prepared by sol-gel process [7]. The UV Visible absorption spectra of these thin films show the existence of one peak located at 625.55 nm due to the presence of the CdSe NCs in the $SiO_2$ amorphous matrix (figure 8).

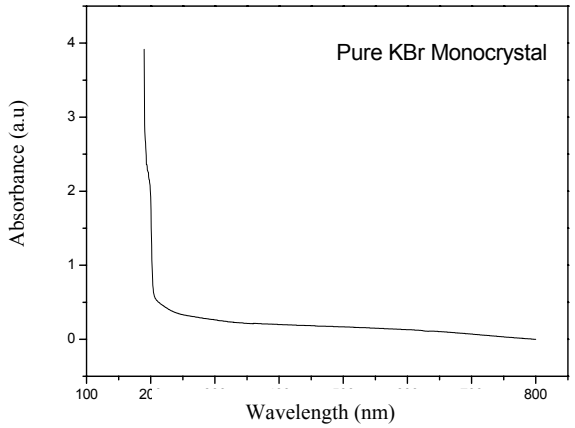


*Figure 6. Pure KBr Monocrystal UV-Visible spectrum.*

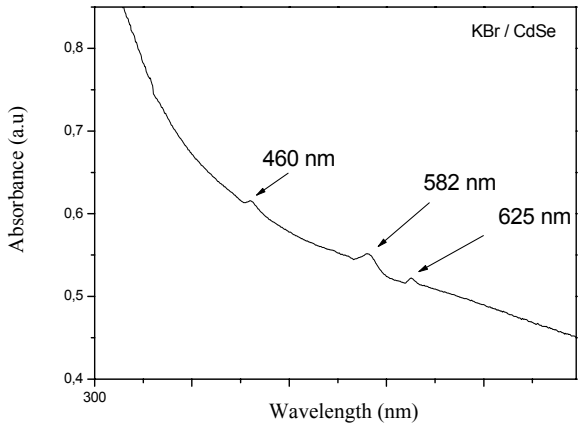


*Figure 7. UV-Visible spectrum of a KBr Monocrystal dopped with CdSe nanocrystals.*

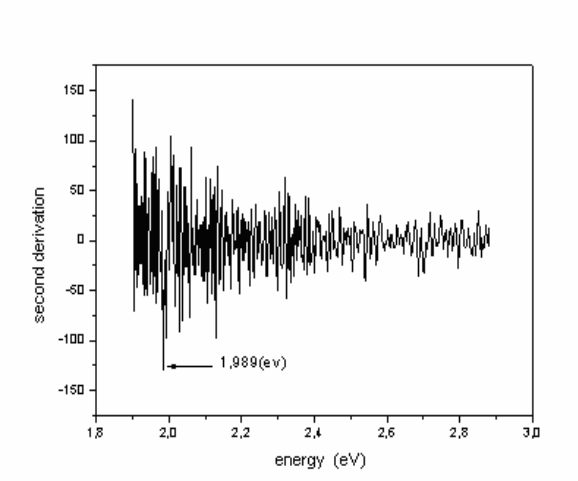


*Figure 9. Bandgap of CdSe NCs in KBr matrix.*

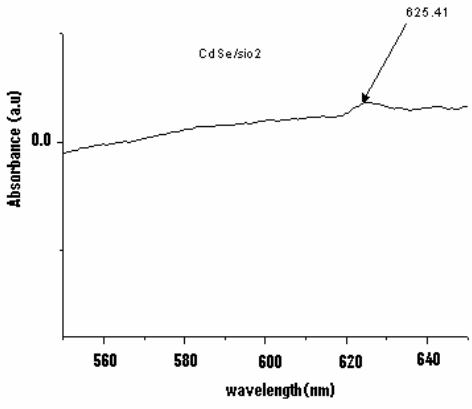


*Figure 8. UV-Visible spectrum of CdSe NCs /.$SiO_2$*

Using the optical analyses, the crystallites size was estimated using the effective masse model [6].

$$E^* = E_g + \frac{\hbar^2 \pi}{2R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) - \frac{1{,}8e^2}{\varepsilon R} \qquad (2)$$

where $E^*$ is the optical gap energy of the NCs; $E_g$ is the optical gap energy of the bulk system; $m_e^*$ and $m_h^*$ are the effective masses of the electron and the hole, respectively; $\varepsilon$ is the dielectric constant of the bulk material; $e$ is the electron charge and $R$ the average radius crystallite size.

According to Dijken *et al*. work [6], we used as data $m_e^* = 0.13\ m_0$, $m_h^* = 0.45\ m_0$ . $\varepsilon = 10$, leading to the relation (3):

$$E^* = 1,7 + \frac{23.36}{R^2} - \frac{1.8}{R}e^2 . \quad (3)$$

By calculating the second derivative of the absorbance of the KBr matrix doped CdSe NCs from absorption spectrum, we determine $E^* = 1,989$ eV (Figure 9) as relative value of the first transition. Including this value in equation 3, we obtain $R = 8.68$ nm as average radius for the CdSe crystallites. Such result shows decreasing the crystallites size leads to an enhancement of the gap energy. The bandgap variation $\Delta E = 0.308$ eV exhibit a blue shift. By comparing the NCs average size of CdSe and the Bohr radius exciton which is about 5.5 nm [6], we conclude that the considered confinement is intermediate.

## 4. CONCLUSION

Sol-gel and fusion techniques of synthesis and the structural and optical analysis show the good incorporation of the CdSe NCs in both host systems: KBr monocrystals and $SiO_2$ thin films. These experiments are reproducible and can be applied for others semiconducting nano dopants and inorganic matrices.

The blue shift confirms the quantum confinement of the CdSe NCs. Nevertheless, the crystallites size determined by XRD and by optical absorption presents a noticeable gap induced by the non-spherical shape of the NCs. $R = 27.5$ nm and 8.8 nm, respectively. These results are in perfect agreement with the recent works of Sarangi *et al*. [4, 5]. In order to complete this work and to confirm the crystallite size and the geometrical shape, we plan to continue our investigation with the electronic microscopy by transmission (MET).

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