Elaboration and characterization of AuCl semiconductor nanocrystals embedded in KCl single crystals

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***Abstract*—In this work, we investigated the structural and the optical properties of AuCl semiconductor nanocrystals embedded in KCl single crystals. The AuCl nanocrystals were obtained by doping the KCl crystalline matrix with gold using the Czochralski method. The X-ray diffraction showed the formation of the AuCl nanocrystals in KCl with a tetragonal structure. The average radius of the AuCl nanocrystals is estimated using the Scherrer formula. The photoluminescence spectra presented a band emission situated at 580 nm leading to the formation of the AuCl nanocrystals within KCl.**

Keywords-AuCl; Semiconductor nanocrystals; X-ray diffraction; Photoluminescence.

I. INTRODUCTION

Semiconductor nanocrystals embedded in wide gap matrices, such as alkali halides [1, 2] have in recent years a great interest for both fundamental research and technical application. From the technological point of view, the main motivation for studying nanocrystals is to search new applications by controlling their physical properties as a function of size [3]. The nanocrystals are characterized by a dominant surface effect and they have a considerable surface/volume [4]. In that respect, the optical properties of semiconductor considerably change when their sizes become comparable to the bulk Bohr radius of exciton [3]. This change permits to get the quantum confinement of the electronic excitations [5]. The confinement in three dimensions of the exciton could be at the origin of strong nonlinear properties, which make them suitable materials for use in laser devices.

Gold(I) chloride (AuCl) belong to the family of elements I-VII having semiconductor properties, was the subject of little studies. The optical properties of AuCl were studied by Claude Schwab [6] and T. N. Silukova [7]. They showed that the luminescence of the gold monochloride has a narrow band and a broad band situated respectively at 472,2 nm (2,62 eV) and 632 nm (1,96 eV). But their crystallographic properties were studied by E. M. W. Janssen. He found that the AuCl has a body-centered tetragonal structure with a space group $I4_1/amd$ [8].

The aim of this work is to elaborate and study the structural and the optical properties of AuCl nanocrystals embedded in a KCl crystalline lattice; which is a dielectric material and transparent in the visible range. It is the range of optical response of AuCl nanocrystals. The characterization of AuCl nanocrystals in KCl has been studied by using the X-ray diffraction and the photoluminescence (PL).

II. EXPERIMENTAL

The samples of KCl single crystals doped AuCl nanocrystals are elaborated using the Czochralski method, which consists of melting the gold thin films deposited on pure KCl pastilles. The growth process is performed by using a seed oriented [100]. The obtained single crystals have cylindrical shape and transparent colour. The single crystals are cleaved perpendicularly to the crystallographic direction [100]. The cleavage permits to obtain samples with 1 mm thickness. The thermal treatment of samples is performed at 650°C during 3 hours. After the annealing, the samples are cooled slowly at room temperature.
The crystalline structure was analysed with X-ray diffraction (XRD) by a Bruker D8 Advanced diffractometer system with Cu irradiation ($\lambda_{k\alpha} = 1{,}54056\,\overset{o}{A}$) at 40 kV and 40 mA in the 2θ range (10-80°). The photoluminescence (PL) spectra were measured with a Jobin-Yvon spectrofluorometer Fluorolog-3 using a Xenon lamp (450 W).

III. RESULTS AND DISCUSSION

A. X-ray diffraction

Figure 1 exhibits the X-ray diffraction of pure KCl samples. We observe two very intense peaks situated at $2\theta = 28{,}37°$ and $2\theta = 58{,}68°$, corresponding to (200) plane and its harmonic (400) of KCl single crystals, as identified by using JCPDS file 41-1476.
X-ray diffraction of KCl doped AuCl nanocrystals after annealing at 650°C for 3 h, is showed in Fig. 2. The spectrum shows the intense peaks of KCl single crystals and two diffraction peaks with a weak intensity, situated at $2\theta = 31{,}74°$ and $2\theta = 65{,}83°$. These peaks are attributed respectively to (211) and (422) planes of

AuCl tetragonal structure with a space group $I4_1/amd$, comparing with the literature data of JCPDS file 30-0603. We note that the AuCl presents a preferential orientation along (211) and (422) planes, because of the oriented growth of KCl single crystals obtained by the Czochralski method. We observe that the (400) peak of KCl is very intense that (200) comparing with those of spectrum of pure KCl. This change may be due to doping of the KCl matrix by the AuCl.

A slight shift of the AuCl peak angular positions towards higher angles can be noticed in comparison to the standard position indicated in the JCPDS file 30-0603. This shift may be attributed to the contraction of the AuCl nanocrystals cells in KCl lattice [9].

Therefore, X-ray diffraction results confirm the formation and the embedding of AuCl nanocrystals in KCl matrix.

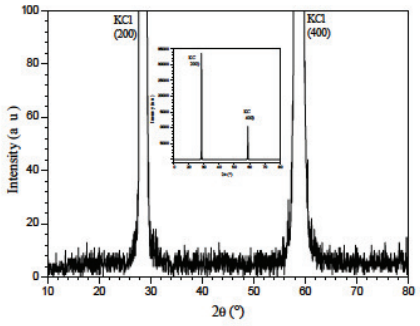

Figure 1. X-ray spectrum of pure KCl single crystals.

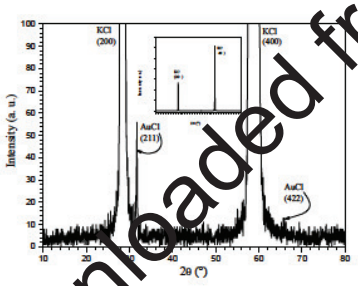

Figure 2. X-ray spectrum of KCl single crystals doped AuCl after annealing at 650 C for 3 h.

We assume that the shape of AuCl nanocrystal embedded in KCl was spherical. The average radiuses (R) of AuCl were estimated using Scherer's formula [10]:

$$D = 2R = \frac{0.9\,\lambda}{\Delta(rad)\cos\theta} \qquad (1)$$

Where:

D is the average diameter of the nanocrystals,

λ is the wavelength of the X-ray radiation,

θ is the Bragg angle diffraction,

Δ is the full-width at half-maximum (FWHM) of the peak.

The average radius of AuCl nanocrystals in KCl corresponding to each diffracting plan is reported in Table I. We note a large dispersion of AuCl nanocrystals size in KCl. It is varied between 3,4 and 18,7 nm.

Table I. Nanocrystal sizes of AuCl calculated from XRD.

2θ(°)	(hkl)	Δ (°)	R (nm)
31,74	(211)	0,22	18,7
65,83	(422)	1,36	3,4

B. Photoluminescence

PL spectra of pure KCl and KCl doped AuCl nanocrystals after annealing at 650°C for 3 h and excited with $\lambda_{ex} = 360\,nm$ at room temperature, are reported in Fig. 3. Indeed, for the spectrum of pure KCl single crystals (Fig. 3◆(a)), no emission band could be detected. However, the spectrum of KCl doped AuCl (Fig. 3 (b)) shows a emission band centered at 580 nm (2,14 eV). We assign this band to AuCl nanocrystals with a shift from the bulk equal 52 nm (0,18 eV) [6]. The enlargement of this band can be explained by the presence of size dispersion of AuCl nanocrystals inside KCl (Table I).

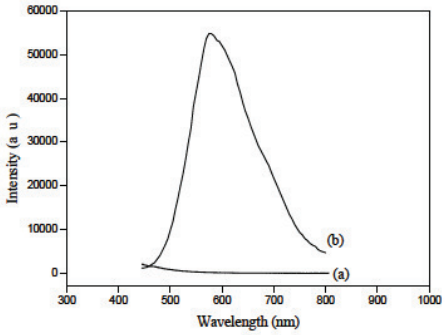

Figure 3. PL spectra ($\lambda_{ex} = 360\,nm$) of: (a): pure KCl and (b): KCl doped AuCl nanocrystals.

IV. CONCLUSION

KCl single crystals doped AuCl nanocrystals were prepared by the Czochralski method. Structural characterization by XRD shows the formation of AuCl nanocrystals in KCl with a tetragonal structure. However, the PL measurements exhibit the characteristic emission band of AuCl nanocrystals situated at 2,14 eV (0,18 eV shift from bulk of AuCl).

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