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X-ray Diffraction of AuCl Semiconductor Nanocrystals Embedded in NaCl Single Crystals Grown by Czochralski Method

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The AuCl nanocrystals embedded in NaCl single crystals are elaborated using the Czochralski method. The X-ray diffraction has confirmed the formation of the AuCl nanocrystals with a tetragonal structure inside the NaCl matrix. The average radius of the AuCl nanocrystals is estimated using the Scherrer formula.

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1. Introduction

The synthesis and characterization of small particles of materials is currently an area of intense theoretical and experimental research. The revelation is that physical properties of such systems are bound to be appreciably different from those of the bulk crystal. In general, the physical properties of crystals become very different when their size becomes very small.

Semiconductor nanocrystals embedded in wide gap matrices, such as alkali halides, have drawn considerable interest in recent years because of their special electronic and optical properties as compared to those of the bulk materials [1]. It was found that semiconductor nanocrystals dispersed in transparent matrices represented three-dimensionally confined quantum wells of electronic excitations.

During the past decade, a considerable effort has been spent in the preparation and investigation of the I–VII family of semiconductor nanocrystals. Various methods of the production of I–VII nanocrystals embedded in wide gap matrices have been reported [2–4]. Among all the I–VII compounds, gold monochloride or AuCl is one of the interesting materials because it is characterized by the interesting optical absorption and emission in the visible region [5, 6].

In the present study, we report the growth of AuCl nanocrystals dispersed in NaCl matrix and study their structural characterisation using X-ray diffraction.

2. Experimental

The NaCl single crystals doped AuCl nanocrystals are elaborated by the Czochralski method, from the fusion of the gold thin films deposited on pure NaCl pastilles. The growth is carried out by using a seed oriented following the crystallographic axis [100]. The obtained single crystals are cleaved parallel to the plane (100) in order to prepare samples with 1 mm thickness. Some pastilles have been annealed at 650 °C and 300 °C, then cooled slowly at room temperature.

The X-ray diffraction (XRD) of AuCl embedded in NaCl matrix is performed by using the K_α line of copper of a D 8 advanced diffractometer at 40 kV and 40 mA.

3. Results and discussion

We report in Fig. 1 the XRD diffractogram of the NaCl single crystals doped AuCl nanocrystals, before and after annealing. We observe that all the spectra included two intense peaks located at $2\theta = 31.79°$ and $2\theta = 66.33°$. These peaks correspond respectively to the (200) reflection of NaCl single crystal and its harmonic (400), which were consistent with the literature data of JCPDS file 40-0628. Before annealing (Fig. 1a), we note the presence of another peak with a weak intensity, situated at $2\theta = 28.38°$. This peak is attributed to the (112) plane of the AuCl tetragonal structure with a space group

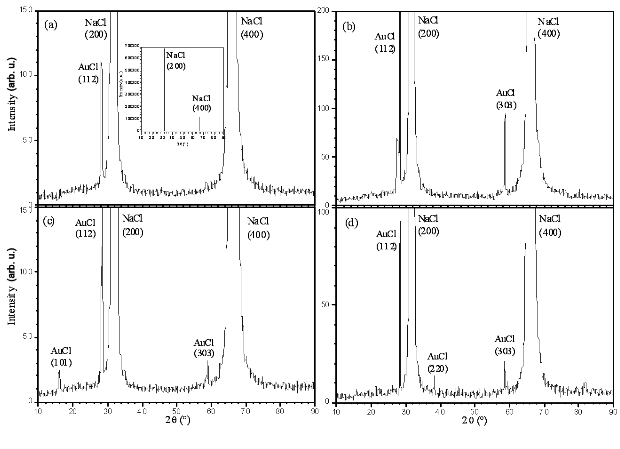

Fig. 1. XRD of AuCl nanocrystals in NaCl single crystal before and after annealing: (a) before annealing, (b) annealing at 650 °C for 3 h, (c) annealing at 650 °C for 6 h, and (d) annealing at 300 °C for 24 h.

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$I4_1/amd$, as identified by using JCPDS file 30-0603. We note that the AuCl nanocrystals in NaCl before annealing presents a preferential orientation along (112) plane.

The XRD spectra of AuCl in NaCl samples annealed at 650 °C during 3 h and 6 h are represented respectively in Fig. 1b and c. Moreover, among the intense peaks of NaCl we observe two peaks with a weak intensity situated at $2\theta = 28.39°$ and $2\theta = 58.77°$, which were assigned to (112) and (323) planes of AuCl tetragonal structure. However, for the annealing 650 °C for 6 h, we observe a third peak located at $2\theta = 15.97°$, that corresponds to (101) plane of AuCl tetragonal structure.

The spectrum of AuCl in NaCl annealing at 300 °C for 24 h is illustrated in Fig. 1d. This spectrum shows three peaks at $2\theta = 28.38°$, $2\theta = 38.28°$ and $2\theta = 58.61°$, which are attributed respectively to the (112), (220) and (323) planes of AuCl tetragonal structure.

The X-ray diffraction results confirm the formation and the incorporation of AuCl nanocrystals in NaCl matrix and it shows also that the NaCl single crystal has not been deformed after the formation of AuCl nanocrystals. A slight shift of the AuCl peak angular positions can be noticed comparing to the standard positions indicated in the file for AuCl (JCPDS file 30-0603). This shift may be attributed to the contraction of the AuCl nanocrystal cells in the NaCl matrix [4].

Based on the Scherrer formula applied to X-ray diffraction patterns, we assume that the shape of the nanocrystals embedded in NaCl matrix is spherical. In order to determine the average radius (R) of the AuCl nanocrystals, we calculated the full-width at half maximum (FWHM) at different peaks [7]:

$$D = 2R = \frac{0.9\lambda}{\Delta[\mathrm{rad}]\cos\theta},$$

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.

We note that the average radii of AuCl nanocrystal in NaCl are:

Before annealing:

2θ [°]	(hkl)	Δ [°]	R [nm]
28.38	(112)	0.12	34.1

After annealing at 650 °C for 3 h:

2θ [°]	(hkl)	Δ [°]	R [nm]
28.39	(112)	0.10	40.9
58.77	(323)	0.21	21.7

After annealing at 650 °C for 6 h:

2θ [°]	(hkl)	Δ [°]	R [nm]
15.97	(101)	0.46	8.7
28.38	(112)	0.12	34.1
58.77	(323)	0.13	35

After annealing at 300 °C for 24 h:

2θ [°]	(hkl)	Δ [°]	R [nm]
28.38	(112)	0.12	34.1
38.28	(220)	0.21	21
58.61	(323)	0.16	28.4

4. Conclusion

In conclusion, we investigated AuCl nanocrystals embedded in NaCl single crystals elaborated by the Czochralski method. The X-ray diffraction has confirmed the formation of the AuCl nanocrystals inside the NaCl matrix with a tetragonal structure.

This work indicated that the Czochralski method allows the fabrication of semiconductor nanocrystals embedded in alkali halide matrices with a high crystalline quality.

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