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Short Communication

Effect of Indium Doping on the Structural Properties of Calcium Fluoride Powders

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Abstract

In doped calcium fluoride transparent conducting powder were prepared by solid state reaction method. Structural properties of the samples were investigated as a function of various In-doping levels (x=0.00-0.04-0.05-0.06). The results of x-ray diffraction have shown that the samples are polycrystalline structure in cubic phase, with preferential orientations along the (112) for In for all samples, and show presence (111), (220), (311), (400) planes in pure CaF_2 sample and The preferred orientation is (220) for pure CaF_2, and we have peaks correspond to (101), (002), (110), (112), (200), (202) for In for all samples and The preferred orientation is (112) for In for all samples. The average of crystallite size is within the range [5.148-1.041 nm] for all samples. The relative intensities, distance between crystalline planes (d), crystallite size (D) and lattice parameters (a) were determined.

INTRODUCTION

Calcium fluoride (CaF_2) density is 3.18 (g/cm^3) melting at 1633 (K) and crystalize in cubic structure with lattice constants a = 5.432 Å.

CaF_2 is presently the fastest known scintillator. It has an emission component with subnanosecond decay time [1,2].

CaF_2 has several scintillation emission bands. The fast scintillation light is emitted in the UV bands centered at 220 and 200 nm.

The decay time of the fast component varies between 600 and 800 ps [3].

CaF_2 has attracted much attention because of its wide range of potential applications in optoelectronic and microelectronic devices [4-6,8].

CaF_2 compounds doped with rare-earth ions have been reported to display unique luminescence properties and can thus be used as scintillators [7,9-11].

EXPERIMENTAL METHOD

CaF_2: In powders (x = 0.00, 0.04, 0.05, 0.06) (Tables 1-4) were prepared by a solid state reaction method, were accurately weighed in required proportions and were mixed and ground thoroughly using an Agate mortar and pestle to convert to very fine powders.

The grinding of the mixtures was carried out for 3 hours for all the powder samples. The ground powder samples were firing at 700°C for 3 hours.

RESULTS AND DISCUSSIONS

Structural properties

The X-ray diffraction (device type XRD-PW 1840 PHILIPS production is connected to a computer with software for diffraction spectrum processing) patterns of undoped and In doped CaF_2 powders prepared with various In concentration 0 wt%, 4 wt%, 5 wt% and 6 wt% are shown in Figure 1.

The XRD reveals that all samples are having polycrystalline nature with cubic structure.

The relative intensities of undoped and in doped CaF_2 powders are calculated. The distance between crystalline planes values (d) are calculated by using following relation:

$$2d.\sin\theta = n\lambda \quad (1)$$

Where d is distance between crystalline planes (A°), θ is the Bragg angle, λ is the wavelength of X-rays (λ=1.78897 A°).

The crystallite size is calculated from Scherrer's equation [12]:

$$D = \frac{0.94\lambda}{\beta\cos\theta} \quad (2)$$

where, D is the crystallite size, λ is the wavelength of X-ray, ß is full width at half maximum (FWHM) intensity in radians and θ is Braggs's angle.

The dislocation density is defined as the length of dislocation lines per unit volume and calculated by following equation [13]:

$$\delta = \frac{1}{D^2} \quad (3)$$

The lattice constants a for cubic phase structure is determined by the relation [14]:

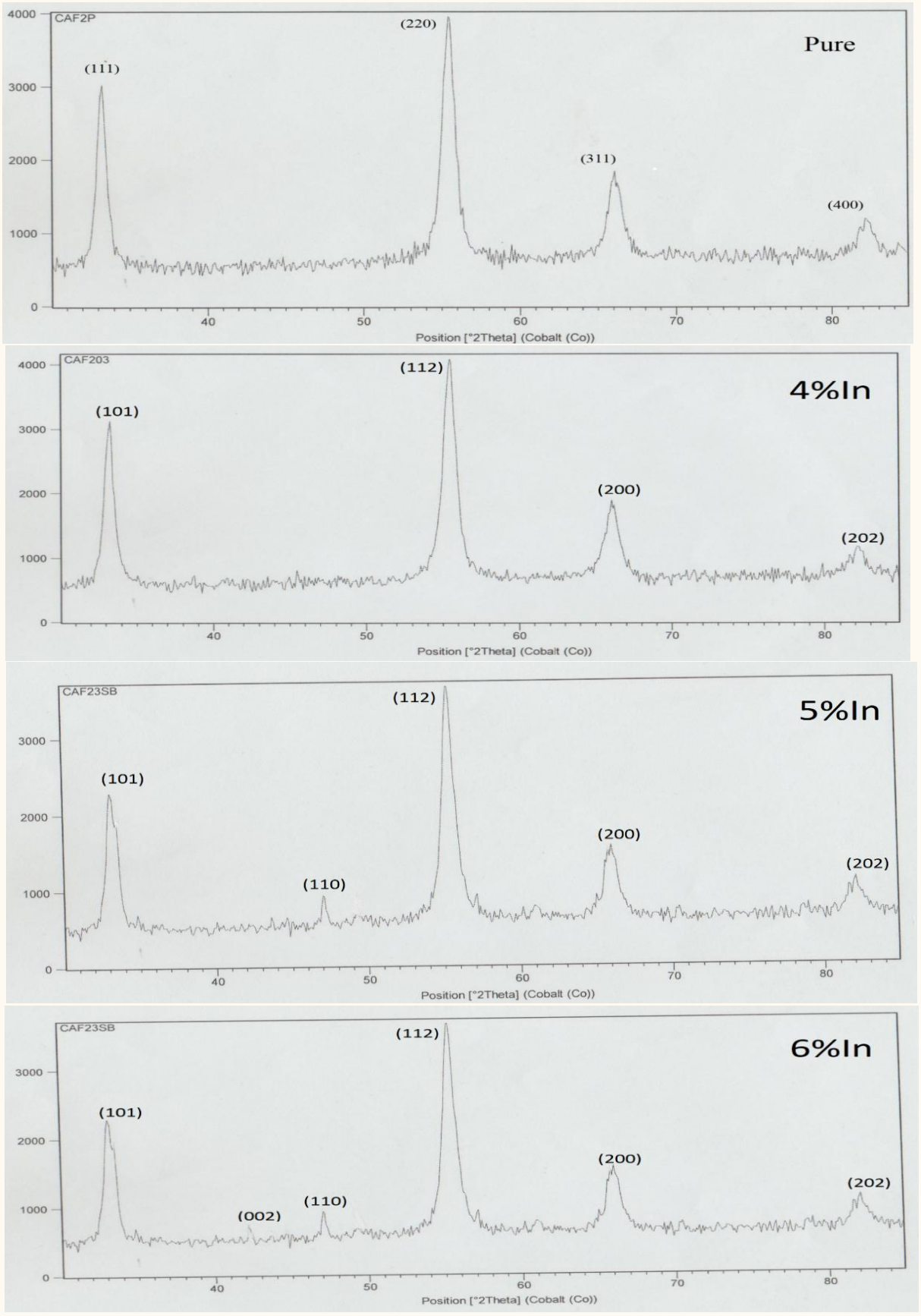

Figure 1 XRD results of pure CaF_2, 4 wt% in doped CaF_2, 5 wt% in doped CaF_2, 6 wt% in doped CaF_2.

Table 1: shows results of structural values of undoped CaF_2 sample.

Samples S	2θ (deg)	(hkl)	d (A°)	Rel. int. [%]	β (deg)	D (nm)	Average D(nm)	Δ 10^{15}line/m^2	Lattice const. a(Å)
CaF_2	33.12	(111)	3.138	80	1.250	1.403	1.504	508.024	5.456
	55.23	(220)	1.929	100	1.720	1.103		821.956	
Pure	65.78	(311)	1.647	48	1.350	1.483		454.692	
	82.23	(400)	1.360	33	1.100	2.029		242.904	

Table 2: shows results of structural values of In doped CaF_2 samples (x=0.04).

Samples	2θ (deg)	(hkl)	d (A°)	Rel. int. [%]	β (deg)	D (nm)	Average D(nm)	Δ 10^{15}line/m^2	Lattice const. a(Å)
CaF_2:In	33.06	(101)	3.144	82	1.335	1.294	1.520	597.216	4.759
	54.82	(112)	1.943	100	1.650	1.148		758.780	
(4 wt%)	65.72	(200)	1.648	46	1.550	1.291		416.233	
	82.14	(202)	1.361	28	0.950	2.347		181.540	

Table 3: shows results of structural values of In doped CaF2 samples (x=0.05).

Samples	2θ (deg)	(hkla)	d (A°)	Rel. int. [%]	β (deg)	D (nm)	Average D(nm)	Δ 10^{15}line/m^2	Lattice const. a(Å)
CaF_2: In	32.83	(101)	3.166	63	1.320	1.328	2.091	567.702	4.754
	47.01	(110)	2.242	25	0.420	4.366		52.460	
(5 wt%)	54.88	(112)	1.941	100	1.820	1.041		922.780	
	65.92	(200)	1.644	46	1.260	1.599		391.113	
	82.08	(202)	1.362	31	1.050	2.123		221.870	

Table 4: shows results of structural values of In doped CaF_2 samples (x=0.06).

Samples	2θ (deg)	(hkl)	d (A°)	Rel. int. [%]	β (deg)	D (nm)	Average D(nm)	Δ 10^{15}line/m^2	Lattice const. a(Å)
CaF_2:In	32.91	(101)	3.158	65	1.450	1.209	2.561	684.143	4.747
	42.12	(002)	2.489	22	0.350	5.148		37.733	
(6 wt%)	46.96	(110)	2.245	27	0.450	4.075		60.220	
	54.98	(112)	1.938	100	1.750	1.152		753.520	
	66.96	(200)	1.621	38	1.230	1.639		372.256	
	82.06	(202)	1.362	29	1.040	2.143		217.748	

$$a = d\sqrt{h^2 + k^2 + l^2} \quad (4)$$

where d and (hkl) are distance between crystalline planes and Miller indices, respectively.

CONCLUSION

This paper presents a study of structural properties of, in doped CaF_2 powders prepared by solid state reaction method. X-ray diffraction patterns confirm that the samples have polycrystalline nature with cubic structure and show presence (111), (220), (311), (400) planes in pure CaF_2 sample. The preferred orientation is (220) for pure CaF_2.

For 4% in we have peaks correspond to (101), (112), (200), (202) .The preferred orientation is (112).

For 5% In We noticed appearance of this orientation (110).

For 6% In We noticed appearance of these orientations (002), (110).

The average of crystallite size is within the range [5.148-1.041 nm] for all samples. It was defined that the lattice constants a for all the samples, were almost identical with JCPDS values.

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