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Physical Science & Biophysics Journal
ISSN: 2641-9165

Studying the Structural Properties of Compounds Fluoride that Blotched by Sb

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Research Article
Volume 6 Issue 2
Received Date: November 09, 2022
Published Date: November 25, 2022
DOI: 10.23880/psbj-16000224

Abstract

Sb 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 Sb-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 and show presence (111) ،(220) ،(311) ،(400) planes in pure CaF2 sample and The preferred orientation is (220) for pure CaF2 and we have peaks correspond to (012), (015), (024), (122) for Sb for all samples and the preferred orientation is (015) for Sb for all samples. The average of crystallite size is within the range [4.063-0.915 nm] for all samples. The relative intensities, distance between crystalline planes (d), crystallite size (D) and lattice parameters (a) were determined.

Keywords: Powder; Calcium fluoride; Solid state reaction; Structural properties; Rare-earth ions

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 sub nanosecond 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 [4,5,6]. CaF_2 compounds doped with rare-earth ions have been reported to display unique luminescence properties and can thus be used as scintillators [7-11].

Experimental

CaF_2: Sb powders (x = 0.00,0.04,0.05, 0.06) 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.

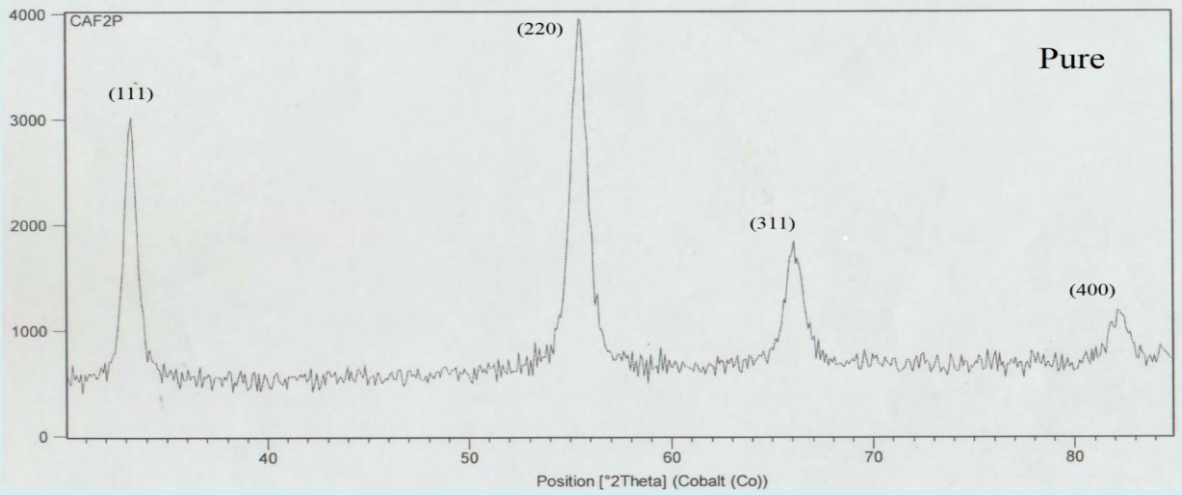
Results and Discussions

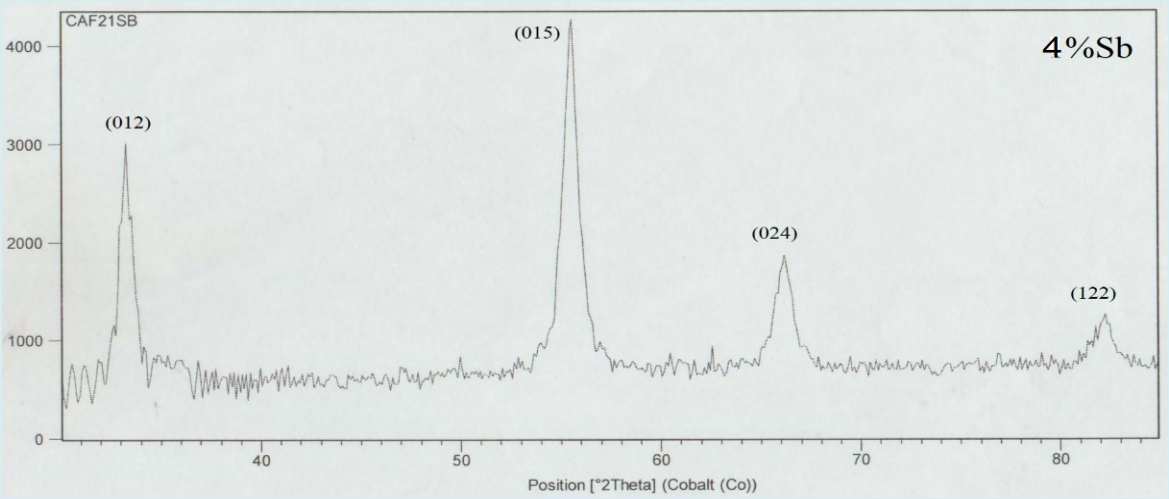
Structural properties

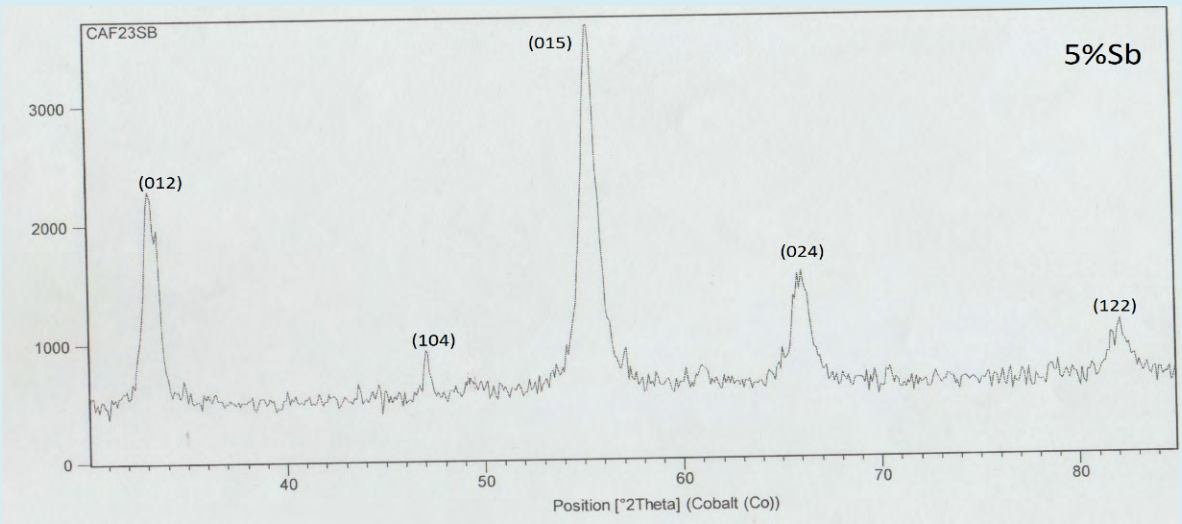
The X-ray diffraction patterns of undoped and Sb doped CaF_2 powders prepared with various Sb concentration 0

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.







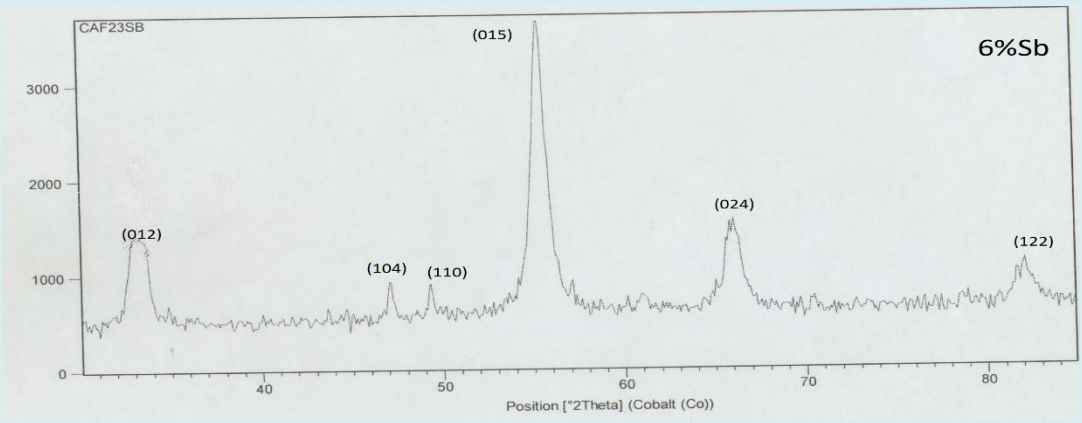


Figure 1: XRD results of pure CaF_2, 4 wt% Sb doped CaF_2, 5 wt% Sb doped CaF_2, 6 wt% Sb doped CaF_2.

Samples S	2θ (deg)	hkl	d (A°)	Rel. int. [%]	β (deg)	D (nm)	Average D(nm)	Δ 10^{15}line/m²	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 1: The results of structural values of undoped CaF_2 sample.

Samples	2θ (deg)	hkl	d (A°)	Rel. int. [%]	β (deg)	D (nm)	Average D(nm)	Δ 10^{15}line/m²	Lattice const. a(Å)
CaF_2:Sb	32.94	(012)	3.155	76	1.160	1.511	1.517	437.996	9.881
	54.96	(015)	1.938	100	1.755	1.080		857.338	
(4 wt%)	66.12	(024)	1.639	44	1.525	1.315		578.293	
	82.12	(122)	1.347	33	1.040	2.162		223.938	

Table 2: The results of structural values of Sb 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/m²	Lattice const. a(Å)
CaF_2:Sb	32.33	(012)	3.212	68	1.325	1.321	1.829	573.052	9.734
	47.12	(104)	2.237	26	0.630	3.010		110.374	
(5 wt%)	55.92	(015)	1.909	100	2.130	0.915		1194.422	
	65.96	(024)	1.643	44	1.565	1.280		610.351	
	81.98	(122)	1.363	32	1.040	1.620		381.039	

Table 3: The results of structural values of Sb doped CaF_2 samples (x=0.05).

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:Sb	33.10	(012)	3.144	39	1.370	1.280	2.104	610.351	9.846
	47.14	(104)	2.238	23	0.625	2.935		116.087	
(6 wt%)	49.12	(110)	2.152	22	0.455	4.063		60.057	
	55.22	(015)	1.931	100	1.710	1.109		813.086	
	65.98	(024)	1.642	43	1.505	1.332		563.626	
	82.08	(122)	1.362	30	1.170	1.905		275.556	

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

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

$$2d\sin\theta \quad (1)$$

Where d is distance between crystalline planes (A°), è is the Bragg angle, ë is the wavelength of X-rays (ë = 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, ë is the wavelength of X-ray, ß is full width at half maximum (FWHM) intensity in radians and è 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]:

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

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

Conclusion

This paper presents a study of structural properties of Sb 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%Sb we have peaks correspond to (012), (015), (024), (122). The preferred orientation is (015).

For 5%Sb We noticed appearance of this orientation (104).

For 6%Sb We noticed appearance of these orientations (104), (110).

The average of crystallite size is within the range [4.063-0.915 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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