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Effect of Chromium Doping on the Structural Properties of Strontium Fluoride Compound

Ahmad Khoudro[1] Mufid diab[2] Omar al-aboush[3]
1. Professor, Department of Physics, Faculty of science, Tishreen University, Syria
2. Professor, Department of Physics, Faculty of science, AL-Baath University, Syria
3. Phd Student, Department of Physics, Faculty of science, AL-Baath University, Syria

Abstract
SrF_2: Cr (x = 0.00-0.1-0.15-0.2-0.25-0.3-0.35 wt%) powder has been successfully prepared using the solid-state reaction method. The phosphors were characterized by differential thermal analysis (DTA), X-ray diffraction (XRD). The samples were annealed at $750℃/6h$. The structural properties of strontium fluoride samples doped with different Cr ratios were investigated. The results of the X-ray diffraction patterns showed that the samples are polycrystalline structure in the cubic phase and show the presence of (111), (020), (022), (131), (222), (040) levels in the pure SrF_2 sample and the preferred orientation is (111) for pure SrF_2. The distance between the crystal planes (d), the crystal size (D), and the lattice constant (a) were determined.
Keywords: powder, SrF_2, solid state reaction, Structural properties, DTA, XRD
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INTRODUCTION

Alkaline earth fluorides are among the important materials that are an important basis in the applications of condensed matter physics and materials science [1,2]. Alkaline earth fluorides have attracted great attention of researchers due to their distinctive properties such as high ions, low energy photons, high resistivity, anionic conductivity as well as electron acceptor behavior [3,4]. Strontium fluorine (SrF_2) crystallizes in a cubic fluorite structure with a closely spaced cubic Fm3m space group of cations with anions occupying tetrahedral sites [5]. SrF_2 has a wide band gap (11ev), it is insulating and optically transparent, energy Low photon, low index of refraction, high radiation resistance and good mechanical strength. It has a face-centered cubic structure (Fcc), its density is 4.277g/cm^3, its molecular weight 152.62 g/mol, its melting point 1477 ℃, and the crystal lattice constant 5.798 A [6].SrF_2 is considered the fastest flashes known today and has a rate of radiation emission less than a fraction of a nanosecond and emits several light beams and the fastest in the field of ultraviolet radiation within the range (200-220 nm) and has a decomposition time for the fastest components of 600-800 ps. Modifying the fluorescence characteristics of crystals doped with doping elements plays an important role in the development of photodetectors based on fluorides. For this reason, research has been directed for years on fluorescent compounds of fluorides, especially those that have phosphorescence and give a flux photon emission [7,8]. Milad Al-Hassan et al. studied the effect of indium doping as well as Antimony on the structural properties of calcium fluoride powder with different concentrations of impurities [9,10].

EXPERIMENTAL

The SrF_2:Cr (0.0,0.1,0.15,0.2,0.25,0.3,0.35wt%) powders were synthesized by using Solid State Reaction Method [11], Accurately weighed in the required proportions and thoroughly mixed and ground using an agate slurry and pestle to convert into very fine powders. Acetone was used to help the solid compounds mix during the sample preparation process in relatively small quantities. The previous materials were ground and mixed with an agate mortar to ensure obtaining a homogeneous mixture after adding an amount of acetone in order to improve the homogeneous mixing process for it for about 15 minutes until the acetone dried. This process was repeated three consecutive times for each of the samples. After that, the resulting mixture was dried by heating it to a temperature of 100°C for a period of time sufficient to ensure the removal of moisture. The samples were annealed at $750℃$ a temperature for 6 hours, after which the samples were gradually cooled in the heating oven to room temperature at a rate of 1°C/min.

RESULTS AND DISCUSSIONS

Structural properties

A significant thermal change that spreads heat was observed at the temperature $741.3℃$ shown in the fig (1), which is due to the entry of chromium into the crystalline structure of SrF_2, and this was confirmed by charts XRD of the annealed samples at this temperature. As for the annealed samples at lower temperatures, they showed two separate crystalline phases for each of chromium and strontium fluoride, and thus we conclude that chromium does

not enter the crystalline structure.

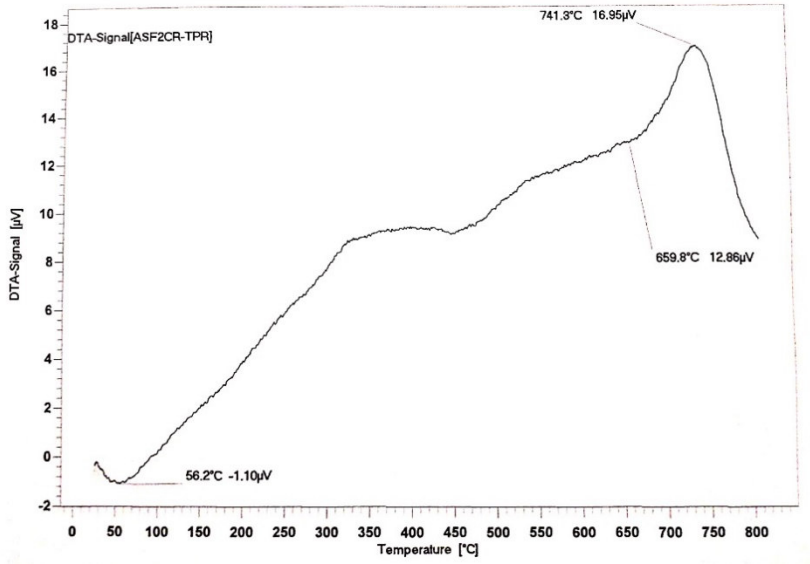

Fig (1): Differential thermal analysis spectrum of a compound SrF_2:Cr

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 Cr doped SrF_2 powders prepared with various Cr concentration (x = 0.00-0.1-0.15-0.2-0.25-0.3-0.35%) are shown in Fig (2).

XRD analysis shows that all samples are polycrystalline in nature with cubic structure.

The relative intensities of undoped and Cr doped SrF2 powders was calculated. The distance values between crystal planes (d) were calculated using the following Bragg's law [12]:

$$2dsin\theta = n\lambda \qquad (1)$$

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 [13]:

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

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 Bragg's angle.

The dislocation density is defined as the length of dislocation lines per unit volume and calculated by following equation [14]:

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

The lattice constants a for cubic phase structure is determined by the relation [15]:

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

Where (hkl) Miller indices.

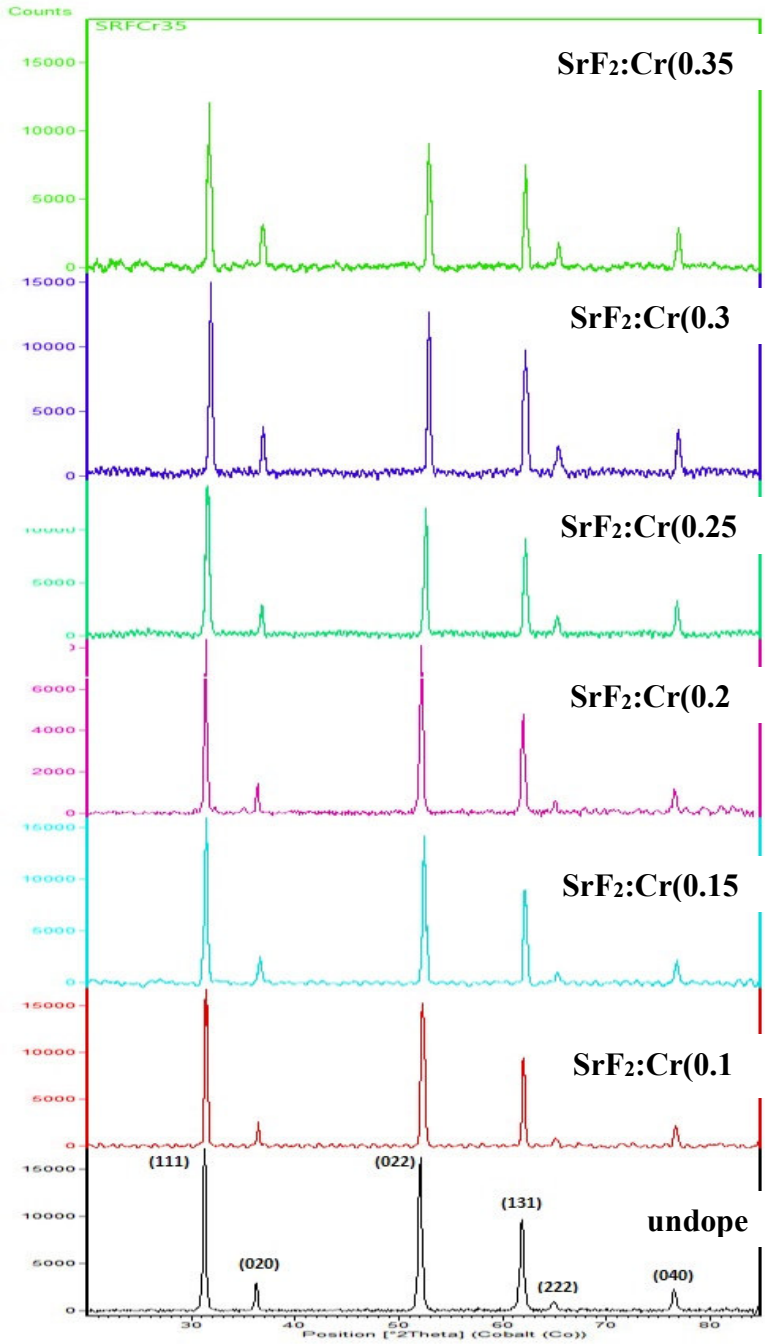

Fig (2): XRD patterns of pure and doped SrF_2

Table 1: *shows results of structural values of undoped SrF_2 sample*

$2\theta°$	$\theta°$	(hkl)	$d_{exp}(A°)$	$\beta\ (deg)$	$D\ (nm)$	$\Delta\ 10^{15} line/m^2$	*Lattice const.* a (Å)	V (Å^3)
31.2477	15.62385	(111)	3.321337	0.3936	4.4364	50.8074	50.8074	190.3798
36.2069	18.10345	(020)	2.878687	0.2952	5.9934	27.8389	27.8389	190.8417
52.02	26.01	(022)	2.03979	0.2952	6.3387	24.8884	24.8884	192.0398
61.83017	30.915085	(131)	1.741071	0.3936	4.9800	40.3210	40.3210	192.5477
64.89764	32.44882	(222)	1.667154	0.492	4.0504	60.9538	60.9538	192.6191
76.50739	38.253695	(040)	1.444743	0.3936	5.4407	33.7811	33.7811	192.9977
Average					5.2066	39.7651	5.768023	191.9043

Table 2: shows results of structural values of Cr doped SrF_2 samples (x=0.1%)

$2\theta°$	$\theta°$	(hkl)	$d_{exp}(A°)$	$\beta\ (deg)$	$D\ (nm)$	$\Delta\ 10^{15} line/m^2$	*Lattice const.* a (Å)	V (Å^3)
31.3097	15.65485	(111)	3.314924	0.2952	5.916174	28.5705	5.7416	189.2792
36.2689	18.13445	(020)	2.873931	0.2422	7.306218	18.7333	5.7478	189.8974
52.082	26.041	(022)	2.037531	0.2422	7.727838	16.7449	5.7630	191.4025
61.89217	30.946085	(131)	1.739499	0.3936	4.981666	40.2949	5.7692	192.0268
64.95964	32.47982	(222)	1.665737	0.3938	5.062188	39.0232	5.7702	192.1282
76.56939	38.284695	(040)	1.443753	0.2952	7.257495	18.9856	5.7750	192.601
Average					6.3752	27.0587	5.7611	191.222

Table 3: shows results of structural values of Cr doped SrF_2 samples (x=0.15%)

$2\theta°$	$\theta°$	(hkl)	$d_{exp}(A°)$	$\beta\ (deg)$	$D\ (nm)$	$\Delta\ 10^{15} line/m^2$	*Lattice const.* a (Å)	V (Å^3)
31.3317	15.66585	(111)	3.312655	0.2924	5.9731	28.0280	5.737687	188.8907
36.2909	18.14545	(020)	2.872248	0.2212	8.0003	15.6236	5.744495	189.5639
52.104	26.052	(022)	2.036731	0.2212	8.4622	13.9644	5.760744	191.1771
61.91417	30.957085	(131)	1.738943	0.2924	6.7065	22.23285	5.76742	191.8425
64.98164	32.49082	(222)	1.665235	0.3632	5.4893	33.1861	5.768543	191.9545
76.59139	38.295695	(040)	1.443402	0.2924	7.3281	18.6215	5.773607	192.4605
Average					6.9933	21.9428	5.7587	190.981

Table 4: shows results of structural values of Cr doped SrF_2 samples (x=0.2%)

$2\theta°$	$\theta°$	(hkl)	$d_{exp}(A°)$	$\beta\ (deg)$	$D\ (nm)$	$\Delta\ 10^{15} line/m^2$	*Lattice const.* a (Å)	V (Å^3)
31.36511	15.682555	(111)	3.309215	0.2624	6.6565	22.5681	5.731728	188.3028
36.33682	18.16841	(020)	2.86874	0.2018	8.7706	12.9999	5.73748	188.8703
52.13336	26.06668	(022)	2.035664	0.2018	9.2769	11.6195	5.757727	190.8768
61.94462	30.97231	(131)	1.738173	0.2624	7.4745	17.8990	5.764867	191.5878
65.0221	32.51105	(222)	1.664312	0.3234	6.1663	26.2996	5.765347	191.6356
76.57834	38.28917	(040)	1.44361	0.2624	8.1651	14.9991	5.77444	192.5438
Average					7.7517	17.7309	5.7552	190.636

Table 5: shows results of structural values of Cr doped SrF_2 samples (x=0.25%)

$2\theta°$	$\theta°$	(hkl)	$d_{exp}(A°)$	$\beta\ (deg)$	$D\ (nm)$	$\Delta\ 10^{15} line/m^2$	*Lattice const.* a (Å)	V (Å^3)
31.38711	15.693555	(111)	3.306954	0.2624	6.6569	22.5656	5.727812	187.917
36.35882	18.17941	(020)	2.867063	0.2018	8.7711	12.9982	5.734126	188.5392
52.15536	26.07768	(022)	2.034865	0.2018	9.2778	11.6173	5.755468	190.6523
61.96662	30.98331	(131)	1.737617	0.2624	7.4754	17.8949	5.763024	191.4041
65.0441	32.52205	(222)	1.663811	0.3234	6.1670	26.2932	5.763611	191.4626
76.60034	38.30017	(040)	1.443259	0.2624	8.1664	14.9946	5.773036	192.4034
Average					7.7524	17.7273	5.7528	190.396

Table 6: shows results of structural values of Cr doped SrF_2 samples (x=0.3%)

$2\theta°$	$\theta°$	(hkl)	$d_{exp}(A°)$	$\beta\ (deg)$	$D\ (nm)$	$\Delta\ 10^{15} line/m^2$	*Lattice const.* a (Å)	V (Å^3)
31.40611	15.703055	(111)	3.305003	0.2416	7.2304	19.1281	5.724434	187.5848
36.37782	18.18891	(020)	2.865616	0.1886	9.3855	11.3521	5.731232	188.2539
52.17436	26.08718	(022)	2.034176	0.1886	9.9279	10.1455	5.753519	190.4586
61.98562	30.99281	(131)	1.737137	0.2416	8.1198	15.1673	5.761433	191.2456
65.0631	32.53155	(222)	1.663379	0.3028	6.5873	23.0453	5.762112	191.3133
76.61934	38.30967	(040)	1.442956	0.2428	8.8268	12.8348	5.771824	192.2823
Average					8.3463	15.2789	5.7507	190.189

Table 7: shows results of structural values of Cr doped SrF_2 samples (x=0.35%)

$2\theta°$	$\theta°$	(hkl)	$d_{exp}(A°)$	$\beta\ (deg)$	$D\ (nm)$	$\Delta\ 10^{15} line/m^2$	*Lattice const.* a (Å)	V (Å^3)
31.41701	15.708505	(111)	3.303885	0.2284	7.6484	17.0942	5.722497	187.3945
36.38872	18.19436	(020)	2.864787	0.1866	9.4864	11.1119	5.729573	188.0905
52.18526	26.09263	(022)	2.033781	0.1866	10.0348	9.9306	5.752401	190.3477
61.99652	30.99826	(131)	1.736862	0.2412	8.1337	15.1154	5.760521	191.1548
65.074	32.537	(222)	1.663131	0.2886	6.9118	20.9320	5.761253	191.2277
76.63024	38.31512	(040)	1.442782	0.2284	9.3840	11.3559	5.771129	192.2128
Average					8.5999	14.2567	5.7495	190.071

The fig (3) shows a clear increase in the crystalline size with an increase in the concentration of chromium impurity.

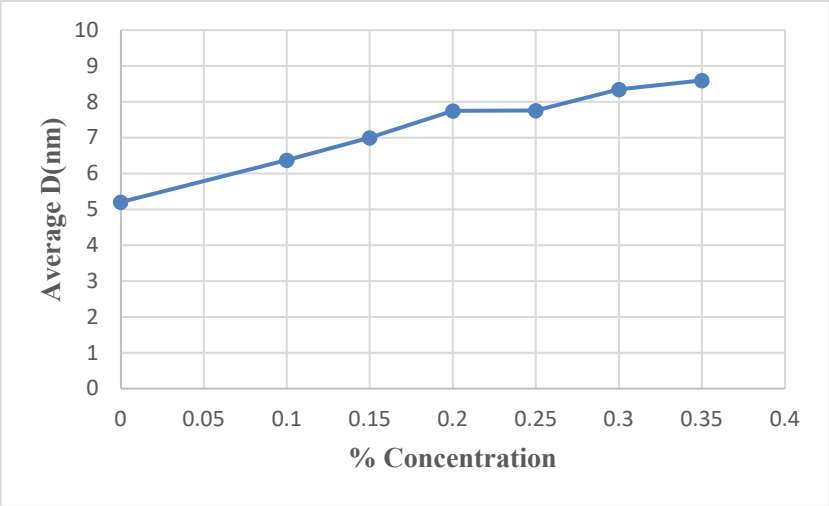

Fig (3): variation of the average grain size with concentrations (0,0.1,0.15,0.2,0.25,0.3,0.35 wt%) of Cr doped SrF_2 powders.

CONCLUSION

This article presents a structural study of pure SrF_2 powder doped with different low concentrations of chromium and prepared by solid reaction method. The X-ray diffraction patterns confirmed that the samples had a polycrystalline nature with a cubic structure where peaks appeared for the pure SrF_2 sample (111), (020), (022), (131), (222), (040). The preferred orientation of the pure sample is (111). No new peaks appeared when strontium fluoride was doped with low chromium concentrations with a slight shift of the peaks SrF_2: Cr (0.1,0.15,0.2,0.25,0.3,0.35). Crystalline size increased with increasing doping of SrF_2 by Cr. It was found that the crystal lattice constant for all samples was almost identical to the values of JCPDS.

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