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Photoluminescence and Band gap energy of Ca-Sr Tartrate

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ABSTRACT

Mixed Crystals of Calcium-strontium tartrate were grown by a gel technique using single diffusion method. The effect of various parameters like pH of gel, gel density, gel aging, and concentrations of reactants etc. on the growth of these crystals was studied. Faint yellowish, semi-transparent, whitish, rhombohedra shaped maximum size 3 mm × 5 mm, thickness 2mm crystals were obtained. The crystals grown were characterized by SEM, UV, and PL. The results of these observations are described and discussed.

Keywords: Gel technique, Calcium strontium tartrate, PL, UV, and SEM.

INTRODUCTION

A series of pure and mixed crystals have been grown by several researchers with the aim of identifying new materials for practical and industrial purposes [1-5]. Single crystals are the backbone of the modern technological revolution. Compounds of tartaric acid find several practical applications in science and technology because of their interesting physical properties such as dielectric, ferroelectric, piezoelectric and non-linear optical properties [6-10]. The art of growing crystals in gel is not new for researchers because of its simplicity, inexpensiveness and crystals can be grown at ambient temperature. But the challenges and opportunities in understanding the growth features and morphology of grown crystal remain there. Crystals of great interest from both solid state sciences as well as technological point of view has been reported by many investigators using gel method. Tartrate crystals are of considerable interest, particularly for basic studies of some of their interesting physical properties. Some crystals of this family are ferroelectric [11-13], some others are piezoelectric [14] and quite a few of them have been used for controlling laser emission [15].

In the literature survey, to the best of our knowledge, there is no report on the systematic growth of Ca-Sr tartrate crystals. The purpose of the present paper is to report for the first time the growth of mixed single crystals of Calcium Strontium tartrate in silica gel at ambient temperature. These crystals have identified and characterized by SEM, UV, and PL. The results of these observations are described and discussed.

MATERIALS AND METHODS

The single diffusion method was employed in the present work for the growth of Calcium Strontium tartrate crystals. The growth process involves the diffusion of mixed Calcium chloride-Strontium chloride solution in to a gel in which tartaric acid is impregnated beforehand. The silica gel was used as a growth media. The chemicals used for growth mixed tartrate were $C_4H_6O_6$, $CaCl_2$, $SrCl_2$ and Na_2SiO_3 all chemicals were of AR grade. The crystallization apparatus consist of borosilicate glass test tubes of length 20 cm and diameter 2.5 cm placed vertically on wooden stands. Tartartic acid, Calcium chloride and Strontium chloride solution were prepared by dissolving these compounds in an appropriate amount of distilled water to give the required molarities. Gels of required specific gravity were prepared by adding to the solution of sodium metasilicate, a calculated amount of redistilled water and a stock solution was kept ready for doing further experiments. Tartaric acid solution of particular strength was taken in a 100ml beaker and sodium metasilicate solution of a suitable gravity was added drop wise using a tephlon cock burette, constantly stirring the solution in a beaker by magnetic stirrer. Stirring is done to avoid the excessive local ion concentration which may otherwise cause premature local gelling and make the final medium inhomogeneous and turbid. Here tartaric acid acted as a lower reactant. The systronic digital pH meter model number 335 was used to measure the pH. The solution after noting pH values, being allowed to fall along the side of a test tube without giving chance for the formation of the bubbles. Test tubes were then closed with rubber corks or cotton to prevent evaporation and contamination of the exposed surface of the gel by dust particles of the atmosphere. The solution was found to be strongly depends on pH. High pH value gel takes lower time to set than low pH value, depending on the environmental temperature. After ensuring firm gel setting, the saturated mixed solution of Calcium chloride and Strontium chloride (supernatant) of particular strength was poured over the set gel with the help of a pipette. The solution being allowed to fall along the wall of the test tube to prevents the gel surface from cracking. The supernatant ions (Ca^{++} and Sr^{++}) slowly diffused in to the gel medium where it reacts with inner reactant.

The following reaction is expected to take place in the formation of Calcium Strontium tartrate crystals.

$$2C_4H_6O_6 + x\ Cacl_2 + (1-x)Srcl_2 \rightarrow Ca_xSr_{(1-x)}\ (C_4H_4O_6)_2.xH_2O + 4Hcl.$$

RESULTS AND DISCUSSION

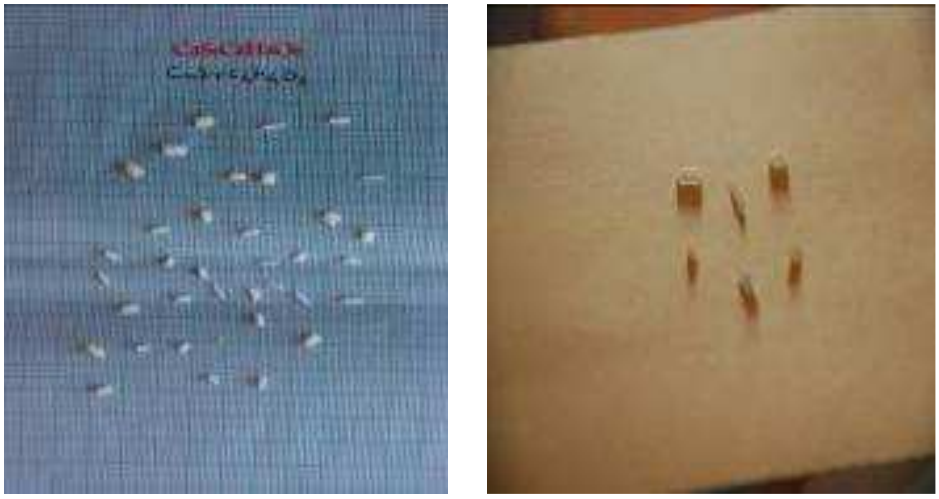
The systematic growth experiments were performed by adding $CaCl_2$, $SrCl_2$ as feed solution of strength varying from 0.2 M to 1.2M over the set gel of pH range 4 to 4.5 and gel density range 1.02 gm/cm^3 to 1.05 gm/cm^3. mixed crystals of Ca-sr tartrate are pale yellowish, semi transparent, some are whitish, rhombohedra shaped, maximum size of the grown crystals are

3mm×5mm and thickness 2mm are obtained. The optimum growth conditions for various parameters were found and are reported in table1

Table 1. Optimum conditions for growth of Calcium strontium tartrate

Calcium Strontium tartrate	Conditions
Density of sodium metasilicate solution	1.04gm/cm^3
Concentration of tartaric acid	1.25M
Volume of tartaric acid	7ml
Volume of sodium metasilicate solution	19
pH of the gel	4.2
Concentration of $CaCl_2$	1M
Concentration of $SrCl_2$	1M
Temperature	Room temperature
Gel setting time	96 hours
Gel aging time	72hours
Period of growth	4weeks

Different parameters such as concentration of reactants, pH of gel, impurities in the solvent, gel setting time, gel aging time, etc have considerable effect on growth rate. Figure 1(a), (b), illustrates different morphologies of pure Calcium Strontium tartrate crystals grown under different conditions of growth.



(a) **(b)**

Figure 1. Optical photograph illustrating varied morphology of Calcium strontium tartrate crystals under different growth conditions (a) Whitish, some are needle shaped.(b) Semitransparent crystals of Calcium strontium tartrate

4. Characterization:

Calcium Strontium tartrate crystals were characterized by UV, PL, SEM.

4.1 UV Absorption spectroscopy:

Absorption spectra of Calcium Strontium tartrate crystals were recorded using a SHIMADZU UV-2450 UV-Vis spectrophotometer over the wavelength range 200 – 700 nm at Nano Research Laboratory, Department of Physics; Pratap College Amalner. Figure 2 shows UV absorption spectra of Calcium Strontium tartrate crystals. From the spectrum, it has been inferred that

Calcium strontium tartrate crystals have sufficient transmission in the entire visible and IR region. The absorption coefficient is high at lower wavelength and the wide transparency from 340 nm suggesting their suitability for second and third harmonic generations of the 1064 nm radiation [16-17].

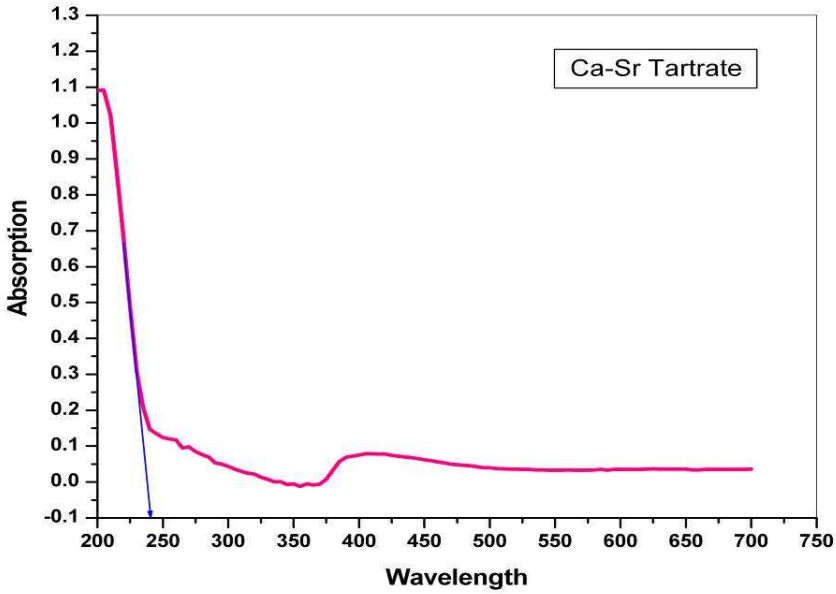


Figure 2: Optical absorption spectra of Calcium Strontium tartrate

The band gap energy of the Calcium strontium tartrate crystals with the obtained wavelength are calculated using the following simple conversion equation; Band gap energy (eV) = 1240/wavelength (nm).Band gap Energy is presented in the table2

Table 2: Band gap energy of Calcium Strontium tartrate crystals

Crystal	λ (nm)	Band gap Energy (eV)
Calcium Strontium tartrate	241.29	5.13

Wide band gap energy is obtained in gel grown mixed Calcium Strontium tartrate crystals.

4.2 Photoluminescence (PL) characteristics:

A photo luminance spectrum was performed using Perkin Elmer LS55 florescent spectrophotometer at Nano Material Research Laboratory, Department of Physics Pratap College Amalner.

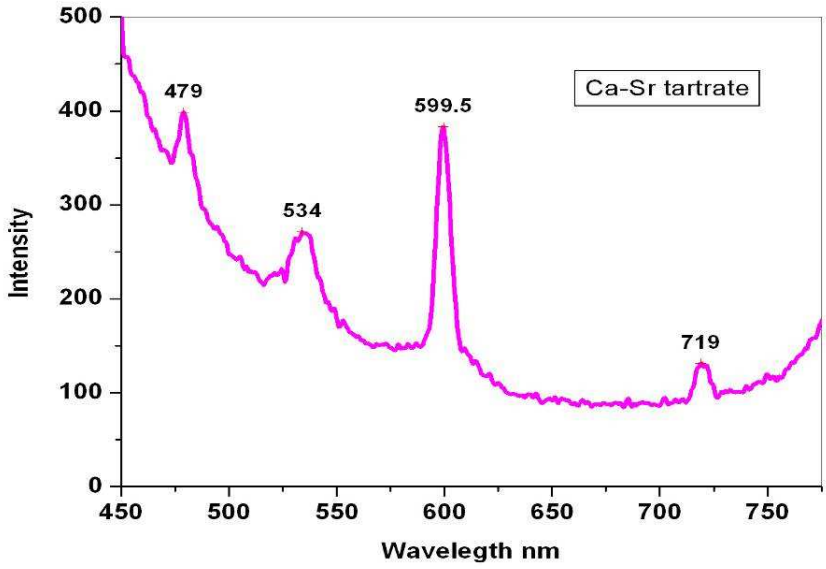


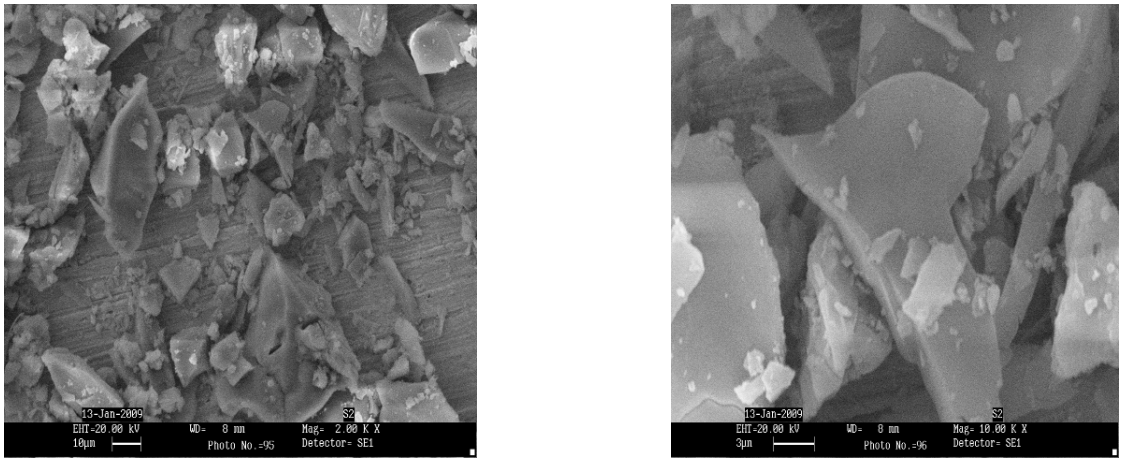
Figure 3: Emission spectrum of Calcium strontium tartrate

Figure 3 shows the emission spectrum of Calcium strontium tartrate crystal was recorded at room temperature. The emission spectrum shows the peaks mainly at 479nm, 534nm, 599.5 nm, and 719 nm when excited with 400 nm. Of these, the cyan emission at 479nm is the most intense of all emission, green emission at 534nm. The peak of orange emission at 599 nm is sharp and the peak of red emission at 719nm.

4.3 Scanning Electron Microscopy (SEM):

This technique combines of the resolution and analytical power with much ease of operation. Images can be formed from a very wide range of materials. From metals to ceramics, semiconductors to polymers. These materials can be examined with low energy secondary electrons, with high energy back scattered electrons or with other emission such as light, heat and sound. The high depth of field of the SEM images makes it especially suitable for the study of the fracture surfaces and complex microstructures such as those found in composite materials.

In the present work powdered sample of Calcium Strontium tartrate crystals was examined by using SEM technique at the National Chemical Laboratory, Pune. The study of the surface of the crystal gives valuable information about its internal structure. Figure 4 (a) illustrates SEM photographs of single crystals of Calcium Strontium tartrate crystal. An enlarged SEM image is shown in Figure 4 (b). It shows plate like crystal morphology. These crystals are grown by layer deposition. Thick and thin layers are seen in figure. The individual plates of samples are flat and the plates with the sharp edges were observed. On some plates further plate like growth was observed.



(a) **(b)**

Figure 4 (a): SEM image of Calcium Strontium tartrate crystal. (b) Magnified SEM image.

CONCLUSION

Gel growth technique is suitable for growing crystals of Calcium Strontium tartrate. Different habits of Calcium Strontium tartrate crystals can be obtained by changing parameters like gel density, gel aging, pH of gel, concentration of reactants, etc. Calcium Strontium tartrate crystals show the Cyan, green, orange and red emission when excited with 400 nm. SEM photographs shows plate like crystal morphology of the Calcium Strontium tartrate. Wide band gap energy is obtained.

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