

STRUCTURAL PROPERTIES OF $\text{Sr}_2\text{Al}_2\text{SiO}_7$ PHOSPHORS USING SOLID STATE REACTION METHOD

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ABSTRACT

The crystal and electronic structures, as well as the luminescence properties of $\text{Sr}_2\text{Al}_2\text{SiO}_7$ are reported. The crystal structure of $\text{Sr}_2\text{Al}_2\text{SiO}_7$ (Sr-gehlenite) is tetragonal with space group $-4 21 m$, Space group number:113, a (Å) = 7.8200, b (Å) = 7.8200 c (Å) = 5.2640, $Z = 2$ and Calculated density (g/cm^3) = $3.81 \text{ g} \cdot \text{cm}^{-3}$. First-principles calculations confirm that the Al and Si atoms are in partial ordering in the 2a and 4e sites in $\text{Sr}_2\text{Al}_2\text{SiO}_7$. In addition, the band structure calculation shows that $\text{Sr}_2\text{Al}_2\text{SiO}_7$ has an indirect band gap with an energy gap of about 4.01 eV, which is in good agreement with the data (5.3 eV) available in literature.

KEYWORDS: Crystal structure; Luminescence; Phosphor; Sr-gehlenite; $\text{Sr}_2\text{Al}_2\text{SiO}_7$

INTRODUCTION

Luminescent materials with long afterglow are kinds of energy storage materials that can absorb both the UV and the visible lights from the sunlight and gradually release the energy in the darkness at a certain wavelength. These kinds of long persistent phosphors have been widely studied by many researchers (Kimura et al. 2000, Takasaki, *et al.*, 1996, Yamamoto *et al.*, 1997, Holsa *et al.*, 2001, Kimata, M *et al.*, 1984). A wide variety of host materials are used as luminescent compounds, but when it comes to persistent luminescence, the number of known hosts is relatively low. For instance, the materials which absorb the moisture from the surrounding environment to form sulphate and that destroy the sulphide structure, these materials no longer show long afterglow. Thus the majority of research is concentrated around the aluminates, such as (Sr-Al-Si-O): RE system (P. Yang, et al. 2002, T.L. Barry, 1968). These new types of materials have overcome the shortcoming of the above- mentioned sulphides and therefore are widely used as the phosphorous pigment for various applications (Y. Lin, et al. 2001, Yuelei Ding *et al.*, 2009). In this paper, long-lasting silicate phosphors, $\text{Sr}_2\text{Al}_2\text{SiO}_7$ were synthesized by solid-state reaction around 1450°C in a reducing atmosphere. The phase composition, crystal structure, and afterglow properties were investigated. A detailed investigation why the phosphor shows such a difference in afterglow behaviour was also discussed.

EXPERIMENTAL METHODS

Synthesis of $\text{Sr}_2\text{Al}_2\text{SiO}_7$

Un-doped $\text{Sr}_2\text{Al}_2\text{SiO}_7$ were prepared by a solid-state reaction method. Appropriate amount of the starting materials of SrCO_3 (99.90 %), Al_2O_3 , SiO_2 (99.99 %), were weighed and mixed using mortar and pestle. The grinded sample was placed in an alumina crucible and subsequently fired at 1450°C for 3 h in a weak reducing atmosphere. The weak reducing atmosphere was generated with the help of activated charcoal.

Characterization

The structural data were collected using an X-ray powder diffractometer (NIT Raipur) with a Graphite monochromator using Cu-K α radiation ($1 \frac{1}{4} 1.54056 \text{ \AA}$ or 0.15 nm), The synthesized sample was observed by moving radiation detector with scan speed of $2^\circ/\text{min}$ at the range of 10° - 80°C . The XRD patterns show very broad peaks. The broadening of the diffraction peaks of the sample indicates that the particle size is in the order of nano-scale.

First-principles calculation method

The calculations of the total energy and electronic structure of $\text{Sr}_2\text{Al}_2\text{SiO}_7$ were carried out on the basis of density

functional theory. The exchange-correlation functional generalized gradient and the structural data of $\text{Sr}_2\text{Al}_2\text{SiO}_7$ obtained from the present study by the Rietveld refinement of the X-ray powder diffraction data were used in the calculations. [8,9]

RESULTS AND DISCUSSION

Crystal and electronic structures of $\text{Sr}_2\text{Al}_2\text{SiO}_7$

As discussed above, the distribution of Al/Si in $\text{Sr}_2\text{Al}_2\text{SiO}_7$ is partial ordering. When Si–N is introduced to partially replace Al–O, the distributions of Al/Si and O/N are also problematic issues (i.e., the ordering of Al/Si and O/N), not only for X-ray diffraction analysis but also for first-principles calculations. By X-ray powder diffraction analysis, all the possible structural models were considered in the course of the refinement, producing very for the accurate determination of the distributions of Al/Si and N/O in $\text{Sr}_2\text{Al}_2\text{SiO}_7$, further study by neutron diffraction is needed.

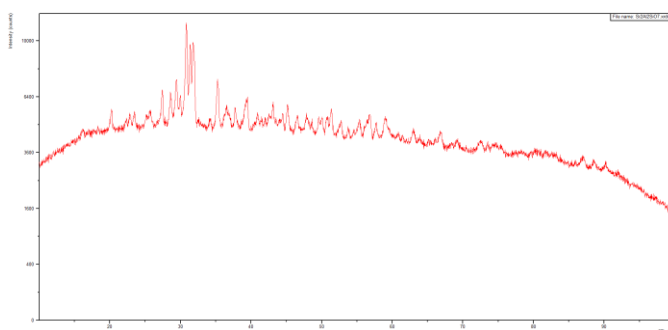


Fig-1: XRD pattern of $\text{Sr}_2\text{Al}_2\text{SiO}_7$

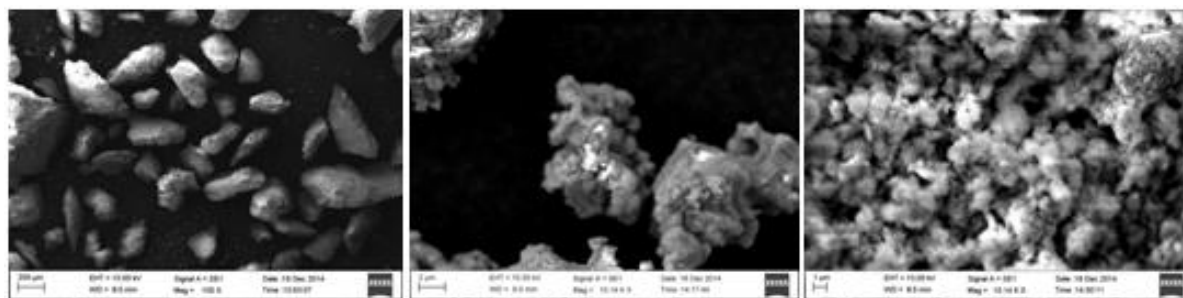


Fig-2: EXD pattern of $\text{Sr}_2\text{Al}_2\text{SiO}_7$

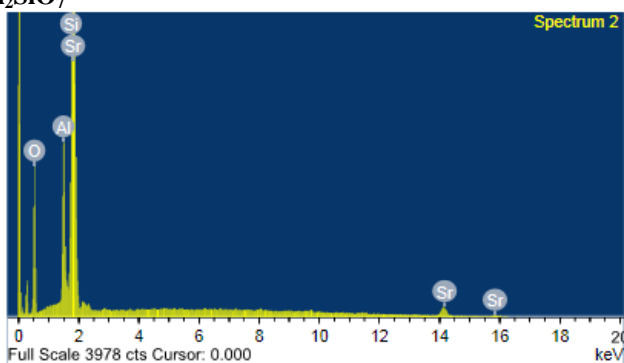


Fig3

CONCLUSIONS

We concluded that the partial ordering of Al and Si in $\text{Sr}_2\text{Al}_2\text{SiO}_7$ has been confirmed by first-principles calculations based on density functional theory. The electronic structure shows that $\text{Sr}_2\text{Al}_2\text{SiO}_7$ has an indirect band gap of about 4.07 eV, in good agreement with the optical band gap (5.3 eV)

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