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Crystal Structure Analysis of $Sr_2MgSi_2O_7$ Doped with Eu^{2+} and Dy^{3+} using Rietveld Refinement

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Abstract: ***This study examines the crystal structure of Sr2MgSi2O7 doped with Eu2+ and Dy3+ using the Rietveld refinement method. The phosphor was synthesized via solid-state reaction and characterized using X-ray diffraction XRD. The observed XRD patterns matched the crystallographic database, confirming the structure. Rietveld refinement revealed the impact of doping on lattice parameters, with a slight increase in cell volume. The refinement showed good convergence, highlighting the methods effectiveness in studying luminescent materials.***

Keywords: XRD, Phosphor, Rietveld refinement, $Sr_2MgSi_2O_7$.

1. Introduction

Materials of different kinds are to be studied for different technological development. Various materials, Semiconductors in the electronic industry, zeolites as catalysts in the petrochemical industry, ceramics in medicine and engineering are few of the examples of extensively investigating materials. In the near future, it may be necessary to study high temperature superconductors in applied science and engineering. In order to understand the properties of these materials and to improve them, the atomic structure has to be known. An effective way to do this is by means of diffraction techniques using neutrons from nuclear reactors and particle accelerators or X-rays from X-ray tubes and synchrotrons. The single crystal diffraction technique, using relatively large crystals of the material, gives a set of separate data from which the structure can be obtained. However, most materials of technical interest cannot grow large crystals, so one has to resort to the powder diffraction technique using material in the form of very small crystallites **[1-2]**. The drawback of this conventional powder method is that the diffraction peaks grossly overlap, thereby preventing proper determination of the structure. The "Rietveld Method" creates a virtual separation of these overlapping peaks, thereby allowing an accurate determination of the structure. Most of the silicate and oxide-based hosts exhibits white light emission when doped with Dysprosium (III) but in many host materials such as $Ba_5CaAl_4O_{12}$, BaY_2ZnO_5, $Sr_3Y(PO_4)_3$, $Ba_3Y(PO_4)_3$, Li_2SrSiO_4, $NaSrB_5O_9$, $Ca_3Si_2O_7$ and $YAlO_3$ only blue and yellow emission peaks could be observed **[3]**

2. Materials and Methods

The $Sr_2MgSi_2O_7$: Eu^{3+}, Dy^{3+} phosphor powder, with varying concentrations of Dysprosium, was prepared using the solid state reaction technique. The starting materials SiO_2, $SrCO_3$, MgO, Dy_2O_3 and Eu_2O_3 were thoroughly ground for approximately 1 h in a mortar, pre-sintered at 900 ^oC, then fired at 1300 ^oC for approximately 2 h in reducing atmosphere, with H_3BO_3 (1.6 mol%) used as flux **[4-5]**. For taking XRD measurements, Panalytical Xpert PRO MPD with copper k alpha anode of wavelength 1.5405 Angstrom has been used.

3. Results and Discussion

An X-ray diffraction pattern of one of the sample was recorded. The sample which expressed the optimum photoluminescence emission (0.5 mol% concentration of Europium (III) co-doped with 1.5 mol% of Dysprosium (III)) was chosen for X-ray diffraction (XRD) pattern study. Observed XRD was matched well with the standard XRD pattern of $Sr_2MgSi_2O_7$ (crystallographic open database card No. 96-431-7124) with a figure of merit (FoM) of 0.91. The FoM supports the existence of the expected phases in $Sr_2MgSi_2O_7$. The structure refinement of the Di Strontium Magnesium Silicate considered was performed using the Fullprof 2021 suit and the initial parameters of refinement for the said sample were referred from the single crystal data of $Sr_2MgSi_2O_7$ (crystallographic open database card No. 96-431-7124). All atomic positions, fraction factors and temperature factors were refined convergence and well satisfied the refection condition. The final refinement patterns are illustrated in **Fig. 1**.

Table 1: Lattice Parameter of observed and refined parameter

Lattice Parameters	a	b	c	α	β	γ	Vol. (Å)
COD (96-431-7124)	7.9869	7.9869	5.152	90	90	90	328.648
Fullprof	8.0161	8.0161	5.169	90	90	90	332.1486

It can be observed that incorporating Eu^{2+} affects the unit cell parameters. Cell volumes were slightly increased with introducing Eu^{2+} ions. This lattice distortion occurred because of the differences in ionic radius of Sr^{2+} (132 pm) and Eu^{3+} (131 pm). Conventional Rietveld R-factors R_p, R_{wp} and R_{exp} for Pattern were observed to be 36.4, 48.1, and 18.36 whereas Chi^2 was 6.86. Comparison between observed and refined lattice parameters is provided in **Table 1**. **A** 3 – dimensional view of the crystal structure of $Sr_2MgSi_2O_7$ created using Vesta Ver. 3 software is shown in **Fig. 2**.

Element	Atomic No.	Ion	Wyckoff	x	y	z	SOF	B (temp)
Strontium	38	Sr^{2+}	4e	0.3341	0.1659	0.5074	0.03107	0.78
Magnesium	12	Mg^{2+}	2a	0	0	0	0.00834	0.5
Silicon	14	Si^{4+}	4e	0.1353	0.3647	0.9458	0.003191	0.54
Oxygen	8	O^{2-}	2c	0.5	0	0.158	0.01073	1
Oxygen	8	O^{2-}	4e	0.1384	0.3616	0.2506	0.03455	1
Oxygen	8	O^{2-}	8f	0.08681	0.1888	0.8055	0.12772	1

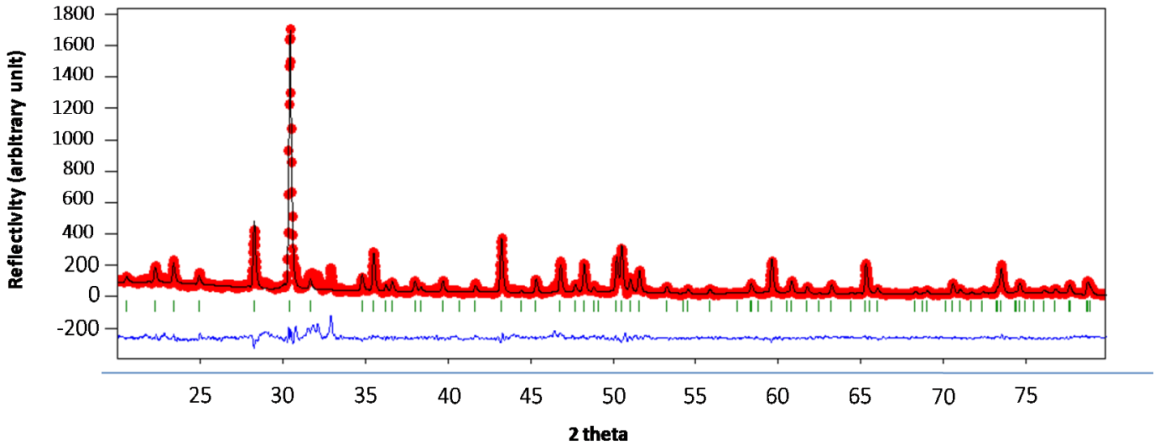

Figure 1: Rietveld Refinement Pattern

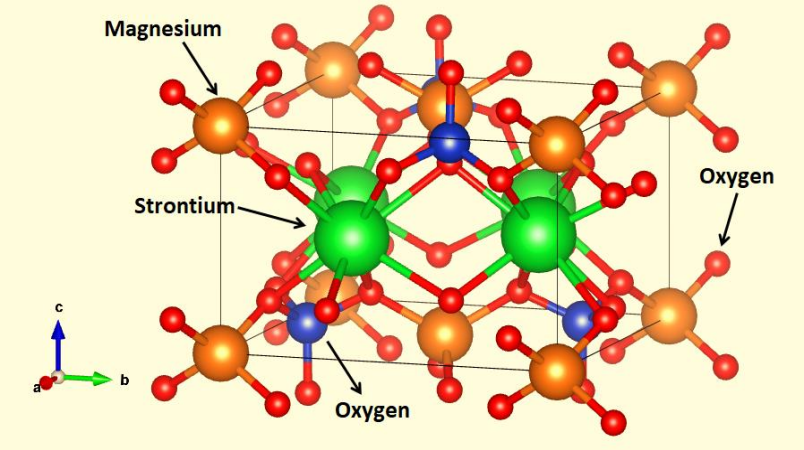

Figure 2: Crystal Structure of $Sr_2MgSi_2O_7$

The crystal structure in **Fig. 02** is created using VESTA (Visualization for Electronic and Structural Analysis) Ver. 3.5.7. Various Bonds expected to be in the crystal structure of $Sr_2MgSi_2O_7$ along with its number and length is provided in **Table 04**

Table 4: Bond length and Bond angles

$Sr_2MgSi_2O_7$			
Atom1	Atom2	Bond Length	No. of Bonds
Strontium	Magnesium	3.9775	8
Strontium	Silicon	3.196	4
Strontium	Oxygen	2.6075	4
Strontium	Oxygen	2.5853	4
Strontium	Oxygen	2.5174	8
Strontium	Strontium	4.2294	4
Strontium	Silicon	3.373	4
Strontium	Oxygen	2.7502	4
Strontium	Oxygen	2.8419	4
Strontium	Magnesium	3.9274	8
Silicon	Oxygen	1.6326	8
Silicon	Oxygen	1.625	4
Silicon	Magnesium	3.1307	8
Oxygen	Magnesium	1.9456	8

4. Conclusion

Structural analysis of Di-Strontium Magnesium Silicate using Rietveld refinement of observed XRD was done using software Fullprof suit 2021. The $Sr_2MgSi_2O_7$ was doped with 1.5 mol% of Eu2+ and Dy3+ for this structural analysis. The observed XRD exhibited great resemblance with the results obtained expressed that there are 05 various lengths bonds between Strontium and Oxygen, 2 various bonds between Strontium and Magnesium, 2 bonds between Strontium and Silicon etc. Total number of Bonds created was 80 out of which many bonds are of same bond lengths as summarized in Table 04.

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