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PHOTOCHROMISM TESTING of BaMgSiO4:Fe WITH DIFFERENT REACTION CONDITIONS

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ARTICLE INFO	ABSTRACT
Article history: *Received: 2025-12-05* *Received in revised form :2025-12-16* *Accepted :2026-01-26* *Available online: 2026-06-26*	*In recent years, there has been an increased focus on the study of tunable inorganic photochromic(color-changing) materials. Most of the silicates have poor photochromic properties. However, by doping these particles with specific dopants, these properties can be enhanced. $BaMgSiO_4$ (BMS) is a member of the silicate salts that are suitable for enhancing photochromism using various dopants. Fe as a dopant was tested under two different reaction conditions (air and N_2/H_2) with photochromic BMS samples. The results revealed that the N_2/H_2 atmosphere is the most effective reaction condition for synthesis.*
Keywords: *Photochromism,* *Color centers, Silicate.*	

1. INTRODUCTION

Photochromism is a reversible color change by exposure to light on the materials. A large number of photochromic materials have extensive uses globally, based on different areas such as light-responsive technologies, ranging from adaptive optical elements to biomedical applications, X-ray intensification, scintillation, dosimetry, etc. [1-3] Some research in this area focuses on the development of novel photochromic materials and the precise control of their photochromic properties to satisfy the requirements of various optoelectronic applications. For example, materials that respond to red or near-infrared light within the biological optical window (700–900 nm) have been widely used in biological applications.[4] Photochromic materials that respond rapidly to light stimuli are desirable for applications such as smart lenses. In contrast, reduced sensitivity to photoirradiation is advantageous in the field of data security, as it helps preserve stored information. Furthermore, the ability to tune the coloration rate on demand can greatly enhance the security of recorded texts, since different information may appear at different irradiation times.[5]

2. EXPERIMENTAL

Fe-ion-doped BMS powders were synthesized using a solid-state reaction approach. High-purity $BaCO_3$ (99.9%), $MgCO_3$ (99.9%), SiO_2 (99.9%), and 0.1 mol% Fe_2O_3 (99%) were used as starting materials. Additionally, 10 mol% H_3BO_3 (99.99%) was added as a flux to facilitate the reaction. [6]

The raw materials were weighed according to the stoichiometric composition of $BaMgSiO_4$ and thoroughly mixed in a mortar with ethanol to ensure a uniform mixture. After drying, the powder blend was transferred into an alumina reaction vessel.

Then the mixtures of these materials were transferred to an aluminum oxide reaction vessel and put into a Lenton LTF 14/25/450 oven at 1170°C for 4 hours with the heating and cooling rate of 20°C/min, under air and reducing atmosphere (12% H_2 and 88% N_2) conditions. After sintering, the reacted material was scraped and collected directly from the alumina vessel for further processing and characterization. $BaMgSiO_4$:X (X= First row transition metals, Eu and Dy) samples were synthesized (reaction 1) following the protocol reported by Akiyama et al. [6]

$$2BaCO_3(s) + 2MgCO_3(s) + 2SiO_2(s) \xrightarrow{1170^{o}} 2BaMgSiO_4(s) + 4CO_2\,(g) \qquad (1)$$

The synthesized materials were then compared using a UVP UVLS-24 EL Series (254/365 nm) and an Analytik Jena UVM-57 (302nm).

3. RESULTS AND DISCUSSION

To ensure uniformity, XRD analyses were conducted. XRD patterns were obtained using a PANalytical Aeris powder X-ray diffractometer operating at 40.0 kV and 7.5 mA, equipped with a PIXcel1D-Medipix3 detector and Cu-Kα_1,α_2 radiation (λ = 1.5406 Å and 1.5444 Å). The optical configuration and data acquisition conditions included a nickel β-filter, 0.04 rad Soller slits, a 1/4° divergence slit, a 13 mm fixed mask, a high beam knife, and a 9 mm anti-scatter slit. During measurements, the sample spinner operated at 1 rps, with a scan rate of 0.201 °/s and a step size of 0.0217°.

The collected XRD data were processed using HighScore together with the ICDD PDF-4+. Background correction was performed with a bending factor of 2 and a granularity value of 20 using smoothed input data. Peak detection parameters included a minimum significance of 3.00, a minimum tip width of 0.01, a maximum tip width of 1.00, and a peak base width of 2.00. Peaks were identified using the minimum second-derivative method and matched against reference patterns from the ICDD PDF-4+ database. For the synthesized materials, the most prominent phase (04-011-361) was identified using the HighScore PANalytical software **(Figure 1)**. The XRD patterns of the doped $BaMgSiO_4$:Fe samples synthesized in an air and reducing atmosphere indicate that the doped samples possessed the primary crystal structure independent of the reaction conditions. Well-defined peaks corresponding to the reference phase indicate successful phase formation without significant secondary phases.

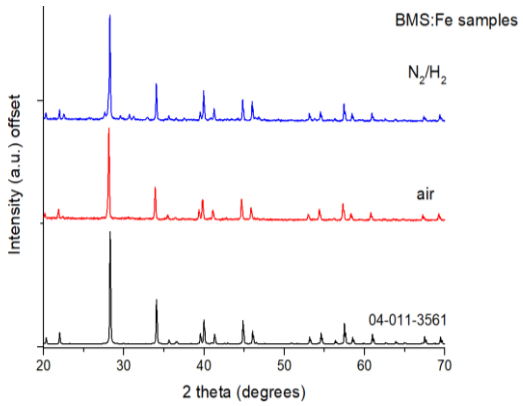


Figure 1: *XRD patterns of the Fe-doped sample synthesized under air and reducing atmosphere, along with the corresponding phase identified from the software.*

The photochromic behavior of Fe-doped $BaMgSiO_4$ was tested by monitoring the reflectance spectra before and after 254 nm UV irradiation for samples sintered under air and reducing atmospheres. The results **(Figure 2a)** clearly demonstrate that the synthesis atmosphere influences the nature of Fe ions and defects present in the material.

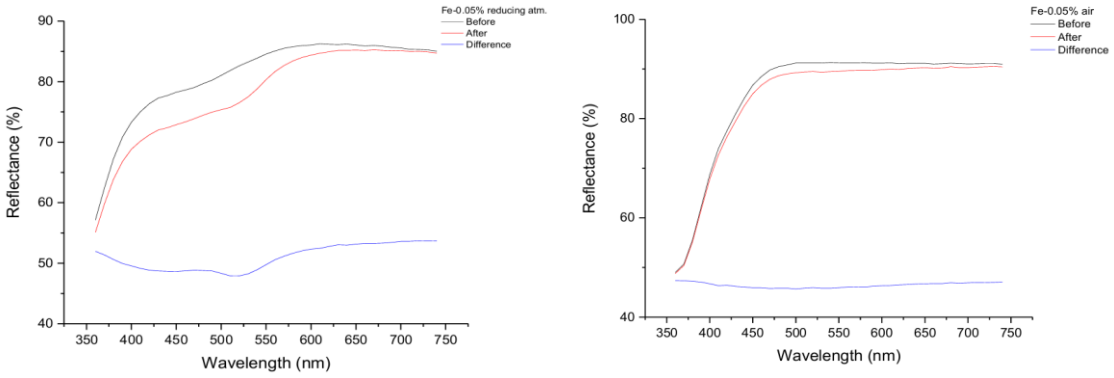
For the sample sintered under a reducing atmosphere, UV irradiation induces a pronounced decrease in reflectance across the visible region (≈350–750 nm). The difference spectrum shows a broad negative feature, with the largest reflectance change occurring in the blue–green region. This behavior is characteristic of strong photochromism and suggests the formation of photo-induced color centers.[6] Under reducing conditions, Fe is more likely to exist partially as Fe^{2+}, accompanied by a higher concentration of oxygen vacancies. Upon UV irradiation, electron transfer processes—such as $Fe^{3+} \rightleftharpoons Fe^{2+}$ transitions or electron trapping at oxygen vacancies—can occur, leading to increased visible-light absorption.

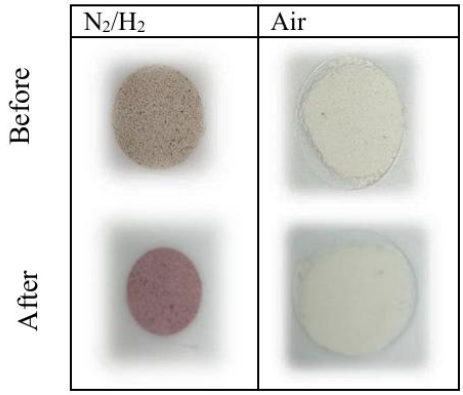
In contrast, the sample sintered in air exhibits a much weaker photochromic response. Although a small decrease in reflectance is still observable after UV exposure, the magnitude of the change is significantly lower and remains nearly constant across the visible range. This subdued response indicates that photo-induced charge transfer processes are less efficient in the air-sintered sample. The dominance of Fe^{3+} species and the lower concentration of oxygen vacancies under oxidizing conditions likely limit the formation of metastable trapped-electron states, thereby suppressing strong photochromism.

Comparing the two atmospheres highlights the role of defect chemistry in photochromic behavior. The stronger response of the sample treated in a reducing atmosphere is due to the combined effect of mixed-valence iron ions and oxygen vacancies. Together, they make it easier for UV radiation to move electrons and stabilize the resulting color centers. Similar mechanisms have been reported in other Fe-doped silicate and oxide-based photochromic systems, where reducing conditions favor reversible optical modulation.

Overall, these results confirm that Fe-doped $BaMgSiO_4$ exhibits photochromism under 254 nm UV irradiation. Sintering under a reducing atmosphere significantly enhances the photochromic contrast, making this material a promising candidate for UV-responsive optical applications such as smart pigments or optical storage, where controllable and reversible color changes are required (Figure 2).

a.





b.

Figure 2: *a. Diffuse reflectance spectra of 0.05%-Fe-doped $BaMgSiO_4$ sintered under reducing and air atmospheres before and after 254 nm UV irradiation; the atmosphere-dependent photochromic response. b. Comparison of the photochromism of two materials with the same composition but with different reaction conditions, with exposure to 254 nm UV light.*

4. CONCLUSION

In this study, $BaMgSiO_4$ (BMS) phosphors doped with Fe were synthesized via a solid-state reaction method under both air and reducing (N_2/H_2) atmospheres, and their photochromic behavior was investigated. Among the examined conditions, the reducing atmosphere proved to be the most effective for inducing photochromism in doped BMS materials.

The XRD results confirm the successful formation of the desired phase independent of the reaction conditions. The diffraction peaks match well with the reference pattern, and no significant secondary phases are observed. This indicates that the sample has good phase purity.

Detailed optical analysis of Fe-doped $BaMgSiO_4$ revealed a clear and reversible photochromic response upon 254 nm UV irradiation, strongly dependent on the sintering atmosphere. Samples synthesized under reducing conditions exhibited a pronounced decrease in diffuse reflectance across the visible spectrum, indicative of strong photo-induced absorption. The enhanced photochromism is attributed to mixed-valence Fe^{2+}/Fe^{3+} ions and increased oxygen vacancies, facilitating efficient UV-induced electron transfer and stable color centers. In contrast, air-sintered samples show weak photochromism due to dominant Fe^{3+} species and fewer defect states.

Overall, the results demonstrate that defect engineering through controlled synthesis atmospheres plays a critical role in activating and enhancing photochromic behavior in silicate-based materials.

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