

Study of XRD Pattern of Mixed Composite of MgTiO₃ and ZnO

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Abstract: In the present work, synthesis of magnesium titanate (MgTiO₃) composite produced by Mg and Ti material with ZnO has been investigated. The objective of present study is to understand how the synthesis parameters influenced the composition and structure of the particles of material. Since a most distinctive feature of fine MgTiO₃ material is the tendency to exhibit a XRD-cubic structure at room temperature. The relationship between the XRD structure and the size for this processing method is reported. Variation of intensity with different composition of material has also been reported.

Keywords: MgTiO₃, ZnO, XRD, Band gap, FWHM

I. INTRODUCTION

In recent years, TiO₃ has been well known as a semiconductor [1] with photocatalytic activities and has a great potential for applications such as environmental purification. The performance of the material (TiO₃) affected by the size of the particles [2]. TiO₃ is mainly applied as pigments, adsorbents, catalyst supports, filters, coatings, photoconductors, and dielectric materials [3]. Thus particle size plays a great role. Zinc oxide (ZnO) [4] has a relatively large energy band gap (~3.3 eV) at room temperature [5]. The band gap of zinc oxide may be increased to nearly 3–4 eV by alloying it with magnesium oxide. Zinc oxide is commonly used in laser diodes and light emitting diodes (LED). Some optoelectronic [6] applications of ZnO overlap with that of GaN, which has a similar bandgap (~3.4 eV at room temperature). Magnesium (Mg) powder (flash powder) [7, 8] was used as a source of illumination in the early days of photography. All the above base materials are taken in different proportion by weight and ground properly in order to make a fine homogeneous mixture. Now different compositions of materials (MgTiO₃ with ZnO) [9] are analyzed by X-ray diffraction (XRD) [10] and comparative study will be observed with the obtained XRD pattern. Magnesium titanate (MgTiO₃) has potential applications such as high frequency capacitors, chip capacitors, and temperature compensating capacitors [11], resonators, filters, antennas for communication, radar and direct broadcasting satellite [12]. Data on particle size can be obtained by X-ray diffraction (XRD) technique as the particle size is related to the diffraction peak broadening.

II. MATERIAL AND EXPERIMENTATION DETAIL

For the preparation of the mixed system, high purity Mg, TiO₃ and ZnO are taken in different proportions. The three base material pure magnesium (Mg), pure titanium oxide (TiO₃) and pure zinc oxide (ZnO) are taken in the powder form. All the three base material are taken in different proportion by weight. These proportions are ground properly in order to get homogeneous mixture. The homogeneous mixture is then fired in a cylindrical furnace (Muffle furnace) at 600°C to 800°C in controlled atmosphere. The heated material is then cooled and again grounded in order to make a fine mixture in the form of powder. In our experiment, we have prepared two samples having different proportions. The first sample is made by taking 40% Mg, 40% TiO₃ and 20% ZnO named as MTZ1 and second sample is made by taking 46% Mg, 46% TiO₃ and 8% ZnO named as MTZ2. XRD measurements were performed on the Bruker D8 Advance diffractometer operating in the reflection mode with Cu-K_α radiation (35 kV, 30 mA) and diffracted beam monochromator, using a step scan mode with the step of 0.075° (2θ) and 2.5 s per step at room temperature 25°C.

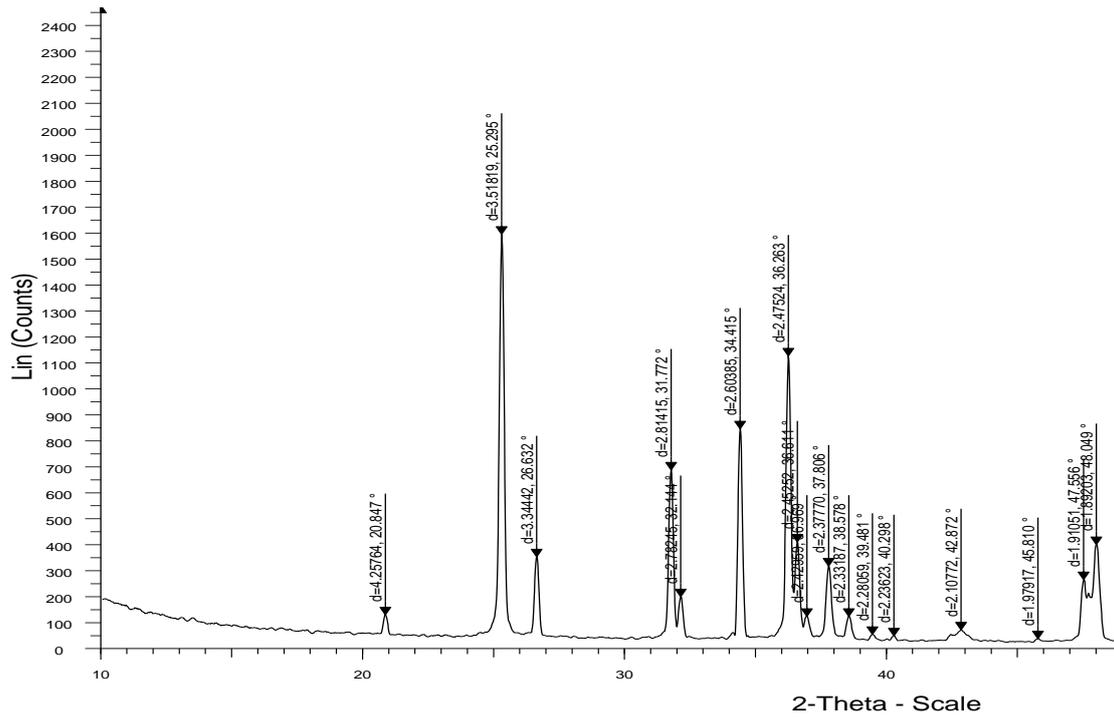


Figure 1: XRD pattern showing variation between intensity (counts) and angle (2θ) for the sample MTZ1

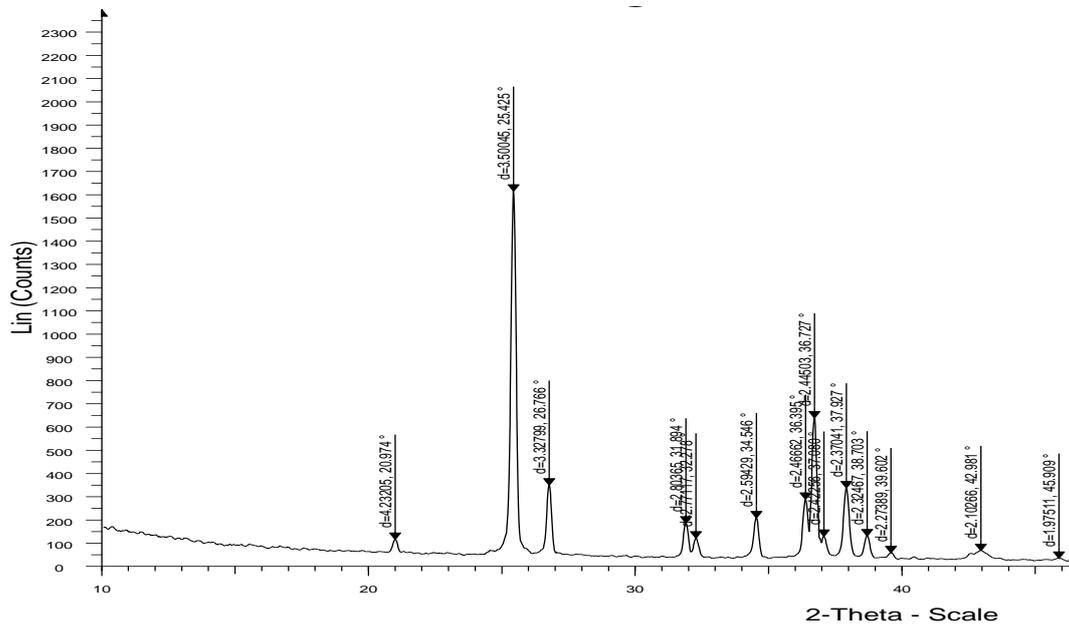


Figure 2: XRD pattern showing variation between intensity (counts) and angle (2θ) for the sample MTZ2

III. RESULTS AND DISCUSSION

In the present paper, the crystallite size is calculated from the observed XRD pattern of different composites of MgTiO₃ and ZnO. XRD is a commonly used technique for the evaluation of crystal structure, because it relies on coherent scattering from many unit cells in a spatially time averaged fashion. The crystallite size of the material can be calculated from the full-width at half-maximum (FWHM) measurement for the prominent X-ray diffraction peaks using Scherrer [13] formula. The finite three dimensional crystal lattice of the material diffracts X-rays in a manner analogous to the reflection from a ruled grating. When the size of particle is of the order of wavelength of incident beam, the diffracted beam becomes diffused. The crystallite size may be obtained from the measured width of the X-

ray diffraction line. The Scherrer formula for the calculation of crystallite size (grain diameter) [14], D , of the sample is

$$D = \frac{k\lambda}{\beta \cos \theta}$$

Where, D is the crystallite size, K is a constant varies with crystallite shape but usually nearly equal to 0.94, λ is the wavelength of source radiation and β is full-width at half maximum (FWHM) of the peak, in radians and θ is the Bragg's angle.

In the present work, measurements have been carried out on the identification of particle size of MgTiO_3 [15] composite with ZnO using XRD technique. The crystallite size calculated using Scherrer formula for the prominent peaks in the diffraction pattern for both sample MTZ1 (Figure 1) and MTZ2 (Figure 2) is same. From the observed results, the XRD patterns (prominent peak) of sample MTZ1 and MTZ2 represented that the material is homogeneous. In Figure 1, XRD patterns for MTZ1 show strong diffraction peaks at 25.295° , 34.415° , 36.263° respectively. In Figure 2, XRD patterns for MTZ2 show strong diffraction peaks at 25.425° , 36.727° respectively. The patterns show sharp and well defined peaks, indicating the crystallinity of the synthesized materials. Intensity of diffraction peaks for the composite MTZ1 is lower than that of composite MTZ2. This implies that the intensity depends on the composition of the material.

IV. CONCLUSIONS

The X- ray diffraction (XRD) analysis of composite MTZ1 and MTZ2 provides good information about the materials. The variation of peaks in diffraction pattern reveals that intensity depends on the composition of material. The measurements carried out for the prominent peaks of diffraction pattern shows that material is homogeneous i.e. the crystallite size (grain diameter) are same in both the sample MTZ1 and MTZ2.

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