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Optical, Structural and Mechanical Properties of a Zinc Magnesium Sulphate Crystal

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Abstract

Single crystals of zinc magnesium sulphate were grown from a non aqueous solution by slow evaporation method at room temperature. Good quality transparent crystals were harvested by slow evaporation technique within 25 days. The crystals were subjected to single X ray diffraction and its structure was determined. UV-Vis spectrum confirms that the material has wide optical transparency. FTIR analysis confirms the vibrational modes of the crystal and the presence of functional groups. The Vicker's hardness property shows its mechanical strength. The surface morphology is studied by SEM technique..

Keywords: MZE–zinc magnesium sulphate crystal, XRD-X-ray diffraction, SEM–scanning electron microscope, FTIR–fourier transform infrared, UV-Vis – ultraviolet-visible.

Introduction

Crystal growth is a highly interdisciplinary area of research. Crystals grown now-a-days find places ranging from microelectronics, optoelectronics, medical instruments, communication systems, defence sources etc., High efficient photovoltaic cells and detectors, fabrication of LEDs, traffic purpose illumination devices widely depend on the crystal growth techniques. Magnesium sulphate crystals have wide application in the field of medicine and in agriculture. To the best of our knowledge this composite crystal zinc sulphate with magnesium sulphate has excellent optical property with good mechanical strength [1-3].

Experimental procedure

Synthesis and growth

High purity salts (99.9%) were used for the crystal growth. Single crystals of Magnesium sulphate mixed Zinc sulphate(MZE) were grown at room temperature by solution growth using slow evaporation method, of an organic solution (ethanol) containing zinc sulphate and magnesium sulphate in equal stoichiometric ratio. The temperature of water in the bath was controlled digitally by using microprocessor. Variation in temperature of the bath can be tuned to an accuracy of ±0.1°C. Transparent good quality crystals of the MZE crystals were harvested in span of 25 days. The photograph of the crystal is shown in Figure 1.

Figure 1. Photograph of MZE crystals

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Characterization

The single crystal X-ray diffraction studies of the grown MZE crystals were carried out using ENRAF NONIUS CAD 4 diffractometer. The UV-Visible spectrum was recorded in the range 190nm-1100nm using Perkin Elmer lambda 35 model. FTIR spectrum analysis was recorded in the range of 4000-400 cm^{-1} using Perkin Elmer spectrum RX I. The hardness property of the crystal was carried out by Vicker's microhardness method and the structural morphology of this material are reported by SEM technique.

Results and discussion

Single crystal X ray diffraction

The structure of the grown MZE crystal was studied by single crystal X ray diffraction method. The crystallographic data obtained from the analysis revealed that the crystal possesses monoclinic structure. The unit cell dimensions were a=10.053 A˚, b= 7.210 A˚, c= 24.378 A˚, α= 90˚, β= 98.21˚, γ= 90˚ and cell volume was 1748.7 $A^{\circ 3}$.

FTIR spectral analysis

The FTIR spectrum was recorded for the sample of the crystals using the KBr pellet technique in the region 4000-400 cm^{-1}. The various functional groups present in the material are identified and confirmed in this study. The FTIR spectrum is shown in Figure 2.

The broad band between 3588 cm^{-1} and 3200 cm^{-1} represents the presence of OH stretching vibrations. The OH inoximes stretching is observed at 3318 cm^{-1} whereas OH stretching is observed at 3246 cm^{-1}. Peaks from 3500-3200 cm^{-1} represent the presence of medium hydrogen bonded OH group. Peaks between 1145-1170 cm^{-1} represent the presence of SO_2 symmetric stretching. Peak at 1081 cm^{-1} represents C-O stretching. Peaks 983 cm^{-1}, 868 cm^{-1}, represents very strong CH out of plane deformation, whereas peak at 762 cm^{-1} intimates the strong CH out of plane deformation. The position of S=O depends on the electronegativity of the attached group and tends to raise the frequency since they tend to stabilize the form S=O and increase stretching vibrations [4-6].

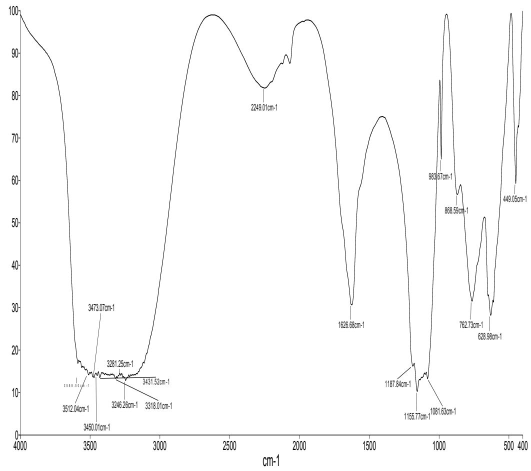

Figure 2. FTIR spectrum of MZE crystal

UV-VIS spectrum analysis

The optical absorption spectra of MZE crystal were recorded in the region 190-1100nm at a scanning speed of 480 nm/min. Figure 3(a&b) shows the absorbance spectra and transmission spectra which hold good in the entire visible region. The lower cutoff wavelength of this crystal was found to be 198.3 nm. The optical behavior of this MZE material is suitable for opto-electronic applications.

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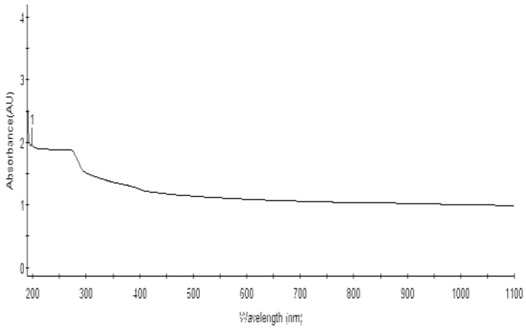


Figure 3(a). Absorption spectrum of MZE

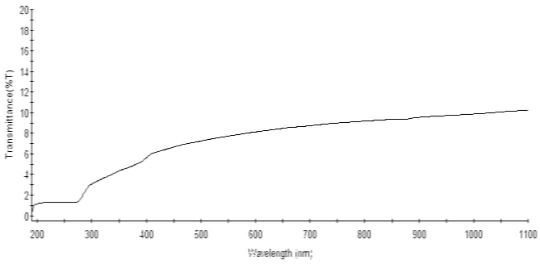


Figure 3(b). Transmission spectrum of MZE

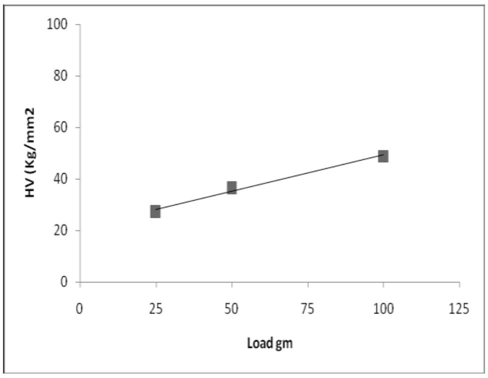


Figure 4(a). Load versus H_v

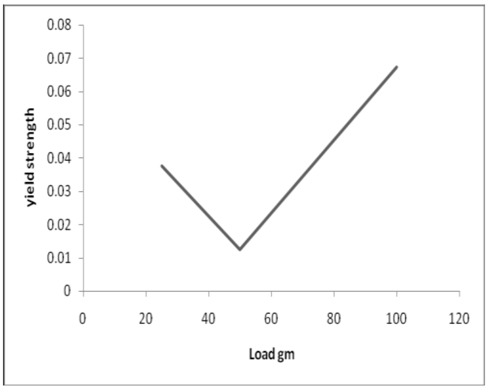


Figure 4(b). Load versus yield strength

Mechanical studies

The micro hardness of a substance is a key property to interpret the mechanical strength of the material which is basically related to the crystal structure and about the atomic package. It also reveals the electronic factors operating to make the stable structure. It is the resistance offered by the crystal for the movement of dislocations and for localized plastic deformation. This test affords useful details about the mechanical properties like elastic constants, yield strength etc., of materials. The variation of H_v with the applied load for the crystals are shown in Figure 4(a). The hardness number was found to increase with increase in applied load, which confirms the hardness.

The calculated values of yield strength σ_v for grown crystals are shown in Figure 4(b). For load 50gm, it decreases and then suddenly for 100gm it reaches a higher value. The elastic stiffness constant C_{11} has been calculated for the crystals using Wooster's empirical relation $C_{11} = H_v^{7/4}$. The calculated stiffness constant for different loads are shown in Figure 4(c). A plot of log p versus log d provides a straight line, the slope of which gives the work hardening coefficient n.

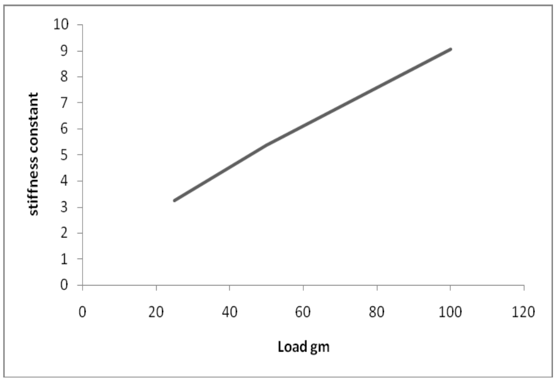


Figure 4(c). Load versus stiffness constant

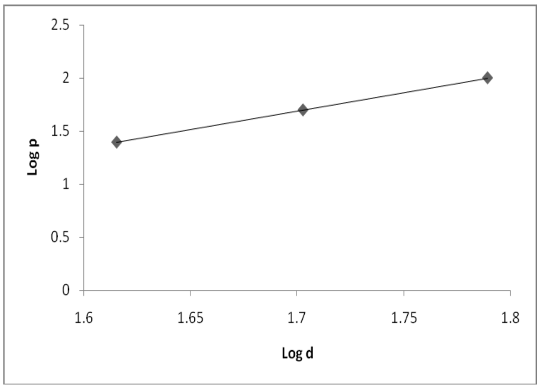
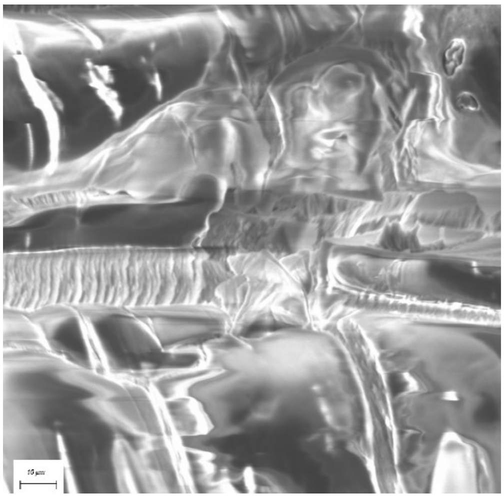


Figure 4(d). Log d versus Log p

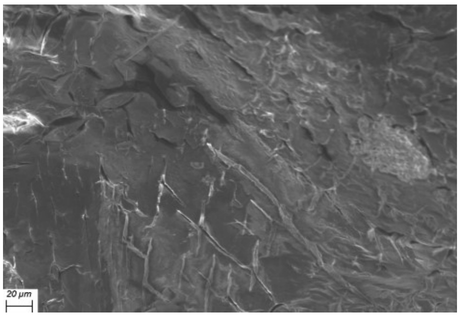
In the present study, work hardening coefficient n is found to be higher than 2 for the sample, indicating that the lattices are soft. MZE crystal has higher microhardness H_v with respect to loads. Figure 4(d) shows that MZE crystal has a linear variation in strength.

SEM analysis

The grown MZE crystal was subjugated by SEM analysis. The quality of the grown crystal can be inferred to some extent by observing the surface morphology of the crystal. The recorded SEM picture Figure 5 (a, b & c) confirmed the formation of smooth surface. But in Figure 5b at higher magnification it is observed that some macro steps with pits and inclusion appeared due to high growth rates. In Figure 5c, plate like crystals show the thick and coarse granular type of growth [7].



(a)



(b)

(c)

Figure 5. SEM pictures of MZE crystals

Conclusion

Single crystals of zinc and magnesium sulphate crystal was grown from an organic solution by slow evaporation method at room temperature. Good quality transparent crystals were harvested by slow evaporation technique within 25 days. The crystals were subjected to single X ray diffraction method. The lattice parameters and structure were found. UV-Vis spectrum confirms that the material has wide optical transparency. FTIR analysis confirms the vibrational modes of the crystal and the expected presence of functional groups were identified. The Vicker's hardness property shows its good mechanical strength. The surface morphology is studied by SEM technique. The crystal has good optical, mechanical and morphological reports and may be considered for optoelectronic applications.

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