Structural, Optical and Magnetic Properties of α-Fe2O3 Nanoparticles


To cite this version:
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B. Balaraju¹, M. Kuppan¹, S. Harinath Babu², S. Kaleemulla¹,a, N. Madhusudhana Rao¹, C. Krishnamoorthi¹, Girish M. Joshi³, G. Venugopal Rao⁴, K. Subbaravamma⁵, I. Omkaram⁶, D. Sreekantha Reddy⁷

1 – Thin films Laboratory, Centre for Crystal Growth, VIT University, Vellore-632014, Tamilnadu, India
2 – Department of Physics, Annamacharya Institute of Technology and Sciences, New Boyanapalli, Rajampet-516 126 andhra Pradesh, India
3 – Polymer Nanocomposite Labortory, Centre for Crystal Growth, VIT University, Vellore-632014, Tamilnadu, India
4 – Materials Physics Division, Indira Gandhi Centre for Atomic Research, Kalpakkam-603102, Tamilnadu, India
5 – Department of Physics, AMET University, Kanthur, Chennai-603112, Tamilnadu, India
6 – Department of Electronics and Radio Engineering, KyungHee University, Yongin-si, Gyeonggi-do 446-701, Republic of Korea
7 – Department of Physics and Sungkyukwan Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University, Suwan – 440746, Republic of Korea
a – skaleemulla@gmail.com

DOI 10.2412/mmse.22.88.233 provided by Seo4U.link

Keywords: iron oxide, nanoparticles, XRD profile, oxide semiconductors.

ABSTRACT. High purity Iron oxide (α-Fe₂O₃) powder was grinded for 16 hours using mechanical milling and studied for its physical properties. The micro structures, crystallite size of the nanoparticles were examined using X-ray diffractometer (XRD). From this it was found that the particles were in rhombohedral structure with average crystallite size of 39 nm. The optical absorbance and reflectance spectra were recorded using UV–Vis-NIR spectrophotometer in the wavelength range of 200 – 2500 nm. From this it was found that the optical band gap of the nanoparticles as 2.08 eV. The magnetic measurements were carried out using vibrating sample magnetometer at 100 K. From the magnetic studies it was found that the magnetic moment of the nanoparticles increased with increase of applied field and saturation was not observed even at high applied magnetic fields.

Introduction. Now-a-days, wide band gap oxide semiconductors, tin oxide, tungsten oxide, nickel oxide, chromium oxide, iron oxide etc. are finding great interest in many potential applications such as magnetic devices, sensors, lithium ion batteries, etc.[1-5]. Moreover much focus in being paid on nanoparticles of these oxide materials as they are best suited for the device applications as the nanoparticle find peculiar properties. More efforts were put for the synthesis of nanoparticles using different physical and chemical methods. Among the various types of nanomaterials, the magnetic materials of iron oxides such as α-Fe₂O₃ and Fe₃O₄ are the most popular and promising materials due their many technological applications. Among the other metal oxide materials, α-Fe₂O₃ finds in many applications such as pigment, electrode material, magnetic materials etc.[6-10]. Further it finds applications in many photovoltaic devices [11-15]. In the present investigation, synthesis of α-Fe₂O₃ nanoparticles were done using mechanical milling method and subjected to structural, optical and magnetic properties.
Experimental. The commercially available $\alpha$-Fe$_2$O$_3$ powder was procured from Sigma Aldrich (India). $\alpha$-Fe$_2$O$_3$ nanoparticles were prepared by simple mechanical milling method. The powder was milled using Agate mortar and ground thoroughly for 16 hours using pestle. After that the samples were characterized for structural, optical, magnetic and photoluminescence properties. X-ray diffraction (X-ray diffractometer, D8 Advance, BRUKER) patterns were used to study the structural aspects. The optical reflectance spectra were recorded using UV-VIS spectrophotometer (JASCO-V-670) in the wavelength range of 200 nm to 2500 nm and the magnetic studies were studied using vibration sample magnetometer (VSM Lakeshore 7404).

Results and discussion.

Structural properties. Fig. 1 shows the X-ray diffraction profile of the Fe$_2$O$_3$ nanoparticles. The diffraction peaks such as (0 1 2), (1 0 4), (1 1 0), (1 1 3), (0 2 4), (1 1 6), (1 2 2), (2 1 4) and (3 0 0) were found in their respective diffraction angles. From this the structure of the nanoparticles was found to be in rhombohedral structure. These are in good agreement with that of standard XRD pattern of $\alpha$-Fe$_2$O$_3$ derived from the JCPDS Card No. 33-664 [16]. No other diffraction peaks related to either FeO or Fe$_3$O$_4$ were found in the profile indicating that the source material is pure from any kind of impurities.

![XRD profile of $\alpha$-Fe$_2$O$_3$ nanoparticles](image)

Fig. 1. XRD profiles of $\alpha$-Fe$_2$O$_3$ nanoparticles.

The crystallite size ($G$) was calculated by using the Debye-Scherer formula,

$$G = \frac{k\lambda}{\beta \cos \theta}$$  \hspace{1cm} (1)

where $k$ - particle geometry dependent constant (for spherical shape $k \sim 1$), $\lambda$ - wavelength of used ($\lambda = 1.5406$ Å), $\beta$ - full width at-half maximum (FWHM) and $\theta$ - the diffracted angle, respectively. The estimated average crystallite size is found to be 39 nm.

Optical properties. Fig. 2 shows the optical absorbance spectrum of $\alpha$-Fe$_2$O$_3$ nanoparticles. From the optical absorbance and reflectance data, the optical band gap of the nanoparticles was estimated.
The optical band gap $E_g$ was obtained by plotting $(\alpha h\nu)^2$ versus the photon energy $(h\nu)$ and by extrapolating the linear region $(\alpha = 0)$. The optical band gap was estimated using the Tauc equation

$$\alpha h\nu = A \sqrt{(E_g - h\nu)} \tag{2}$$

where $h\nu$ – the photon energy, $\alpha$ – the absorption coefficient and $n$ – either $1/2$ for a direct transition or $2$ for an indirect transition.

An optical band gap of 2.08 eV was observed for $\alpha$-Fe$_2$O$_3$ nanoparticles. The observed optical band gap is inconsistent with that of published work [9].

**Fig. 2. Optical absorbance spectrum of $\alpha$-Fe$_2$O$_3$ nanoparticles.**

**Magnetic Properties.** Fig. 3 shows the magnetization versus magnetic field curve of the $\alpha$-Fe$_2$O$_3$ nanoparticles calibrated at 100 K in the external magnetic field of $-10$ kOe to $+10$ kOe. From the Fig. it is clear that the nanoparticle exhibits ferromagnetism. But the strength of magnetization is less. Fig. 4 shows the magnetization versus magnetic field curve of the Fe$_2$O$_3$ nanoparticles calibrated at 100 K in the external magnetic field of $-70$ kOe to $+70$ kOe. Here also the magnetic hysteresis measurements for synthesized samples were carried out using vibrating sample magnetometer (VSM) at 100 K. It can be seen that the magnetization increases almost linearly under an applied magnetic field. The saturation in the magnetization could not be observed even under the high magnetic field of 40,000 Oe. This observation is similar to the earlier study [17]. The linear increase in the magnetization represents the contribution of the $\alpha$-Fe$_2$O$_3$ antiferromagnetic core [18].
Summary. Nanoparticles of highly purified α-Fe₂O₃ have been synthesized by solid state method. The average crystallite size has been found as 39 nm. The optical properties of the sample show that the optical bandgap is at 2.08 eV. The magnetic studies of the sample confirm the ferromagnetic nature of sample with the absence of saturation even at high fields.

References


Cite the paper