Extended Abstract

Investigation of Structural, Magnetic and Optical Properties of thin Films of Iron Oxide Doped with Tungsten Cation Prepared by Spray Pyrolysis Method

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ABSTRACT

In this study, thin layers of pure and tungsten-doped iron oxide α-phase (α-Fe_2O_3) were deposited on glass substrates using the spray pyrolysis method and investigated. Due to their diverse properties, these thin layers have a wide range of applications in catalysts, sensors, solar cells, and magnets. Structural (XRD, FTIR, AFM), Magnetic (VSM), and Optical Analyses were performed. The results showed that tungsten doping increased particle size (85-120 nm), improved surface smoothness, reduced surface roughness and hardness, and led to significant changes in magnetic and optical properties. In particular, the saturation magnetization increased, and the band gap of the material increased. It appears that tungsten doping provides good potential for optical and magnetic applications in these thin layers.

Keywords: Magnetic Nanoparticles, Iron Oxide, Spray Pyrolysis, Thin Layers, Tungsten

INTRODUCTION

The performance of thin films is determined by factors such as atomic structure, defects, impurities, surface roughness, thickness, and mechanical properties [1]. These films can range from sub-nanometer to micrometer thicknesses and typically consist of a deposited layer on a substrate, producing properties distinct from either material alone [2]. Thin films are characterized by their minimal thickness, high surface-to-volume ratio, and growth-dependent structure. Tungsten is widely used in electronics due to its conductivity, serving as an interconnect material in integrated circuits (ICs) and as a coating in thin metal layers. Its electronic properties also make it ideal for X-ray targets. This study focuses on iron oxide thin films, particularly the stable alpha phase, investigating the effects of tungsten cation substitution. Thin film synthesis methods are broadly classified into physical vapor deposition (PVD) and chemical vapor deposition (CVD), each offering unique advantages in nanoparticle fabrication [2]. By combining substrate engineering and dopant integration (e.g., tungsten in iron oxide), thin films can be tailored for enhanced electronic, optical, or mechanical performance.

MATERIALS AND METHODS

The spray pyrolysis method is a versatile and cost-effective technique used for depositing thin and thick layers of various materials, including semiconductors, insulators, magnetic materials, and superconductors. It is widely applied in research and industry for producing optical filters, solar cells, sensors, hard coatings, and dielectric layers. Unlike physical deposition methods, spray pyrolysis offers higher stability, simplicity, and the ability to coat larger surfaces at nanoscale thicknesses. This chemical deposition method involves dissolving the desired material into a solution, which is then sprayed as fine droplets onto a heated substrate using a carrier gas (typically air). The device consists of a nozzle spray system, a rotating hot plate, an adjustable lifting system,

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and controllers for temperature, spray rate, and gas pressure. The substrate must possess high thermal stability, smoothness, and mechanical strength to ensure uniform film deposition [3,4]

Key deposition parameters include spray rate, substrate temperature, carrier gas type and pressure, solution concentration, and nozzle-to-substrate distance. In this study, iron oxide α-phase (α-Fe_2O_3) thin films doped with tungsten ($Fe_{2-x}W_xO_3$, for x = 0–0.10) were prepared using iron nitrate and tungsten chloride dissolved in distilled water. The solution was sprayed onto glass substrates at 450°C, with rotational movement ensuring homogeneity.

The deposited films were analyzed using various techniques:

1- XRD (X-ray Diffraction) – Crystallinity and phase identification.

2- AFM (Atomic Force Microscopy) – Surface morphology and topography.

3- FTIR (Fourier Transform Infrared Spectroscopy) – Structural properties and functional groups.

4- UV-Vis Spectroscopy – Optical transmission and bandgap calculation.

5- VSM (Vibrating Sample Magnetometer) – Magnetic properties under applied fields up to 10,000 Oe.

By optimizing deposition conditions (temperature, rate, time, solution concentration), high-quality crystalline thin films were achieved, demonstrating the effectiveness of spray pyrolysis for functional material synthesis.

RESULTS AND DISCUSSION

This study examines the structural, morphological, magnetic, and optical properties of pure and tungsten (W)-substituted iron oxide (α-Fe_2O_3) thin films synthesized via spray pyrolysis at 450°C. Key techniques—X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, atomic force microscopy (AFM), vibrating sample magnetometry (VSM), and UV-Vis spectroscopy were used to analyze the effects of W substitution (x = 0.000 to 0.100).

XRD ANALYSIS

XRD confirmed a rhombohedral structure (space group R-3c) matching reference data (01-087-1164). W incorporation preserved the crystal structure but increased lattice parameters (a=b: 5.034–5.846 Å; c: 13.720–13.968 Å) and crystallite sizes (52.324–62.424 Å), indicating enhanced crystallinity and lattice expansion [5]. Higher annealing temperatures intensified peak sharpness, suggesting improved crystallite connectivity and sample density (See Fig. 1 and Table 1).

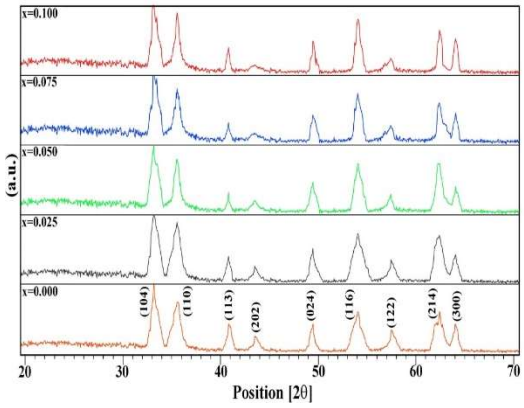


Figure 1- X-ray diffraction spectra of the thin film samples for different substitution amounts at a substrate temperature of 450 °C.

Table 1- Lattice parameters for all samples from X-ray diffraction patterns along with crystallite sizes.

D (Å)	c (Å)	a=b (Å)	Sample (x)
52.324	13.720	5.034	0.000
53.128	13.762	5.124	0.025
56.242	13.822	5.326	0.050
58.264	13.868	5.636	0.075
62.424	13.968	5.846	0.100

FTIR ANALYSIS

FTIR spectra identified Fe–O bonds (472 cm^{-1}, 584 cm^{-1}) and C=O stretching (1220 cm^{-1}). The peak at 522 cm^{-1}, initially attributed to the glass substrate, intensified with W doping, confirming cation integration. Band shifts reflected altered metal-oxygen bond distances due to interstitial site variations, validating structural modifications [6].

AFM ANALYSIS

AFM revealed morphological changes: undoped Fe_2O_3 exhibited quasi-spherical particles, while W doping promoted rod-like, interconnected structures, reducing roughness and enhancing uniformity [7, 8]. Particle sizes grew from ~85 nm (low doping) to ~120 nm (x = 0.100), with smoother surfaces at higher doping levels, indicating improved microstructural cohesion.

VSM ANALYSIS

Magnetic hysteresis loops showed enhanced weak ferromagnetism with W doping. Saturation magnetization (M_s) increased from 0.8 to 8.8 emu/cm^3, and remanence (M_r) from 0.4 to 3.4 emu/cm^3, while coercivity (Hc) decreased from 1180 Oe to 740 Oe [7,9]. These changes were linked to W-induced lattice distortions, spin canting, and reduced magnetic anisotropy due to larger, interconnected particles (See Fig. 2).

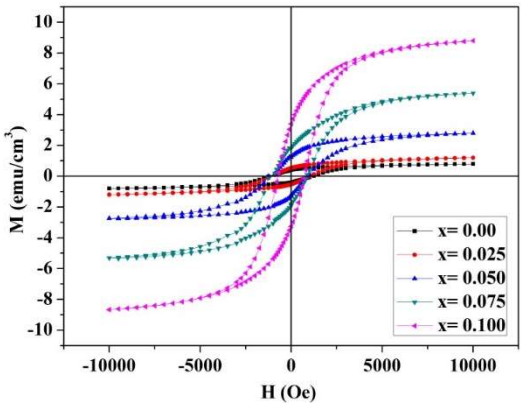


Figure 2- Magnetic hysteresis loops of all prepared samples for different substitution amounts.

UV-VIS SPECTROSCOPY

Transmission spectra (300–1000 nm) showed reduced UV transmission (32% → 6%) but slightly improved visible transmission (63% → 59%) at higher doping (x > 0.050), attributed to smoother surfaces. The band gap (E_g) widened from 2.9 eV to 3.54 eV due to quantum confinement, crystallite growth, and W-induced electronic modifications [9, 10]. Key findings are as follows:

1. Structural Impact**:** W substitution preserved the rhombohedral phase but expanded lattice parameters and crystallite sizes.
2. Morphological Evolution: Doping transformed granular surfaces into denser, rod-like microstructures with reduced roughness.
3. Enhanced Magnetism: Increased M_s and M_r with lowered Hc indicated tunable weak ferromagnetism.
4. Optical Modulation: Doping reduced UV transmission but improved visible light transmittance at higher levels, alongside band gap widening.

The study demonstrates that W doping effectively tailors α- phase of Fe_2O_3's properties for applications in spintronics, photovoltaics, and sensors, where controlled crystallinity, magnetism, and optical responses are critical.

CONCLUSION

Thin films of $Fe_{2-x}W_xO_3$ (x = 0–0.10) were synthesized via spray pyrolysis. XRD confirmed a pure rhombohedral structure (space group R-3c) matching the standard pattern (01-087-1164), with crystallite sizes and lattice parameters calculated via Scherrer's method. FTIR revealed metal-oxygen and other functional bonds. AFM showed dense quasi-spherical/blade-like morphologies (85–120 nm particles). VSM indicated rising saturation magnetization (0.8–8.8 emu/cm³) and decreasing coercivity (1180–740 Oe). UV-Vis displayed increasing transmission and bandgap with higher W content, suggesting tunable optical properties. No impurity phases were detected, highlighting the structural and functional homogeneity of the doped films.

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