

Effect of Different Film Thickness for (Fe_3O_4 - Ni_2O_3) on Crystal Properties and Particle Size Using XRD

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Abstract : In this work, (Fe_3O_4 and Ni_2O_3) Nano-material samples were prepared by sol-gel method with one concentrations (0.1 M solution), and made thin films of this samples on ITO glass substrate by different size (55.25, 78.7, 90.9 144.9 and 263.15) nm. Film thickness was measured by using the weight method. The Nano crystal size of all samples was found by XRD technique, and study effect of different concentrations on the particle Size and crystal properties of all samples. The density particle Size, and d-spacing were increase when thin films thickness increases.

Keywords: Density, d-spacing, XRD technique, Nano Crystal Size. thin films

Introduction

Nickel Oxide (NiO) is an important transition metal oxide with cubic lattice structure. Among the magnetic nanoparticles, fabrication of nickel nanoparticles (NPS) is often more difficult than that of the other particles. This is because they are easily oxidized. To achieve pure nickel nano-crystals, numerous methods have been conducted in organic environments in order to prevent formation of hydroxide or oxidation [1]. Iron oxide nanoparticles (NPs) have attracted much consideration due to their unique properties, such as super paramagnetic, surface-to-volume ratio, greater surface area, and easy separation methodology. Various physical, chemical, and biological methods have been adopted to synthesize magnetic NPs with suitable surface chemistry [2]. Solid materials may be classified according to the regularity with which atoms or ions are arranged with respect to one another. Material is one in which the atoms are situated in a repeating or periodic array over large atomic distances; that is, long range order exists, such that upon solidification, the atoms will position themselves in a repetitive three-dimensional pattern, in which each atom is bonded to its nearest-neighbour atoms. Some of the properties of crystalline solids depend on the crystal structure of the material, the manner in which atoms, ions, or molecules are spatially arranged. There is an extremely large number of different crystal structures all having long-range atomic order; these vary from relatively simple structures for metals to exceedingly complex ones, as displayed by some of the ceramic and polymeric materials.

Sometimes the term lattice is used in the context of crystal structures; in this sense lattice means a three-dimensional array of points coinciding with atom positions. The atomic order in crystalline solids indicates that small groups of atoms form a repetitive pattern. Thus, in describing crystal structures, it is often convenient to subdivide the structure into small repeat entities called unit cells. A unit cell is chosen to represent the symmetry of the crystal structure, wherein all the atom positions in the crystal may be generated by translations of the unit cell integral distances along each of its edges. Thus, the unit cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within [3].

There are three relatively simple crystal structures are found for most of the common metals:

1. The Face-Centred Cubic Crystal Structure. The crystal structure found for many metals has a unit cell of cubic geometry, with atoms located at each of the corners and the centres of all the cube faces. It is aptly called the face-centred cubic (FCC) crystal structure.
2. The Body-Centred Cubic Crystal Structure. Another common metallic crystal structure also has a cubic unit cell with atoms located at all eight corners and a single atom at the cube centre. This is called a body-centred cubic (BCC) crystal structure.
3. The Hexagonal Close-Packed Crystal Structure. Not all metals have unit cells with cubic symmetry; the final common metallic crystal structure to be discussed has a unit cell that is hexagonal. The term hexagonal close-packed brief as (HCP). The top and bottom faces of the unit cell consist of six atoms that form regular hexagons and surround a single atom in the centre [4].

Crystal System: The unit cell geometry is completely defined in terms of six parameters: the three edge lengths a , b , and c , and the three interaxial angles α , β , and γ . and are sometimes termed the lattice parameters of a crystal structure. On this basis there are seven different possible combinations of a , b , and c , and α , β , and γ , each of which represents a distinct crystal system. These seven crystal systems are cubic, tetragonal, hexagonal, orthorhombic, rhombohedral, monoclinic, and triclinic. Crystallographic planes (Miller indices): The orientations of planes for a crystal structure are represented in a similar manner. Again, the unit cell is the basis, with

the three-axis coordinate system. In all but the hexagonal crystal system, crystallographic planes are specified by three Miller indices as (h k l). Any two planes parallel to each other are equivalent and have identical indices [5,6].

Material and Method

Samples Preparation Nickel oxide thin films were prepared by spraying a 0.1 M solution of nickel nitrate of doubly distilled water onto the pre-heated amorphous glass substrates kept at $(390^{\circ}\text{C} \pm 10^{\circ})$ C. Iron oxide thin films were prepared by spraying a 0.1 M solution of ferric nitrate of doubly distilled water onto the pre-heated amorphous glass substrates kept at $(390^{\circ}\text{C} \pm 10^{\circ})$ C. Film thickness was measured by using the weight difference method considering the density of the bulk nickel oxide. This film thickness is proportional to the concentration since we divide the mass by substrate area which gives concentration per unit area. As the density of thin films was certainly lower than the bulk density, the actual film thickness would be larger than the estimated values. The structural characterization of the films deposited at optimized preoperative parameters was carried out.

Results

After prepared Thin film of (Fe_3O_4 and Ni_2O_3) Nano-material deposited on ITO glass substrate with different thicknesses (55.25, 78.7, 90.9, 144.9 and 263.15) nm for each, used XRD to study crystal structural characterization

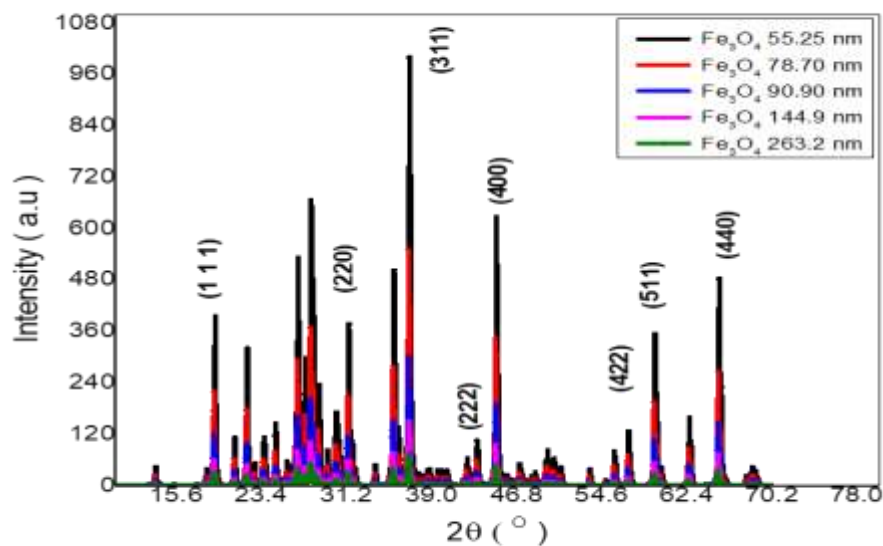


Fig (1): the XRD charts of the five Fe_3O_4 (Iron Oxide) sample

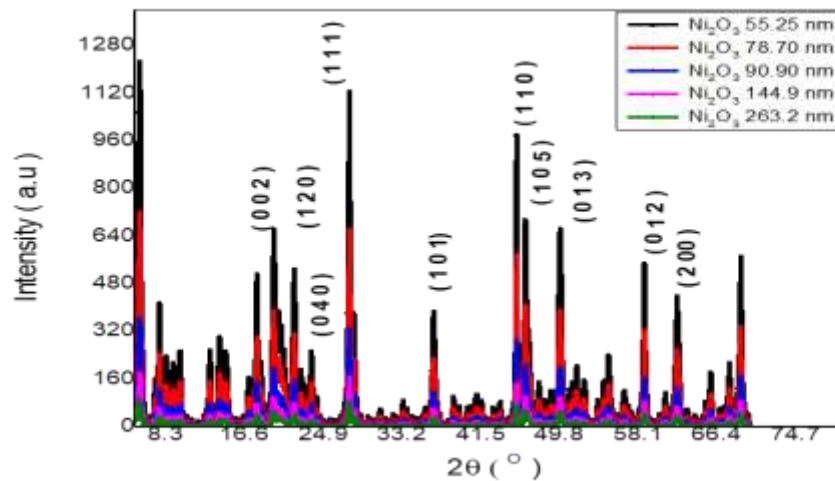


Fig (2): the XRD charts of the five Ni_2O_3 (Nickel Oxide) sample

Table (1) some crystallite lattice parameter (c-form, a,b,c, β , α , γ , density, X_s (nm) and d – spacing) of all samples that made by five Fe_3O_4 (Iron Oxide) sample

Fe_3O_4 : Sample thickness (nm)	a=b=c	$\alpha = \beta = \gamma$	Density(g.cm^{-3})	$X_s(\text{nm})$	d-spacing (\AA°)
55.25	8.09	90	4.857	55.05	2.0297
78.7	8.39	90	5.102	56.06	2.21935
90.9	8.39	90	5.2071	56.10	2.22425
144.9	8.35	90	5.2071	62.95	2.6007
263.2	9.4	90	5.808	64.25	3.59315

Table (2) some crystallite lattice parameter (c- form, a,b,c, β , α , γ , density, X_s (nm) and d – spacing) of all samples that mead by five Ni_2O_3 (Nickel Oxide) sample

Ni_2O_3 Sample thickness (nm)	a=b	c	$\alpha = \beta$	γ	Density(g.cm^{-3})	$X_s(\text{nm})$	d-spacing (\AA°)
55.25	4.61	5.61	90	120	5.3175	53	2.74230
78.7	4.61	5.61	90	120	5.3175	55.75	4.07930
90.9	4.523	7.36	90	120	5.434	56.15	4.07975
144.9	2.955	7.227	90	120	6.803	57.03	4.08000
263.2	2.818	20.56	90	120	7.435	57.44	9.02055

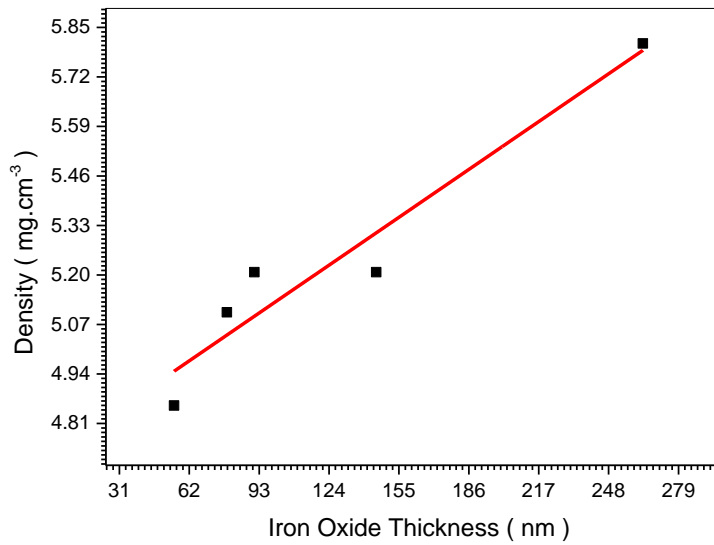


Fig (3): relationship between thicknesses and density of five Fe_3O_4 (Iron Oxide) sample

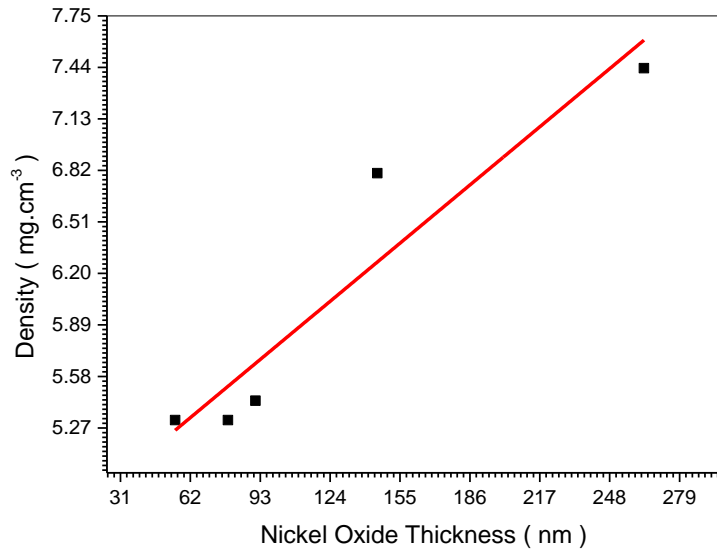


Fig (4): relationship between thicknesses and density of five Ni_2O_3 (Nickel Oxide) sample

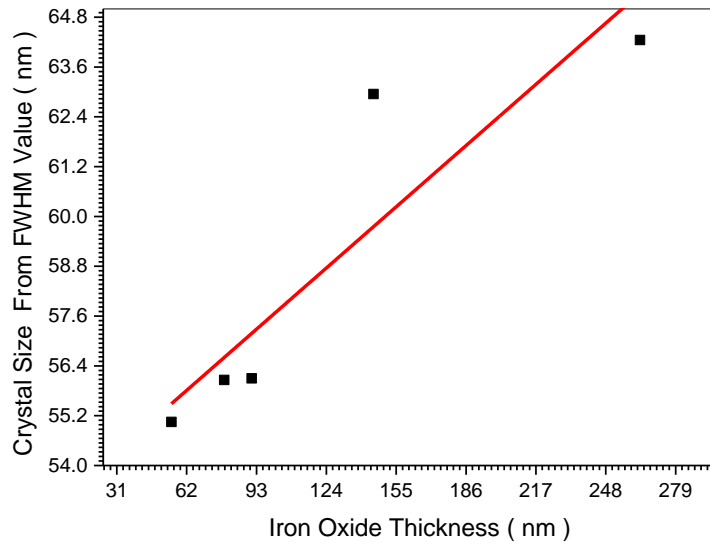


Fig (5): relationship between thicknesses and crystal size from FWHM value of five Fe₃O₄ (Iron Oxide) sample

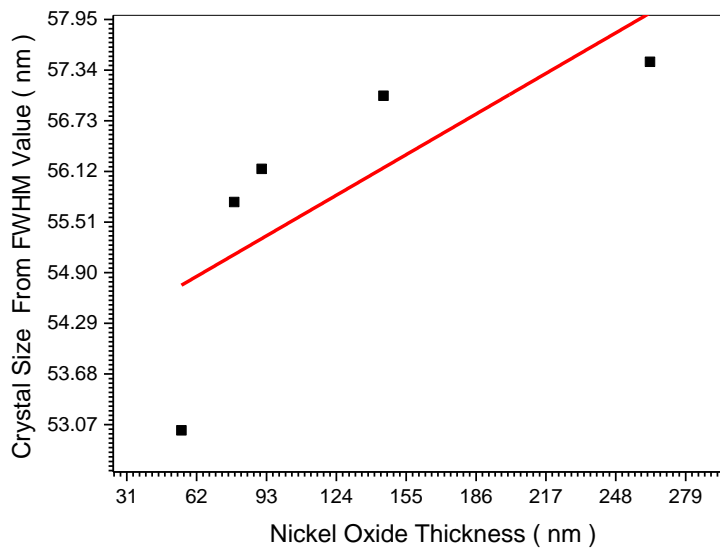


Fig (6): relationship between thicknesses and crystal size from FWHM value of five Ni₂O₃ (Nickel Oxide) sample

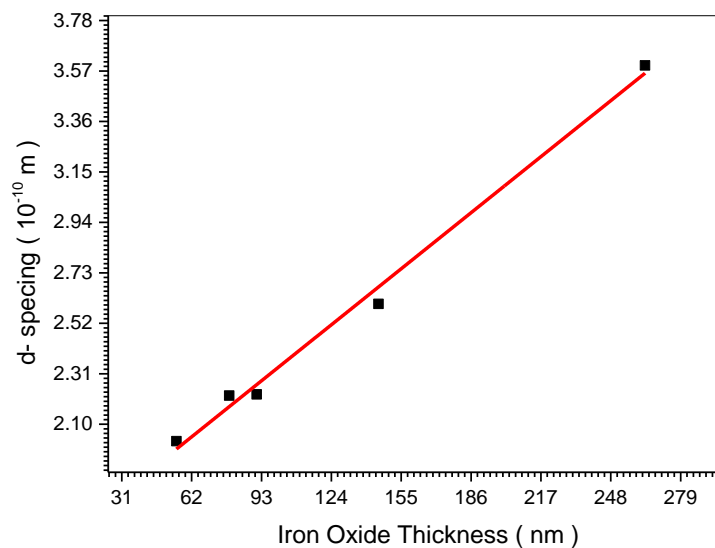


Fig (7): relationship between thicknesses and d-spacing from FWHM value of five Fe_3O_4 (Iron Oxide) sample

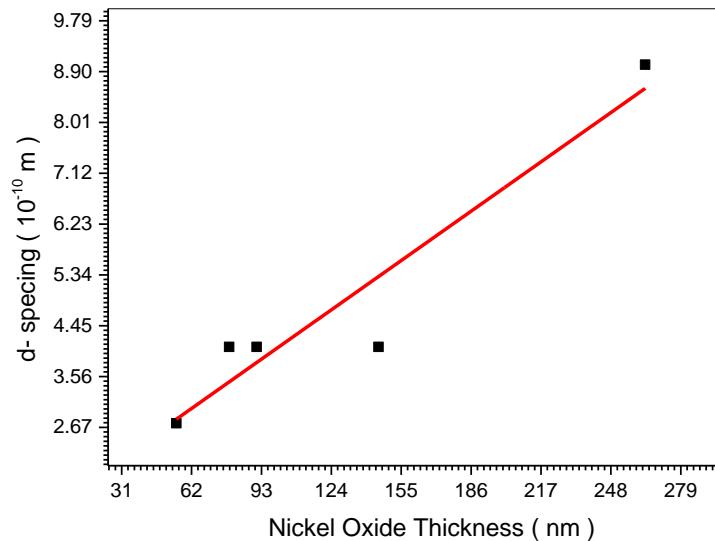


Fig (8): relationship between thicknesses and d-spacing on the five Ni_2O_3 (Nickel Oxide) sample

Discussion

The crystal structure of all samples characterized at room temperature using a Philips PW1700 X-ray diffractometer (operated at 40 kV and current of 30 mA) and samples were scanned between 10° and 80° at a scanning speed of $0.06^\circ/\text{s}$ using $\text{Cu K}\alpha$ radiation with $\lambda = 1.5418\text{\AA}$. The representative XRD charts of all samples (Iron and Nickel) Oxide as show in fig (1) and fig (2). The Miller indices of Iron Oxide are (111) at 19.14° , (220) at 31.39° , (311) at 36.96° , (222) at 38.79° , (400) at 44.96° , (422) at 55.70° , (511) at 59.4° and (440) at 65.35° major lattice planes in the XRD patterns confirms the formation of spinel (Cubic /F-Center),

(Cubic /Primitivity) and (Cubic /I-Center) } . And Miller indices for Nickel Oxide are (002) at 17.5° , (120) at 19.5° , (040) at 22.1° , (111) at 27.7° , (101) at 36.4° , (110) at 45.25° , (105) at 46.14° , (013) at 49.69° , (012) at 58.4° and (200) at 62.38° major lattice planes in the XRD patterns confirms the formation of spinel (Hexagonal/ Primitive) . All peaks for Iron Oxide crystallites with (Cubic-primitive) and for Nickel Oxide was (Hexagonal-primitive) rutile crystal structure. Table (1) and table (2) shows the XRD parameters of all (Iron and Nickel) Oxide samples at various crystalline orientations. Fig (3) and fig (4) describes the relation between thickness of (Iron and Niekcel) Oxide and density of all samples, we showing that increase the density of sample by increasing thickness of Iron Oxide samples by rat ($0.00405 \text{ mg. cm}^{-3}/\text{nm}$), and for Nickel Oxide by rate ($0.001129 \text{ mg. cm}^{-3}/\text{nm}$). The dislocation density (δ) and number of unit cells (n) of (Iron or Nickel) Oxide samples nanoparticles is calculated and listed in table (1) and (2). Dislocation density decreases and the by number of unit cells increases growth and decreasing the defects in crystallites. Fig (5) and fig (6) shows the relation between the (Iron and Niekcel) and crystallite size. On the other hand, it's noticed that the rated of (Iron and Niekcel) thickness increases with increases the crystals size by rated 0.04757 for Iron Oxide samples and 0.01577 for Nickel Oxide samples. Finally, fig (7) and fig (8) describes the relation between the thickness of (Iron and Niekcel) Oxide and d- spasing of all samples, and noticed that the rated of increasing the d- spasing of (Iron and Niekcel) Oxide samples by rated $0.00752 \times 10^{-10} \text{ m / nm}$ for Iron Oxide, but for Nickel Oxide $0.02786 \times 10^{-10} \text{ m / nm}$.

Conclusion

Crystallites with (Iron and Niekcel) Oxide samples are Cubic for Iron Oxide and Hexagonal for Nickel Oxide crystal structure. The density, crystallite size and d-spacing for Fe_3O_4 and Ni_2O_3 were shown to increase when the concentration of Nano crystal increases.

References

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