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Research Paper

Using Mathematical and Experimental Modeling To Calculate Some Physical Properties Of Iron Oxide Thin Film Synthesized By The Spray Pyrolysis Method

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ABSTRACT
This paper examines mathematical and experimental modeling to calculate some physical properties of iron oxide.the results obtained via experiments conducted on samples ofF_2O_3UV-Visible spectrophotometer was used at normal incident of light in the wavelength range of 287–447nm. to knowing how the sample responds to lightwhich obtained that the by Increase the lengthincrease value of substance absorption for the light for all films in the visible (UV) region. It was also increase the extinction coefficient by increasing wave length and it changes due the thickness. the high magnitude of optical conductivity for this sample equal (4.3x1015 sec-1) this confirms the presence of very high photo-response of the thin film.
KEYWORDS: *Thin film, Absorption, energy gap, extinction coefficient*

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I. INTRODUCTION

A mathematical model is a description of a system using mathematical concepts and language. The process of developing a mathematical model is termed mathematical modeling. Mathematical models are used in the natural sciences (such as physics, biology, earth science, chemistry) and engineering disciplines (such as computer science, electrical engineering).A model may help to explain a system and to study the effects of different components, and to make predictions about behavior, Mathematical models can take many forms, including dynamical systems, statistical models [1], differential equations, or game theoretic models. These and other types of models can overlap, with a given model involving a variety of abstract structures. In general, mathematical models may include logical models. In many cases, the quality of a scientific field depends on how well the mathematical models developed on the theoretical side agree with results of repeatable experiments.lack of agreement between theoretical mathematical models and experimental measurements often leads to important advances as better theories are developed. mathematical modeling problems are often classified into black box or white box models, according to how much a priori information on the physical theories are almost invariably expressed using mathematical models[2]

In the physical sciences, a traditional mathematical model contains most of the elements like Governing equations, Defining equations, Constitutive equationsInitial and boundary conditions , Classical constraints and kinematic equations also the application of mathematical model in Anthropology and Astronomy and Biology and in physics[3,4]The sample used in this paper is iron oxide , Iron(III) oxide or ferric oxide is the inorganic compound with the formula Fe2O3[5].It is one of the three main oxides of iron, the other two being iron(II) oxide (FeO), which is rare; and iron(II,III) oxide (Fe3O4), which also occurs naturally as the mineral magnetite. As the mineral known as hematite, Fe2O3 is the main source of iron for the steel industry. Fe2O3 is readily attacked by acids. Iron(III) oxide is often called rust, and to some extent this label is useful, because rust shares several properties and has a similar composition. To a chemist, rust is considered an ill-defined material, described as hydrated ferric oxide[6,7,8].Fe2O3 can be obtained in various polymorphs. In the main ones, α and γ, iron adopts octahedral coordination geometry. That is, each Fe center is bound to six oxygen ligands,Uses of iron oxide in industry The overwhelming application of iron(III) oxide is as the feedstock of the steel and iron industries, e.g. the production of iron, steel, and many alloys [9], also use for

PolishingA very fine powder of ferric oxide is known as "jeweler's rouge", "red rouge", or simply rouge. It is used to put the final polish on metallic jewelry and lenses, and historically as a cosmetic. Rouge cuts more slowly than some modern polishes, such as cerium(IV) oxide, but is still used in optics fabrication and by jewelers for the superior finish it can produce. When polishing gold, the rouge slightly stains the gold, which contributes to the appearance of the finished piece. Rouge is sold as a powder, paste, laced on polishing cloths, or solid bar (with a wax or grease binder). Other polishing compounds are also often called "rouge", even when they do not contain iron oxide. Jewelers remove the residual rouge on jewelry by use of ultrasonic cleaning. Products sold as "stropping compound" are often applied to a leather strop to assist in getting a razor edge on knives, straight razors, or any other edged tool [10]. Iron(III) oxide is also used as a pigment, under names "Pigment Brown 6", "Pigment Brown 7", and "Pigment Red 101".[11] Some of them, e.g. Pigment Red 101 and Pigment Brown 6, are approved by the US Food and Drug Administration (FDA) for use in cosmetics. Iron oxides are used as pigments in dental composites alongside titanium oxides.[12,13]

Hematite is the characteristic component of the Swedish paint color Falu red, Calamine lotion, used to treat mild itchiness, is chiefly composed of a combination of zinc oxide, acting as astringent, and about 0.5% iron(III) oxide, the product's active ingredient, acting as antipruritic. The red color of iron(III) oxide is also mainly responsible for the lotion's widely familiar pink color.

II. THIN FILM PREPARATION

The spray pyrolysis method used here is basically a chemical deposition method in which fine droplets of the desired material are sprayed onto a heated substrate. Continuous films are formed on the hot substrate by thermal decomposition of the material droplets.

TheIron OxideF_2O_3films were deposited onto glass slides, chemically cleaned, using the spray pyrolysis method at 170°C substrate temperature. $Fe_2SO_4.5H_2O$, NaOH, and citric acid were used in the experiments. All the reagents used were of analytical grade purity. Precursor was synthesized by adding 1M NaOH solution drop wise to 0.1M Fe_2SO_4+citric acid solution with vigorous stirring.The precipitate obtained was washed several times with de ionized water to remove possible remnant ions present in the final products and dried .Obtained product was kept at 500^{O}C for 3 hours in a muffle furnace to get the final product of CuO Nano crystalssolvent was used for all the films. The nozzle to substrate distance was 30 cm and during deposition, solution flow rate was held constant at 2 ml/min. The substrate temperature was measured using an Iron-Constantan thermocouple. The thickness of the thin films was measured by weight difference method using a sensitive microbalance. The optical measurements of F_2O_3 film were carried out at room temperature using UV Spectrophotometer in the wavelength range from 287 to 447 nm. The substrate absorption is corrected by introducing an uncoated cleaned glass substrate in the reference beam.

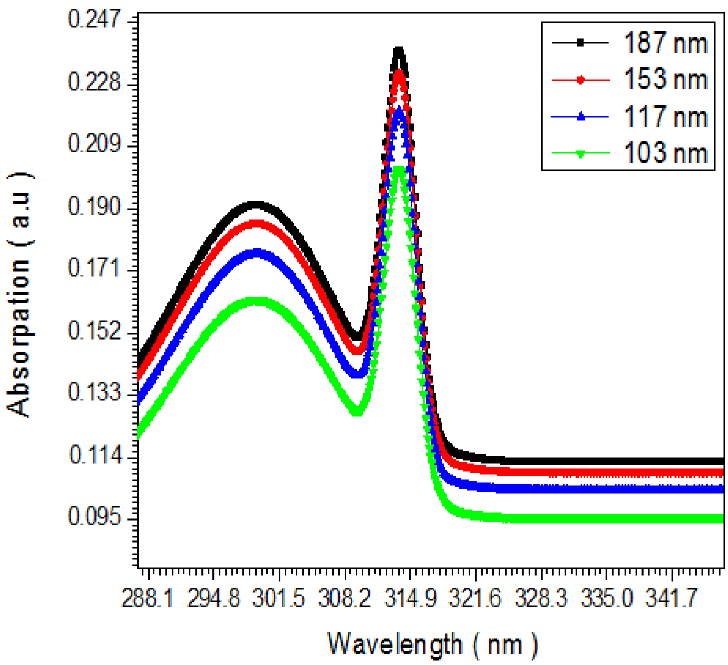

Fig (1) the optical absorption spectra of F_2O_3thin films samples

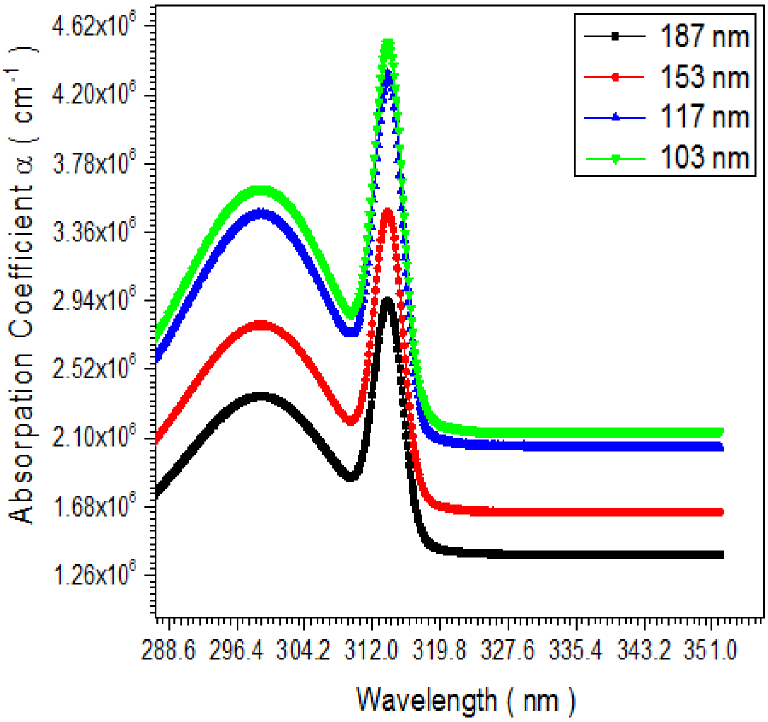

Fig (2) the variation of the Absorption Coefficient t (α) with wavelength of F_2O_3thin films

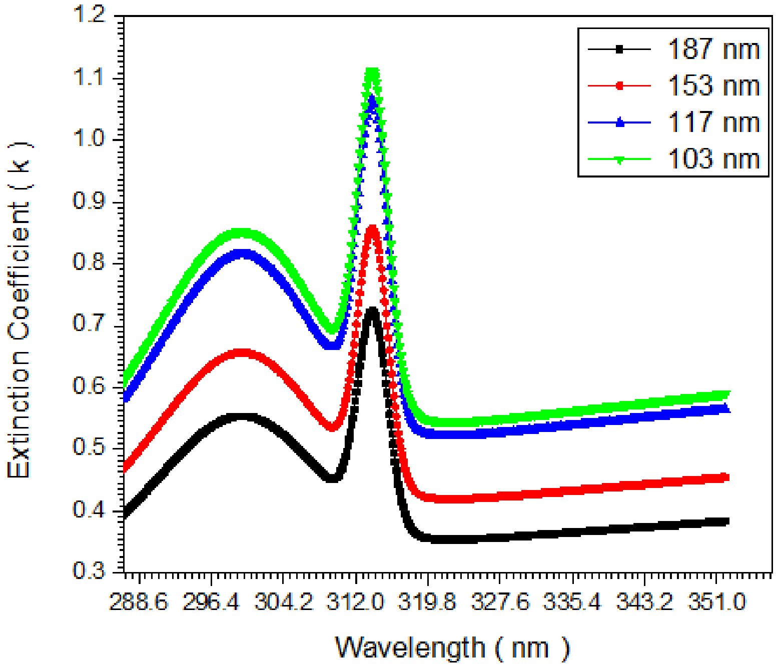

Fig (3) the Extinction coefficient (K) with wavelength (λ) for F_2O_3 thin films

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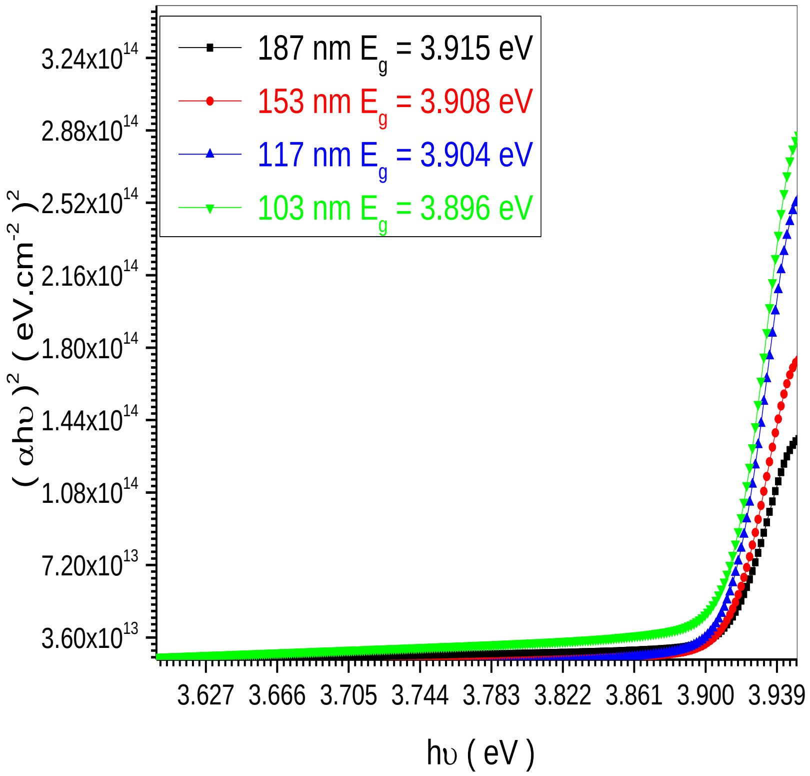

Fig (4) the optical energy gap (E_g) of F_2O_3 films samples

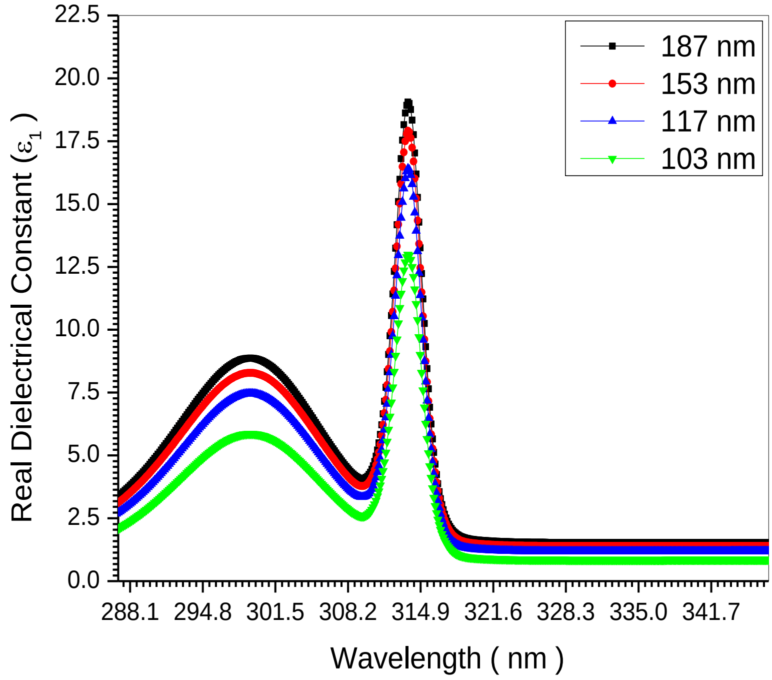

Fig (5) the variation of the real dielectric constant (ε_1) with wavelength of F_2O_3 thin films

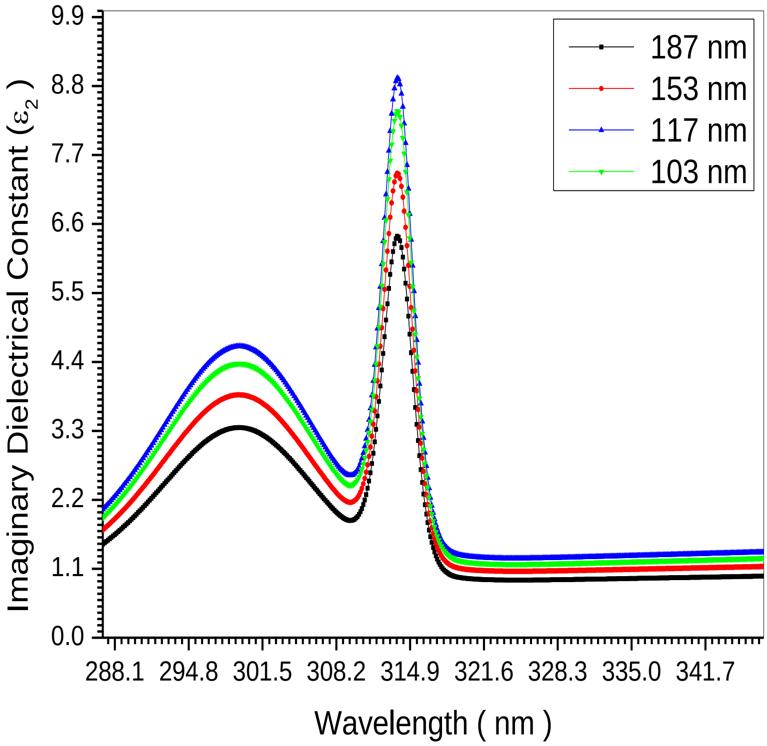

Fig.(6) the variation of the Imaginary dielectric constant (ε_1) with wavelength of Fe2 O 3thin films

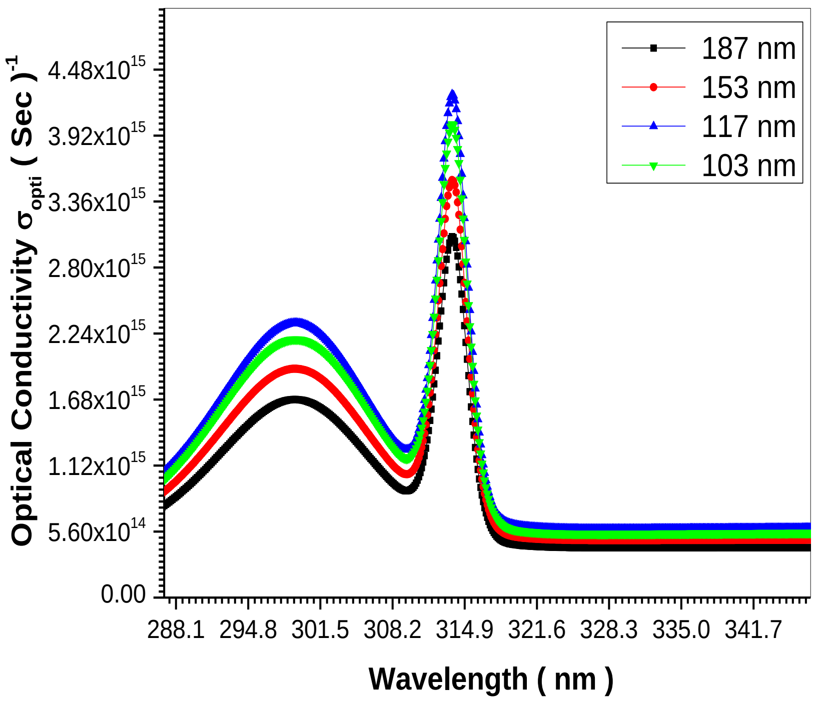

Fig (7) Plot of optical conductivity($o_{pt\sigma}$) as a function of photon energy for F_2O_3thin film.

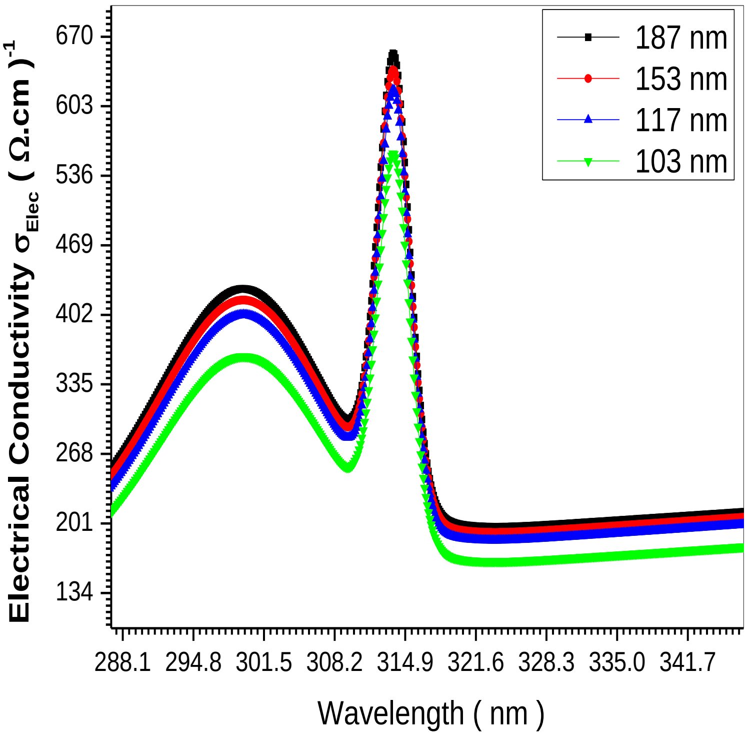

Fig (8) Plot of electrical conductivity(σ_{elc}) as a function of photon energy for F_2O_3thin film.

III. RESULT AND DISCUSSION

Determination of the optical properties of the F_2O_3

The optical absorption spectra in the (287– 447) nm wavelength range for the F_2O_3thin film are depicted in Fig (1) the maximum absorption observed at wavelength (299-314 nm) region then it decreases to (0.095a.u) at wavelength 323 nm. The absorption edge of the film occurs at wavelength (314 nm) corresponding to photon energy (3.95 eV).

The absorption coefficient, (α) is given by

$$\alpha = \frac{2.303xA}{d} \qquad (1)$$

Where (d) is the thickness of the sample and (A). In fig. (2) Shows the plot of (α) with wavelength (λ), which obtained that the value of $\alpha > 4.6x10^{6} cm^{-1}$ for all films in the (UV) region , this means that the coefficient (α) with (λ) for thin films since they are responsible for electrical conduction. Also, fig (2) shows that the value of (α) for 103 nm films are greater than 187 nm films.

The extinction coefficient of Fe2 O 3thin film is given by equation

$$k = \frac{\alpha\lambda}{4\pi} \qquad (2)$$

Where (k) is the extinction coefficient which is shown in the Fig (3) and it is noticed that the extinction coefficient has a maximum value of 1.16 at wavelength 315 nm. The extinction coefficient changesdue the thickness.

The energy band gap of these materials is determined using the absorption spectra. According to the absorption coefficient (α) for direct band gap material is given by the relation

$$\alpha h\nu = B(h\nu - E_g)^n (3)$$

Where E_g the energy gap, constant B is different for different transitions, ($h\nu$) is energy of photon and (n) is an index which assumes the values 1/2, 3/2, 2 and 3 depending on the nature of the electronic transition responsible for the reflection.

And by extrapolating the straight thin portion of the curve to intercept the energy axis, the value of the energy gap has been calculated. The value of (E_g) was (3.915, 3.908, 3.904 and 3.896) eVIt was observed that the different structures of the films confirmed the reason for the band gap shifts as show in fig (4).

Fig (5) shows the variation of the real dielectric constant (ε_1) with wavelength of Fe2 O 3thin films, which calculated from the relation

$$\varepsilon 1 = n^2 - k^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

Where the real the dielectric (ε_1) is the normal dielectric constant .From fig (5) the variation of (ε_1) is follow the refractive index, where increased in the region that λ >350nm, where the absorption of the film for these wavelength is small, but the polarization was increase. The maximum value of (ε1) equal to (19.13) for all films at wavelength near (314) nm. The effect of thickness decrease (ε_1). The imaginary dielectric constant (ε_2) vs (λ) was shown in fig (6) this value calculated from the relation:

$$\varepsilon_2 = 2nK \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

(ε_2) represent the absorption associated with free carriers. As shown in fig(6) the shape of (ε_2)is the same as (ε_1), this means that the refractive index was dominated in these behavior. The maximum values of (ε2)are different according to the thickness, so the maximum value of(ε1)for 187 nm thin film equal (19.13) at (314) nm , while ε2= 6,38 at λ = 314 nm for 187 nm thin film, these behavior related to the different absorption mechanism for free carriers. The effect of thicknessincrease (ε_2).

The optical conductivity σ_{opt} is a measure of frequency response of material when irradiated with light which is determined using the following relation,

$$\sigma_{opt} = \frac{\alpha n c}{4\pi} \qquad (6)$$

Where ***c*** is the light velocity. The electrical conductivity σ_e can be estimated using the following relation.

$$\sigma_{elc} = \frac{2\lambda\sigma_{0pt}}{\alpha} \qquad (7)$$

The high magnitude of optical conductivity ($4.3\text{x}10^{15}$ sec^{-1}) confirms the presence of very high photo-response of the thin film. The increased of optical conductivity at high photon energies is due to the high absorbance of F_2O_3thin film and may be due to electron excitation by wavelengths as it is shown in Figs (7) and (8).

IV. CONCLUSION

After calculating some of the physical properties of the sample, it was found that there is a very high response to the thin film.

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