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Synthesis And Spectroscopic Study Of Nd Doping Tetania With Many Constrations

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Abstract

The TiO_2 and Nd-TiO_2 with many concentrations was prepared in this work by sol-gel pyrolysis methodand calcination was done at 500°C.Analyses confirm that: The XRD pattern 0f prepared TiO_2 nanoparticles exhibitedan anatase crystal structure and has a minimum mean grain size, while Nd-TiO_2samples exhibted anatase and rutile crystal structures.The square root of the roughness measured by AFM showed that the doped TiO_2 sample was rougher than the other samples. UV-Vis measurements ensure that all samples spectra was in UV region and getting blue shift for all Nd-TiO_2 samples.

Introduction

Because of its great chemical stability, easy and low cost methods, and high photosynthetic activity, TiO_2, also known as titania, is widely investigated. These features make TiO_2 a good choice for a variety of useful applications, including solar cells, gas sensors, and water purification, among others [1].TiO_2 is also a promising material for biological applications due to its high biocompatibility [3].The number and type of defects, the presence of doping and the synthesis technique affect the optical properties of titanium dioxide. [5].Due to the huge band gap (3.2 eV), TiO_2 shows excellent transparency in visible/NIR light and absorbs light in the ultraviolet part of the spectrum; The UV region accounts for only 3-5% of the solar spectrum. [2].However, it has been shown that doping titania can alter its optical properties; The impregnation of TiO_2 with lanthanide ions allows excitation of the system with visible light (>400 nm), allowing a large portion of the solar spectrum to be used for Ln^{3+}–TiO_2 excitation. [4].Emission lines for various lanthanides can be seen throughout the spectrum, from ultraviolet (Gd^{3+}), visible (Eu^{3+}, Sm^{3+}), and near infrared NIR)(Nd^{3+},Er^{3+},Yb^{3+}) [1].Electronic transitions in the partially filled 4f orbitals of the lanthanide ions are responsible for the characteristic luminescence features [6].

The emission lines of lanthanides are very narrow, specific, and with long lifetimes, due to the shielded of 4f levels by the 5s and 5p levels that protect the f–f transitions from perturbations caused by the crystalline field of the host matrix. However, the intensity and width of the lines of photoluminescence depend on the host material.[8]. Bearing in mind the information above, choosing among different lanthanides and host matrices, allows the emission of the material to be adjusted for a desired application. [10].Nevertheless, using lanthanides as dopants with high concentrations produces dopant clustering and luminescence quenching , consequently for each host there is a doping limit to avoid clustering, and strategies to detect and analyze low photoluminescence intensity signals must be developed. Among the Ln3+ ions, Nd3+ has obtained particular attention, due to its singular optical and magnetic properties . [9] .It has been reported that the introduction of neodymium atoms into the TiO_2 lattice induces the formation of new sub-bandgap states below the TiO_2 conduction band, due to the properly overlap of the Nd^{3+} energy levels with the conduction band of TiO_2 decreasing the energy of the TiO_2 bandgap .[7]. Additionally, Hassan et al, reported that Nd^{3+}, compared with Ce^{3+} and La^{3+} ions, had led to a higher increase in TiO_2 photoactivity.[3]. While Silva et al. used Nd^{3+}-doped TiO_2 nanocrystals as a luminescent nanothermometer operating within biological windows .[4]. The increased interest in nanometer scale systems, such as in nanoelectronics and nanofluids, has increased the need to monitor local changes in the temperature in nanometric scales, which traditional thermometers are unable to measure.[5]. Different strategies have been developed to tackle this need, one of the most studied is luminescence nanothermometry, which is a technique that uses materials whose luminescent properties, such as luminescence intensity, bandwidth, polarization, decay time, spectral position, and band line shape, are affected by temperature [2].

Preparation

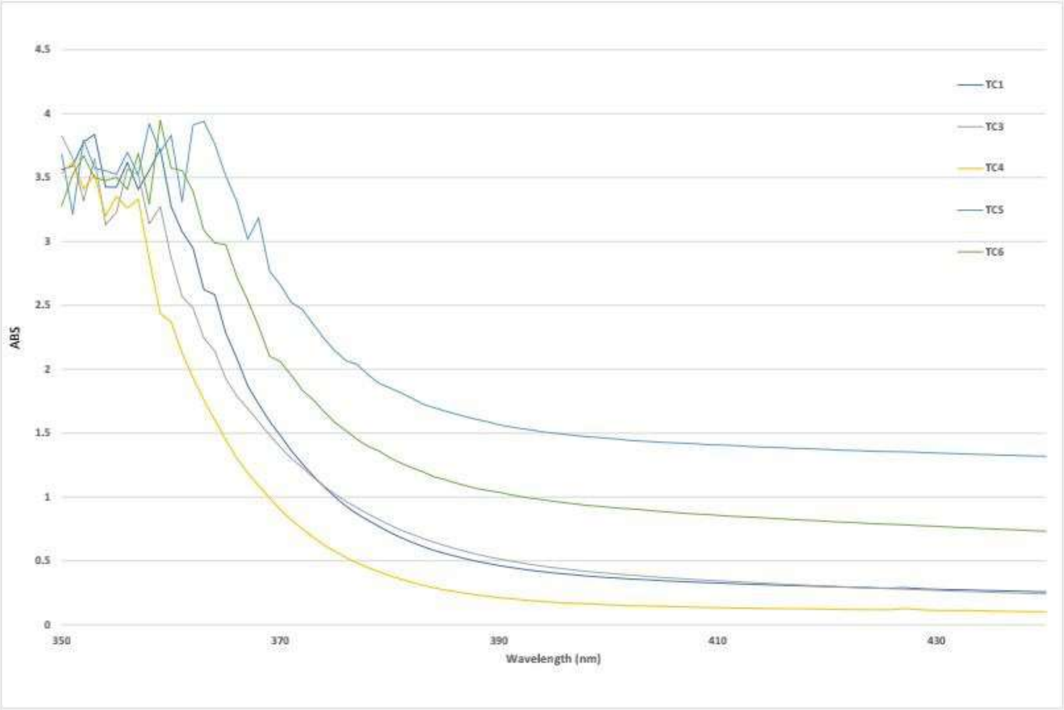
The material was prepared by adding 0.0091 mol of $TiCl_4$ with 10 mL of 1 propanol, adding 20 mL of non-ionic water and adding $NdCl_4$ at certain concentrations and the following proportions were adopted:1%, 2%, 4%, 8%, 16%.The material was sprayed on slices and then placed in afurnace at 500°C.

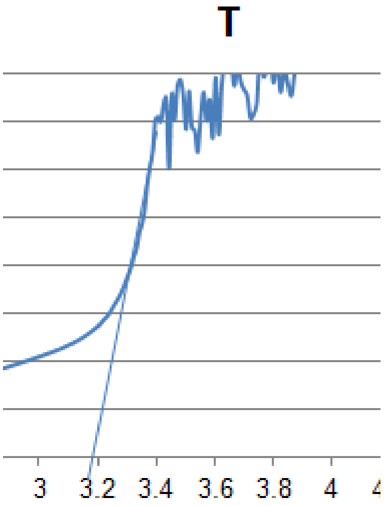
Experimental

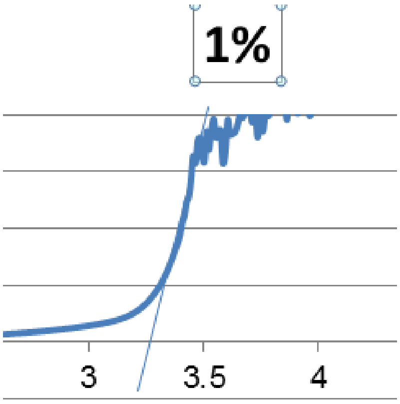
UV-Visible spectrophotometer

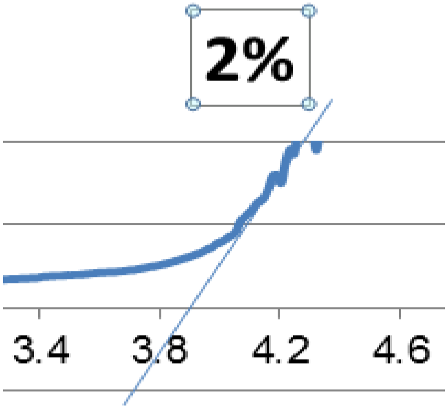
the UV-Visible absorption spectra of bare TiO_2 and Nd-doped TiO_2 samples. Figure shows the UV Visible absorption spectra of bare TiO_2 and Nd-doped TiO_2 samples

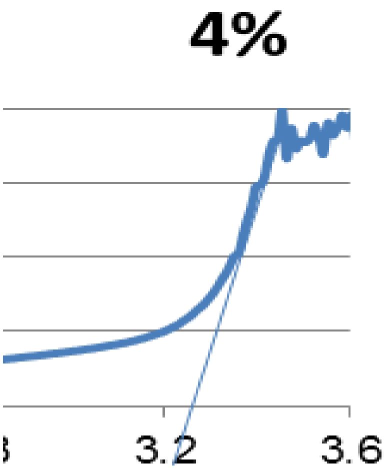
The absorption edge was blue moved as the $NdCl_3$ additive concentration increased, reaching a maximum value of 32% blue.Fig(1).

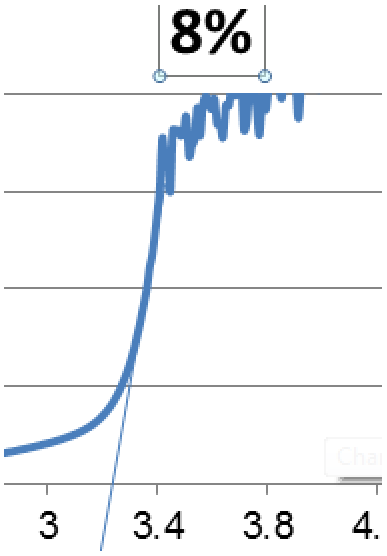


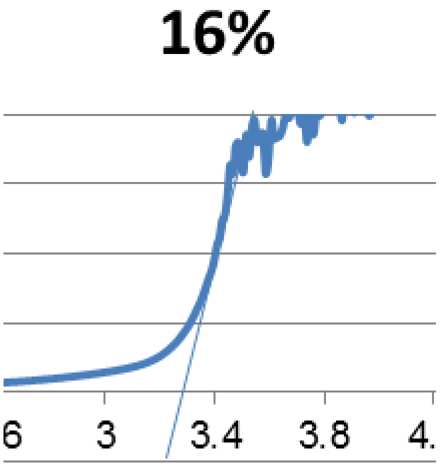












The energy gap values increased with the increase in the concentration of the substance, as shown in the following Table(1) :

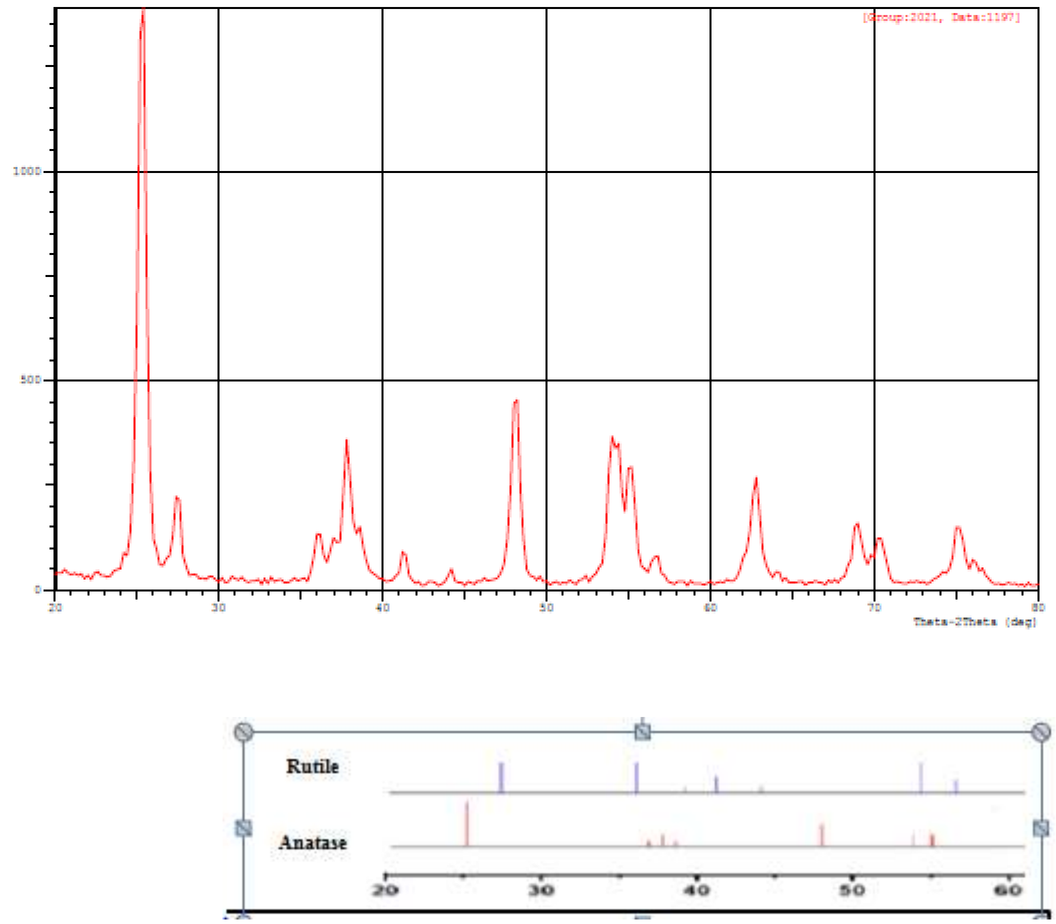
Sample	Wt %	Energy gap
T	0	3.19
TN1	1	3.22
TN2	2	3.84
TN3	4	3.33
TN4	8	3.22
TN5	16	3.32

X-Ray Diffraction (XRD)

The X-ray diffraction patterns for the optimized samples were achieved. The positions of the diffraction peaks in the films were compared with those given in ASTM data card for anatase polymorph**.**

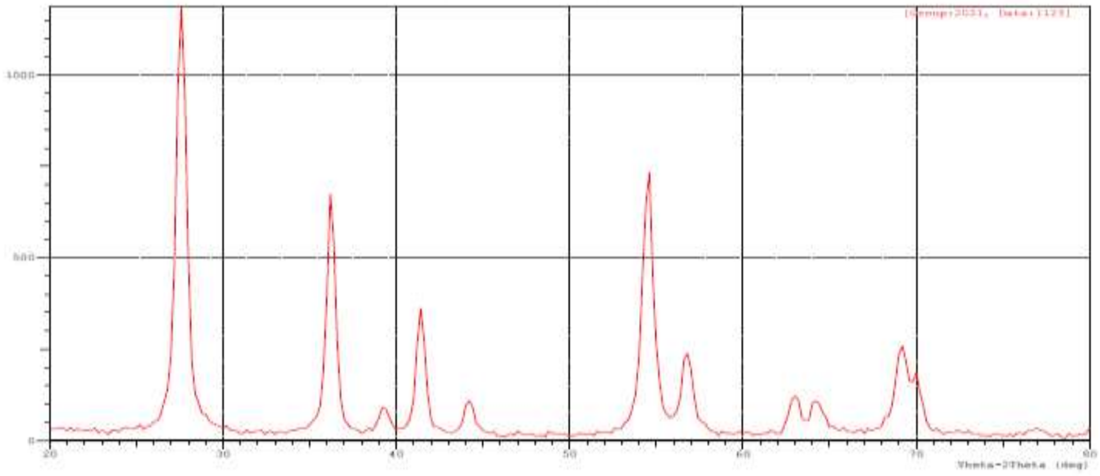
XRD pattern for the sample (T)

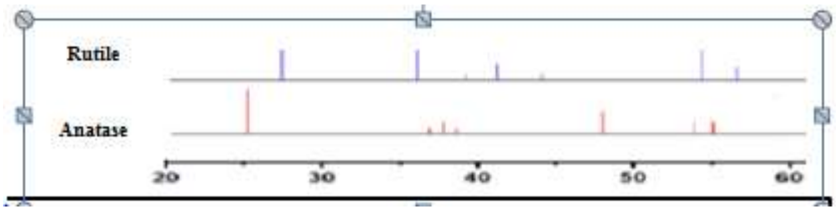
X-ray pattern for (T) sample is shown in the figure(2) . This figure shows that, the film was polycrystalline having totally anatase phase. It is observed that the film exhibited characteristic peaks of anatase crystal plane . The nearly sharp peak detected at (500 Cº) can be related to very weak .



Figure(2) XRD pattern for the sample (T)

The XRD spectrum confirms that the anatase phase is dominated in the pattern. The excess of anatase phase in TiO_2 film is favorable in photocatalyst applications . in this study, the peak fixed at (2Ө) equal to (25.14) was properly exist, this may be attributed to the, relatively, high doping.

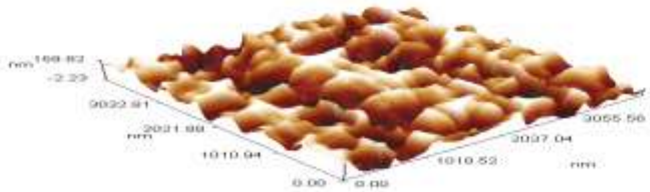




Figure(3) XRD pattern for the sample (TN)

Atomic Force Microscopy (AFM)

In order to evaluate the surface roughness and morphologies of the optimized samples for each group, atomic force microscopy technique has been used. Figures(4) show the (3D)images for pure TiO_2.



The images indicate that; the formations of fine agglomerations consist of compact nanoparticles with non-uniform grain size. Figure (5) shows the histogram of the same sample. The root mean square (rms) roughness of the film equals to (46.8nm), while .the average grain size is (40.5 nm)

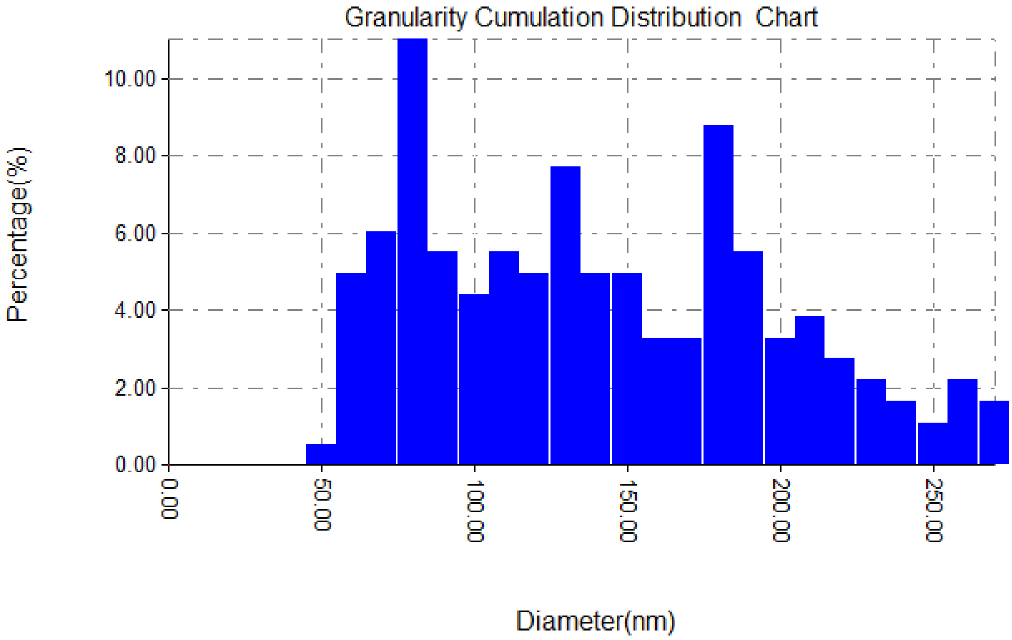
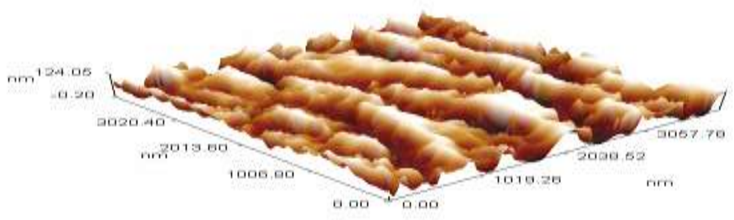
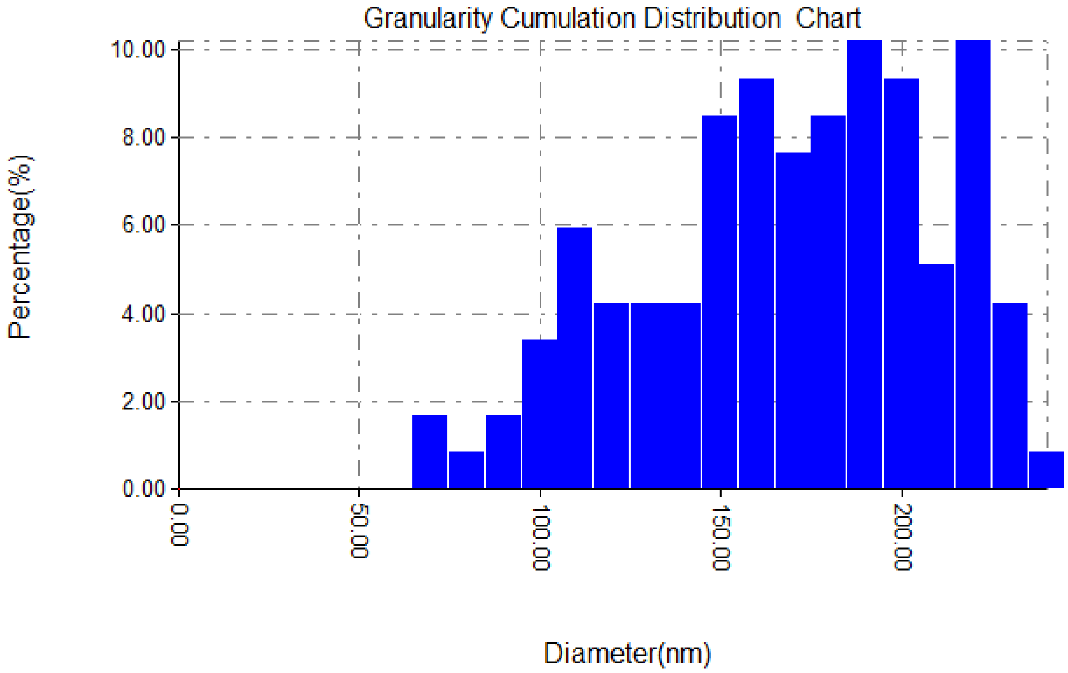


Figure (6) exhibit the surface roughness and morphologies of the optimized sample (T2). The images show that the film became smoother than previous samples; the (rms) roughness became (37nm), while the average grain size is (32.2nm)





Table(2) summarizes the values of root mean square roughness and average particle size for the optimal produced samples

Samples	Root mean square roughness (nm)	Average grain size(nm)
T	46.8	40.5
TN1	42.6	36.8
TN2	57.6	50.3
TN3	38.6	33.5
TN4	43.2	36.3
TN5	37	32.2

Conclusions

The results in this study showed that the Nd-Tio2 mixture is directly proportional to the concentration of the additive with the absorption of visible light, and this UV-visible graph was confirmed. He also proved that the higher the concentration of the substance, the lower the surface roughness, and this was proven in the AFM table.

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