INVESTIGATIONS OF ATOMIC DISORDER AND GRAIN GROWTH KINETICS IN POLYCRYSTALLINE $Gd_2Ti_2O_7$

A DISSERTATION

SUBMITTED IN PARTIAL FULFILMENT OF THE REQUIREMENTS

FOR THE AWARD OF THE DEGREE

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IN

PHYSICS

Submitted By:

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I, Ankita, 2K21/MSCPHY/04 student of M.Sc. Physics, hereby declare that the project Dissertation titled "Investigations of atomic disorder and grain growth kinetics in polycrystalline $Gd_2Ti_2O_7$" which is submitted by me to the Department of Applied Physics, Delhi Technological University, Delhi in partial fulfillment of the requirement for the award of the degree of Master in Science, is original and not copied from any source without proper citation. This work has not previously formed the basis for the award of any Degree, Diploma Associateship, Fellowship or Other similar title or recognition.

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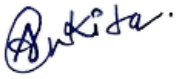

Ankita

DECLARATION

I, Ankita, 2K21/MSCPHY/04 hereby certify that the work which is presented in the Dissertation-II entitled in fulfillment of the requirement for the award of the Master in Science in **Physics** and submitted to the Department of **Applied Physics**, Delhi Technological University, Delhi is an authentic record of my own, carried out during a period from January 2023 to May 2023 under the supervision of **Prof. Vinod Singh.**

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ABSTRACT

Pyrochlores are used for a variety of purposes, including luminescence, ionic conductivity, superconductivity, high temperature thermal battery coatings, nuclear waste immobilization, electrocatalyst, automobile exhaust gas control, electrocatalyst, solid oxide fuel cell, magnetoresistance and many more. The main focus of this study was to examine how the annealing temperature & duration is influencing atomic order/disorder & growth of grains in the pyrochlore $Gd_2Ti_2O_7$. Results indicate that the sample stays in the pyrochlore phase for a relatively longer time at very high annealing temperatures. Designing pyrochlore materials for diverse energy applications may benefit from understanding how atomic order/disorder and grain development affect structural characteristics. The solid state route was used to produce $Gd_2Ti_2O_7$ via uniform heating at distinct temperature level (1100, 1200, and 1300°C) in different time periods (24h & 43h). X-ray diffraction (XRD), Raman spectroscopy, and Scanning electron microscopy (SEM) characterization techniques were performed in order to study both structural & microstructural characteristics associated with $Gd_2Ti_2O_7$. With a rise in heating temperature and time, there is a greater degree of cation-anion order. The production of bigger grains was preferred over coarsening of small grains by curvature. Hence, $Gd_2Ti_2O_7$ grains gradually expand as the heating period and temperature are raised. According to XRD and Raman spectroscopy, grain expansion largely influences the system's periodic ordering through a relaxation

through a of the microstrain and the rise in crystallite size, but there is no discernible impact on the structural ordering, particularly on anion lattice. In order to examine the cation/anion ordering & microstructural changes in pure phase polycrystalline $Gd_2Ti_2O_7$, a quantitative analysis has been given. Therefore, pure phasic GTO has been successfully created using the solid-state reaction method, which was then followed by numerous grinding and heating protocols, and it can now be applied in a variety of fields.

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Firstly, and importantly, I would like to thank my supervisor Prof. Vinod Singh, for allowing and giving us the golden opportunity to work in his Nano fabrication laboratory (NFL). Without his mentoring and unconditional support, this work would not have been possible. We would like to thank him for his valuable time and his feedback and suggestions. We sincerely thank him for his patience in correcting manuscripts and hope to carry forward the various nuances we learned during the writing process. His approach to scientific inquiry kept the joy of research alive during this thesis. Further, we would like to thank all the Ph.D. scholars in our lab to provide us healthy environment: Umang Berwal, Hemendra, Priya, Shivani and Jasveer Singh. The success of work depends upon the nature of the working environment. We also extend our thanks to all the faculty members, M.Sc. (Physics) scholars and members of the Department of Applied Physics, Delhi Technological University for their suggestions and valued support. Lastly, we would also like to thank our parents for their enduring support and for believing in us always

Place: Delhi

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Ankita

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LIST OF ABBREVIATIONS

Gadolinium titanium oxide	$Gd_2Ti_2O_7$
Gadolinium (III) oxide	Gd_2O_3
Titanium (IV) oxide	TiO_2
X-Ray Diffraction	XRD
Scanning electron microscopy	SEM
Williamson-Hall Plot	W-H Plot
Nanocrystalline	nc

CHAPTER-1

INTRODUCTION

1.1 INTRODUCTION

Ceramics are non-metallic, inorganic materials. These are made up of multiple elements. Ceramic materials can be extremely orientated to semi-crystalline, vitrified and are entirely amorphous in terms of crystallinity. Due to their varied crystallinity and the way of electron consumption in the ionic and covalent bonds, most ceramic materials function well as thermal and electrical insulators. These materials are suggested as a host for the immobilization of radioactive waste due to their exceptional radiation stability, good thermal, and mechanical qualities.

1.1.1 Pyrochlores

Pyrochlore materials have the chemical formula $A_2B_2O_7$, in which A(cation) represents trivalent ion (rare-earth) & cation B is 3d, 4d, or 5d element with 1/8th of the oxygen positions vacant.[1] Pyrochlores are ceramics with a cubic structure of the fluorite type.[2] [3] The pyrochlore structure undergoes an order/disorder transformation because of disordering in the cation and anion vacancies. As a result, many scientists are intrigued by the composition, order/disorder transition and high annealing temperature, of pyrochlore materials.[4]–[6]

1.1.2 Properties of Pyrochlores

- Pyrochlores exhibit excellent piezoelectric and ferroelectric capabilities, as well as remarkable dielectric and variable electrical properties.
- They are able to conduct cationic charges efficiently as they are ionic in nature.

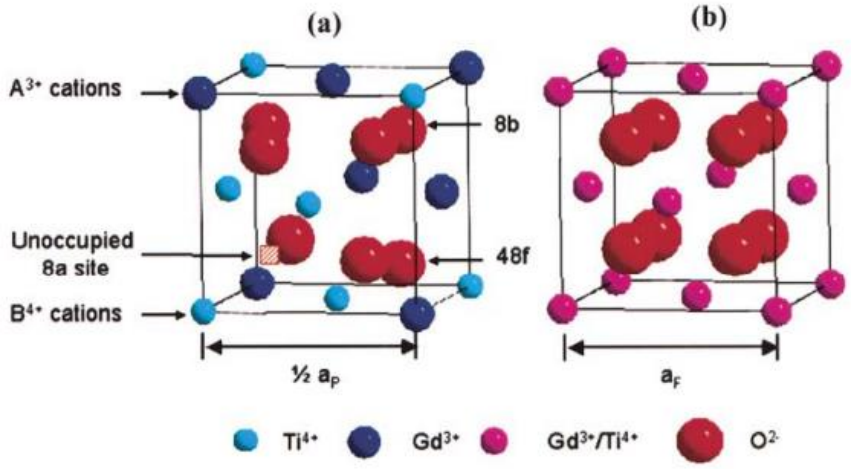

Figure 1.1. Structure of (a) unit cell of pyrochlore and (b) defect- fluorite[7]

1.2 LITERATURE REVIEW

The wide range of physical, chemical, and structural properties of gadolinium titanium oxide, $Gd_2Ti_2O_7$ makes it a technologically crucial material. It is an excellent choice for many applications due to its special qualities, including coatings for high temperature thermal barriers, rapid ion conductors, and catalysts.[8] $Gd_2Ti_2O_7$ is also a possible waste form for immobilizing actinides. For this reason, it is the main component of the current investigation. Because of the high radiation resistance of some compositions, such as $Gd_2Ti_2O_7$, pyrochlores are regarded an inert fuel matrix for actinide transmutation.[9]

[10] The kinetics of microstructural evolution as well as grain growth will significantly influence the structure, phase & physical attributes of the materials, as well as their prospective applications.

1.2.1 Grain growth in pyrochlores

Researching the grain-growth dynamics is very crucial for thorough understanding innovative materials & researching the physical and chemical aspects of pyrochlores, in addition to the atomic ordering or disordering in pyrochlore oxide. [11]Controlling grain growth is also highly helpful in pyrochlore engineering because it is a critical parameter in determining how transformable structural characteristics are.[12] [13] It's interesting to note that structural order/disorder have a substantial impact on physical & chemical characteristics of pyrochlore.[14] [15] Therefore, scientific community continues to make significant efforts to understand order/disorder & grain-growth dynamics in pyrochlore structure.[16] [17]

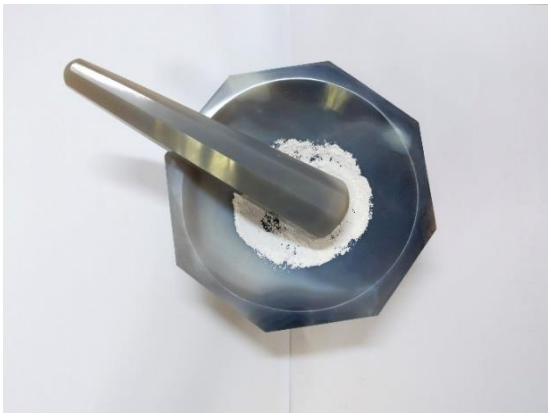

Figure 1.2. Solid state method used to form powered $Gd_2Ti_2O_7$

1.2.2 Types of grain growth

Furthermore, grain growth presents a substantial opportunity for improving radiation-resistant structural materials.[18] Catalytic activities, Ionic conductivity & the capacity to

confine radionuclides are physicochemical features that are influenced by atomic ordering/disordering & grain size.[19] There are two types of grain growth processes: abnormal grain growth & regular grain growth. [10] [20] In general, the usual grain-growth process was preferred by micro-crystalline materials.[21]Rotation and Grain boundary migration/diffusion are driven by curvature during regular grain growth. However, in the case of anomalous grain growth, a bimodal grain size distribution is created when a few energetically advantageous grains grow quickly inside a framework of fine grains.[14] [22] The aggregate crystallites' average grain size grows during the grain growth phase, which reduces the total grain border area and lowers the system free energy.[3][23] Microcrystalline materials show a typical process of grain development.[24] Some grains develop abnormally quickly in comparison to the other grains because of greater atomic mobility near the grain boundaries.[8] [25]This influence is usually noticeable because impurity atoms or defects are present at point of contact.[26] During the synthesis of nanocrystalline-materials utilizing a variety of processes such as spray pyrolysis, sintering & pulsed laser deposition, grain development with extremely low activation energies was also noticed.[6] [27] [28]

Figure 1.3. High Temperature Furnace

Lattice parameter & grain boundary velocity are inversely related.[17] The disorder-order transition phenomena that influences grain development of sample happens during annealing process.[13] [29] Increasing the annealing temperature results in a greater degree of cation order.[30] [31]The $A_2B_2O_7$ pyrochlore structure undergoes an order-disorder transformation which results from the disordering in cations & anion vacancies in the A and B-sites.[20] As annealing temperature and time are increased, atomic order/disorder and grain size also grow.[32] According to experimental findings, the sample spends more time in the pyrochlore phase at higher annealing temperatures.[33] [34] Disorder on the Anion sublattice serves to enhance the quantity of mobile oxygen vacancies by forming Frenkel defects.[9] [35] According to recent modelling findings, cation disorder improves ionic conductivity by raising the concentration of mobile charge carriers and individual mobility.[18] [36]

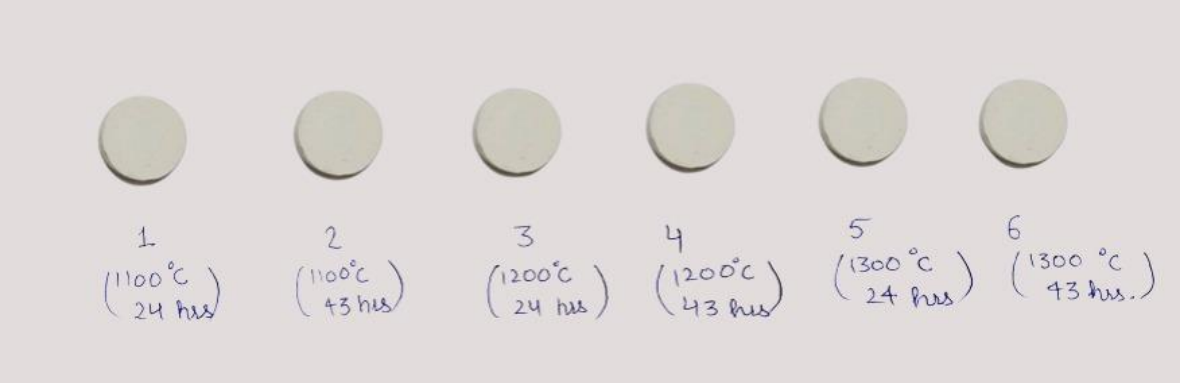

Figure 1.4. $Gd_2Ti_2O_7$ pellets

It might be difficult to gauge the degree of chaos in pyrochlore compounds.[37] [38] Two subsets of patterns make up XRD patterns. The fault fluorite structure, which is present

in all materials regardless of order, gives rise to the first set. [18] [39]The pyrochlore superstructure is responsible for the second subset.[40] Calculating the cation order parameter using the ratio of peak intensities of pyrochlore to fluorites tends to be a standard technique for determining the degree of disorder.[41] However, even in a completely ordered material, the superstructure peaks are far weaker than those of the fluorite phase, and they decline quickly with increasing disorder.[42] As a result, determining order clearly from XRD data alone is challenging. The potential for locally ordered phases in a matrix to exhibit long-range disorder, or vice versa, further complicates structural investigation in polycrystalline materials.[43] [44]

Because of their superior thermodynamic qualities and high-temperature stability under ion irradiation, ceramics having pyrochlore type structure are also a promising contender regarding inert matrix fuel applications.[45] In general, pyrochlore oxides which are basically insulators, heat transport through electronic conduction is almost negligible, and heat transport occurs at high temperatures.[46] According to varied ranges of temperatures, the heat transport in an insulator is mostly caused by the phonon contribution using various scattering events.[47] At low and intermediate temperatures, defect and boundary scattering controls heat transfer; at high temperatures, the phonon-phonon scattering takes control.[48] When compared to similar single crystal materials, nanocrystalline materials have reduced thermal conductivity because of the presence of numerous grain boundaries, which are thought to represent an obstruction to the transfer of heat.[19] [49]

There aren't many published research that discuss how binary oxides, thermoelectric materials, and semiconductors' thermal conductivity varies with grain size.[33], [50] However, it is reported that in pyrochlore, the thermal conductivity is affected by the substitution and cationic mass at very low temperatures.[5] Due to which, it's necessary to

better understand the thermal characteristics of pyrochlore-structured ceramic at room temperature as well as the impact of various scattering mechanisms.[9] [51] This study basically used a solid-state reaction method to create $Gd_2Ti_2O_7$ and studying its atomic ordering/disordering & grain growth dynamics.[52] Designing novel materials regarding technological purposes may benefit from knowledge of the atomic ordering/disordering & grain-growth dynamics.[53]

1.2.3 Applications of pyrochlores

- High permittivity ceramics
- Thermistors
- Thick film resistors for screen printing
- Switching elements
- Oxygen Electrodes
- Radioactive Waste Disposal
- Semiconductor Electrodes for Solar Energy Conversion
- Solid Electrolytes

1.3 OBJECTIVE

- The major aim for this study is to determine how the annealing temperature and time affect the atomic order/disorder and grain development in the pyrochlore $Gd_2Ti_2O_7$.
- Mostly at very high annealing temperatures, the sample is in the pyrochlore phase for a disproportionately longer period of time.

- This study is done in order to understand how atomic order/disorder and grain formation affect structural features which may be useful when designing pyrochlore materials for various energy applications.
- In this paper I've created $Gd_2Ti_2O_7$ using the solid state method by uniformly heating the material at specific temperatures (1100, 1200, and 1300°C) for various lengths of time (24 & 43 hours).
- To study the structural & microstructural properties of $Gd_2Ti_2O_7$ I've used X-ray diffraction (XRD), scanning electron microscopy (SEM) and Raman spectroscopy characterisation techniques.

CHAPTER 2

MATERIALS AND METHODOLOGY

2.1 MATERIALS

Gadolinium (III) oxide (CAS No.: 12,064-62-9, 99.9% purity) and Titanium (IV) oxide (CAS No.:1306-38-3, 99.9% purity). Without further purification, all chemicals were used.

2.2 METHODOLOGY

Grinding a stoichiometric mixture of high purity Gd_2O_3 and TiO_2 using a solid-state reaction route yielded pure phase $Gd_2Ti_2O_7$ samples. The majority of lanthanide sesqui-oxides are extremely sensitive to H_2O and CO_2 in the atmosphere. To assure the retention of intended stoichiometry, the starting chemicals i.e., the existing hydroxides and carbonates were eliminated by mixing Gd_2O_3 and TiO_2 for an hour at 700°C. Following that, a 6g batch of the precursors (Gd_2O_3 and TiO_2) was mixed and grinded for about 7 hours to ensure uniformity and homogeneity in our sample. Using a steel die set and 6t pressure, pellets of 10mm diameter were formed. At varying heating temperatures((a) 1100, (b) 1200 and (c) 1300°C) prepared pellets had been annealed in air for 24 hours and 43 hours. Figure 2.1. illustrates each step of this process in detail.

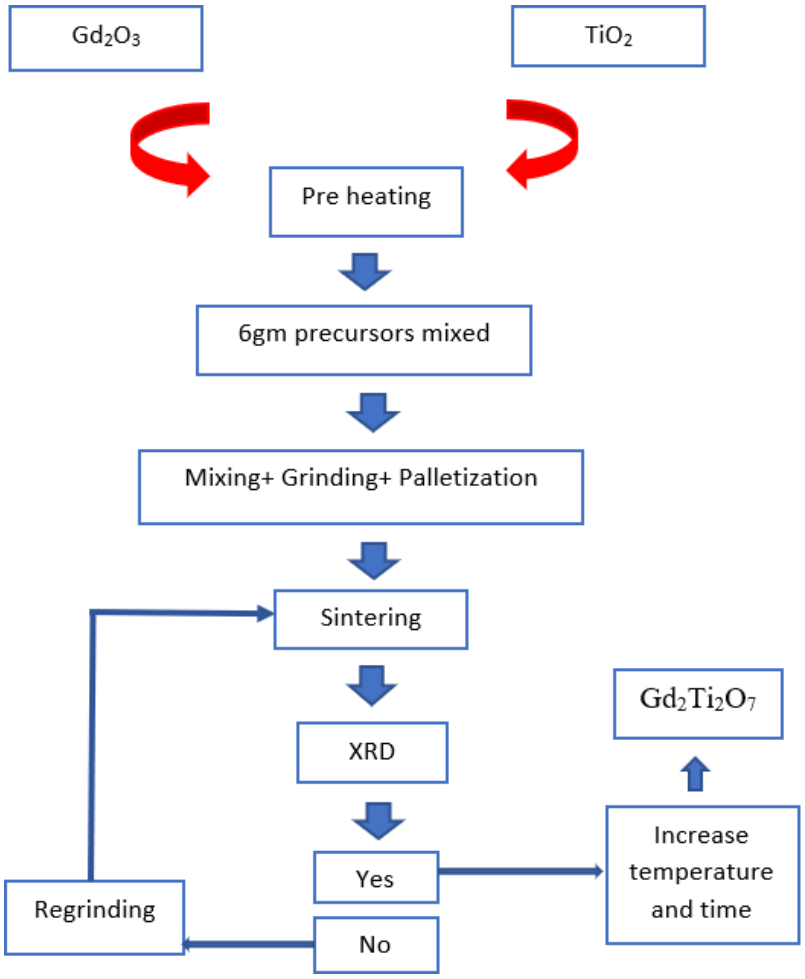

Figure 2.1. Schematic diagram exhibiting solid-state reaction to yield $Gd_2Ti_2O_7$ pyrochlore

CHAPTER 3

CHARACTERIZATION TECHNIQUES

3.1 X-Ray Diffraction

Using the X-ray diffraction, structural analysis of the sintered pellets at various temperatures (1100, 1200 and1300°C) for different annealing time (24 and 43 h) was examined at JNU, Special Centre for Nano sciences, New Delhi. On an XRD machine, Rigaku Diffractometer (Mini flex 600, Japan) the XRD structures of the pellets were captured with at 1° /min in 10°-80° range having Cu diode with Kα radiation of λ = 1.5406A°. X-ray diffraction analysis (XRD) gives precise details of crystallographic structure, physical characteristics and chemical constituents of materials. Basically, XRD is based on constructive interference and incident monochromatic X-rays which are basically electromagnetic radiations having shorter wavelengths, produced due to deacceleration of electrically charged particles having enough energy. In X-ray diffraction, generated X-rays are directed at the sample where the interaction of sample with these incident rays produces diffracted ray which is firstly detected, then analyzed, and then recorded. Sometimes due to the presence of defects the pattern of the diffracted signal can also change. Hence these imperfections are due to the sample's composition, microstrains, crystallite size and even the defects in the crystal structure.

Figure 3.1. XRD machine, Rigaku Diffractometer (Mini flex 600, Japan)

3.2 Raman Spectroscopy

At 532nm excitation wavelength the Raman spectra for each pellet using a Raman analyzer (Enspectr R 532) at JNU, New Delhi was recorded. Raman spectroscopy gives details about phase, crystallinity, morphology, chemical structure and even the molecular interactions. It is a method of scattering of light where a molecule disperses incident light which is coming from a laser light source. When the scattered light has same wavelength as laser light source then it is known as Rayleigh scatter. Whereas when little amount of the incident light is scattered at different wavelengths due to the chemical composition then it is called Raman scatter. The Raman spectrum displays peaks which displays the strength of these peaks at different scattered wavelengths.

Figure 3.2. Raman analyzer (Enspectr R 532)

3.3 Scanning Electron Microscopy

Scanning electron microscopy (SEM-JSM-IT 200, JEOL), at JNU, New Delhi, was used to examine each and every final sintered pellet. SEM creates high resolution images of the sample by scanning via surface using electron beams and making high resolution enlarged images. The electron beam is fired by an electron gun and then passes through the column of microscope where these are focused as they move down through the lenses and apertures. No atoms can interact with this electron beam in the microscope column due to vacuum. SEM ensures images of high quality which provides detailed information of topography, morphology and composition of the sample.

Figure 3.3. Scanning electron microscopy (SEM-JSM-IT 200, JEOL)

CHAPTER 4

RESULTS AND DISCUSSION

4.1 X-Ray Diffraction Analysis

Figure 4.1. displays (a)XRD pattern for the entire series of $Gd_2Ti_2O_7$ milled for approximately 7 hours using a mortar pestle. W-H Plot of $Gd_2Ti_2O_7$ at various temperatures for different annealing time- (b)1100 (24hr) (c)1100 (43hr) (d)1200 (24hr) (e)1200 (43hr) (f)1300 (24hr) (g)1300 (43hr). The milled powder is amorphous in nature, according to the nanopowders XRD pattern. The ball milled nanopowders showed no impurity peaks from residual chemical compounds, proving that all of the reagents were evenly combined. Crystallite size, Strain and Lattice constant of the samples annealed for various time interval (24hr and 43hr) is depicted in the Table 4.1. XRD study has been carried out to investigate grain development and its effects on the structural characteristics of polycrystalline $Gd_2Ti_2O_7$. The sample exhibit unit cell parameter as 9.937598 A° which is calculated and demonstrated in Table 4.1. using XRD data. Because pyrochlore superstructure peaks are seen due to additional allowed reflection conditions, the intensity of these peaks was very low in accordance with the results presented.

There is a rise in peak intensity and alteration in diffraction peak intensity towards high angles is seen due to increase in the temperature. The XRD peaks' full width at half maximum (FWHM) significantly decreased, indicating grain growth brought on by high temperature annealing. Williamson- Hall analysis was used in order to determine crystallite

size & micro-strain of annealed samples. Computed crystallite size for samples that were heated at 1100, 1200 and 1300°C for various time intervals is shown in Table 4.1. During annealing, temperature-induced grain growth caused an increase in crystallite size.

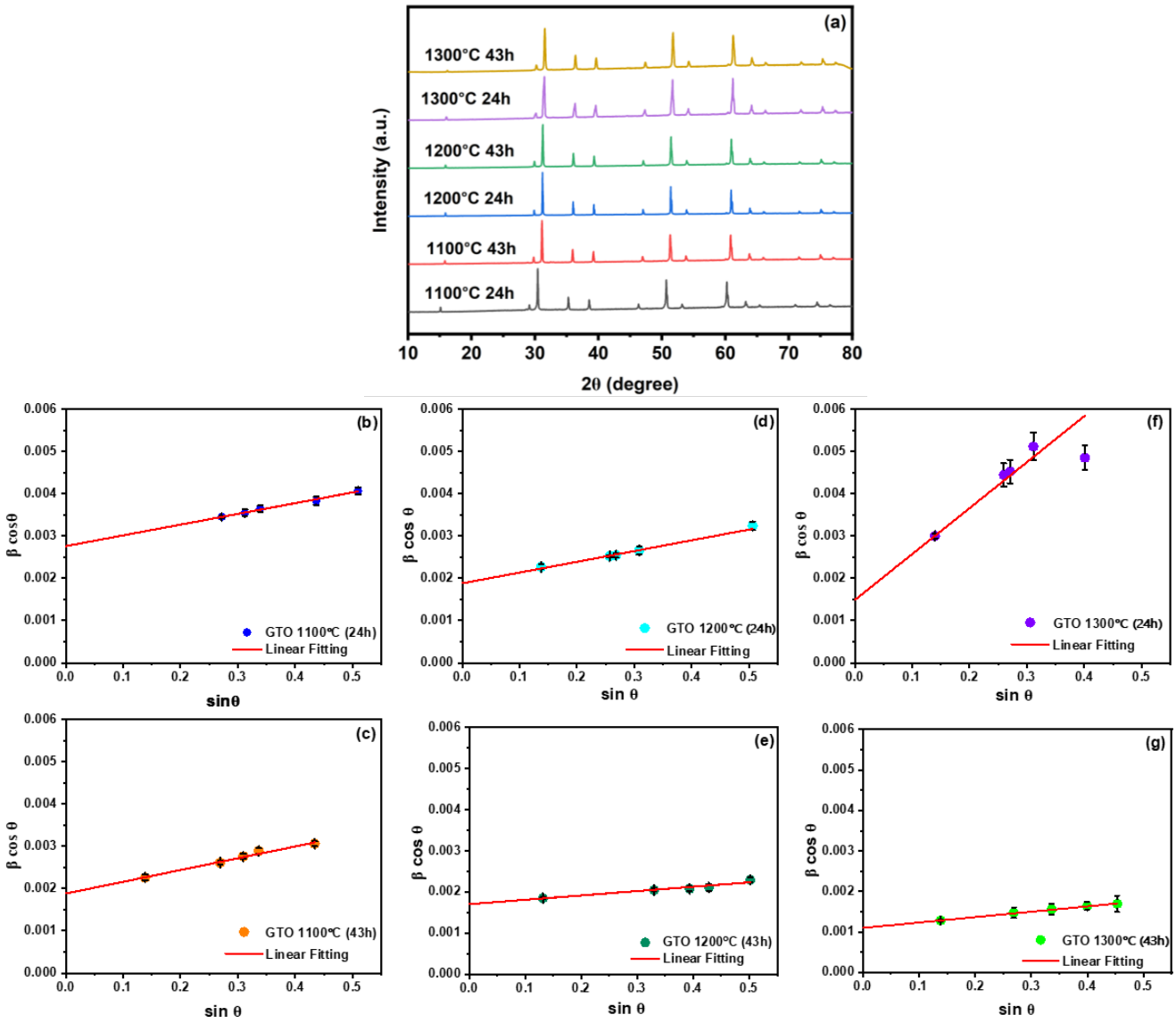

Figure 4.1. (a)XRD pattern for entire series of $Gd_2Ti_2O_7$, W-H Plot of $Gd_2Ti_2O_7$ at various temperatures for different annealing time (b)1100 (24hr), (c)1100 (43hr), (d)1200 (24hr), (e)1200 (43hr), (f)1300 (24hr) and (g)1300°C (43hr)

Table 4.1. Structural variables calculated for $Gd_2Ti_2O_7$ at various temperatures for different time intervals using XRD results.

Temperature (˚C)	Time (hr)	Intercept	Slope	Crystallite size (A°)	Strain	Lattice Constant(A°)
1100℃	24hr	0.00276	0.00254	524.6834783	0.000265	10.16468798
	43hr	0.00188	0.00279	770.28	0.002715	9.950875689
1200℃	24hr	0.00182	0.00280	810.37	0.0003325	9.927795625
	43hr	0.00171	0.00368	846.8575439	0.000475	9.913683901
1300℃	24hr	0.00149	0.01086	971.8969128	0.000635	9.852264018
	43hr	0.0011	0.01178	1316.478545	0.0006975	9.816281546

4.2 Raman Spectroscopy Analysis

To determine the impact of temperature for different time intervals on the sample, the Raman spectra for samples with temperature ranges for annealing i.e., (a) 1100, (b) 1200 and (c) 1300°C at different time intervals (24 hr and 43 hr) were compared. The entire series of $Gd_2Ti_2O_7$ sample's Raman spectra, which were recorded in the 150-750 cm^{-1} wavenumber range, are consistent with the earlier findings. It illustrates that with the increase in annealing time the position of Raman active modes remains unchanged. As a result, XRD and Raman spectroscopy indicates that the system's long-range order is affected by the grain growth primarily through micro-strain relaxation and crystallite size expansion, whereas its effects on structural ordering, particularly on anion lattice, did not seem to be particularly significant. Raman spectroscopy, which we employed to further our research, showed structural alterations brought on by a shift in oxygen's location in the anion sublattice. Theoretically, the $Gd_2Ti_2O_7$ pyrochlore exhibits six Raman active mode of vibration as a result of oxygen

vibrations at the 48f and 8a sites. O-Gd-O bond bending causes the two most noticeable Raman bands i.e., T_{2g} (310 cm^{-1}) & E_g, to appear. Another strong band which is A_{1g} (520 cm^{-1}) attributed to Gd-O stretch through the vibration in 48f (O) which is over <100> cubic axes has been given the oxygen position parameter (x). The intensities of the other four bands are weaker. 3 of the other 4 weak bands- at 212, 545 & 680 cm^{-1} were discernible. Raman active modes associated with Ti-O stretching are frequently not seen at lower wavenumbers because of Ti-O bond's short bond length. The Raman spectra can be used to estimate the blue shift in the pyrochlore, as shown in Figure 4.2. In Figure 4.2, Raman spectra for materials that were annealed for 24 and 43 hours at temperatures of 1100, 1200 & 1300°C are compared.

In as-sintered sample, O-Gd-O bond bending caused four T_{2g} modes to appear at wavenumbers- 200, 308, 320 & 450 cm^{-1}, while the Gd-O stretch caused 1 A_{1g} mode to appear at wavenumber- 516 cm^{-1}. The existence of theoretically predicted modes lends additional support to the XRD findings that the as-sintered sample of Gd2Ti2O7 formed an ordered pyrochlore structure. These peaks might contribute to Raman active modes of Ti-O because of the tight Ti-O length (1.8 A°), which was expected to occur at an elevated frequency range. The position of the Raman active modes during high temperature annealing remained constant as the annealing temperature changed. This demonstrates that during heating, $Gd_2Ti_2O_7$ does not change into a defective fluorite structure. The effect of annealing temperature was better understood through examination of the ratio of intensity (T_{2g}/A_{1g}) of the major peaks. The T_{2g}/A_{1g} ratio scarcely changes with annealing temperature, proving that the oxygen position is unaffected by rising annealing time intervals for specific value of heated temperature. To examine the impact of heating at different time, Raman spectra for

materials that undergo annealing at temperatures of (a) 1100, (b) 1200, & (c) 1300°C for varying periods (24hr and 43hr) were analyzed. Figure 4.2. displays the results for comparison. It illustrates that when the annealing time increases, the positioning of Raman active modes stays unchanged. The illustration of intensity ratio (T_{2g}/A_{1g}) further exemplifies how negligible the annealing period affects the end result. As a consequence, grain expansion impacts the system's long-range order through an increase in crystallite size & a decrease in micro-strain, but has no discernible effect on the structural ordering, especially on the anion lattice which is supported by XRD and Raman spectroscopy.

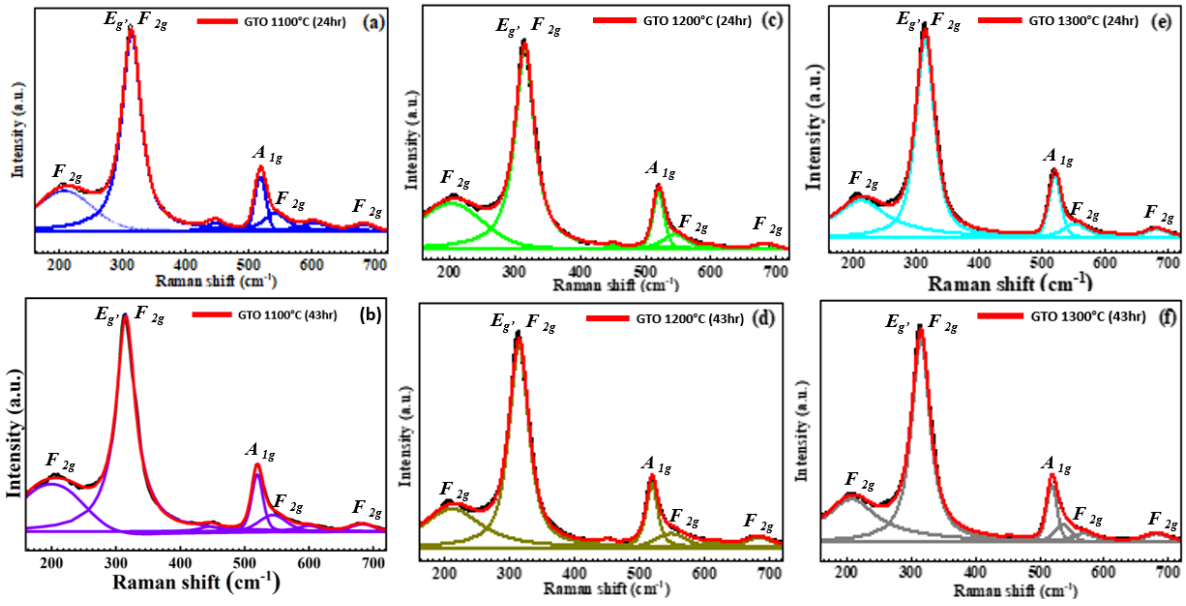

Figure 4.2. (a-f) Raman spectra for entire series of Gd2Ti2O7 at various temperature for different annealing time

4.3 Scanning Electron Microscopy Analysis

SEM images of milled samples show another characteristic of hand milling of micro sized particles which contains nano sized granules. Figure 4.4. shows the systematic SEM

micrographs of $Gd_2Ti_2O_7$ at various temperature for different annealing time i.e. (b)1100 (24hr), (c)1100 (43hr), (d)1200 (24hr), (e)1200 (43hr), (e)1300 (24hr) & (f)1300°C (43hr). The manual milled powder containing micron-size particles including nano-sized granules results in another characteristic of pyrochlores, as seen in SEM images of milled samples. According to SEM data, the average grain sizes were 400-1000 nm, greater than the samples made from milled powder, indicating that grain growth occurred during the sintering process. As heating temperature rose to 1100-1300°C, microstructures were made up of homogenous grains and the average grain size increased which was determined using SEM data. It was found that heating at 1100°C produced a large number of evenly distributed pores along with an increment in grain size.

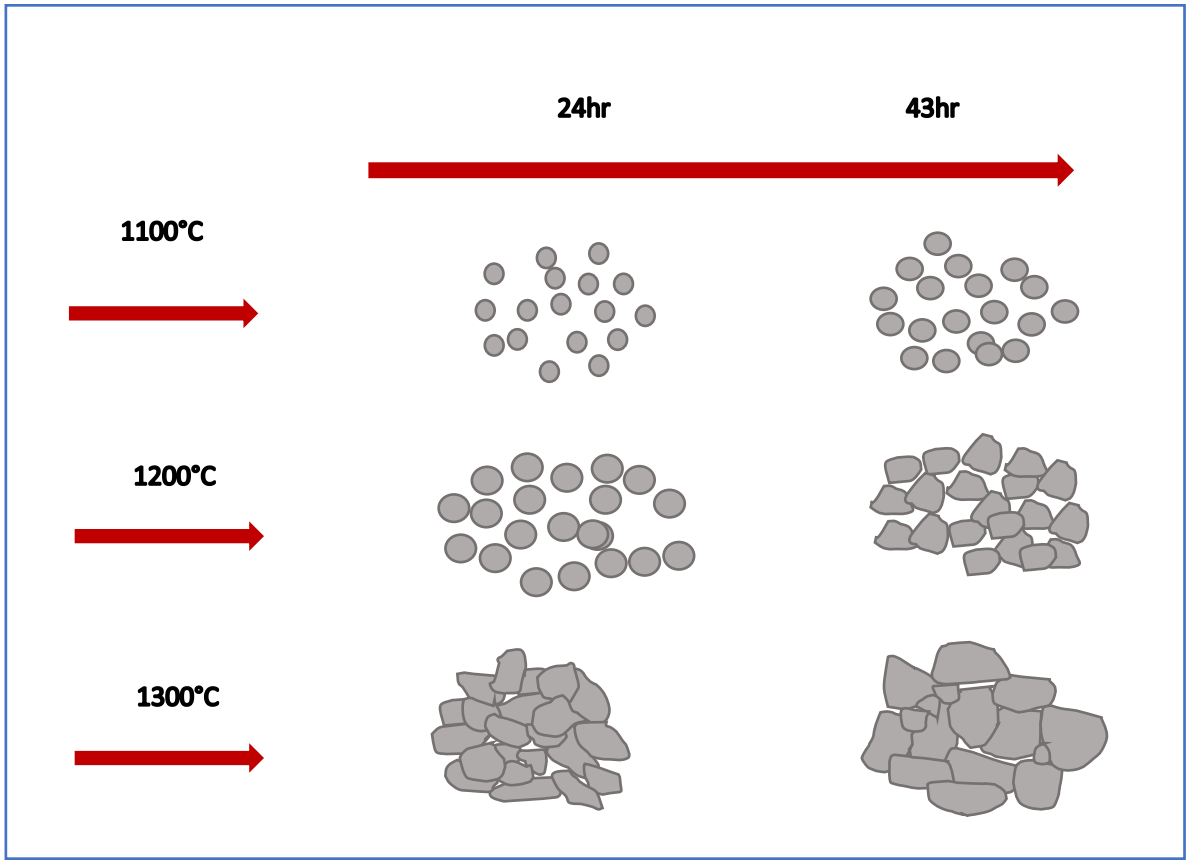

Figure 4.3. Schematic diagram representing grain growth in $Gd_2Ti_2O_7$ at different heating temperatures and time.

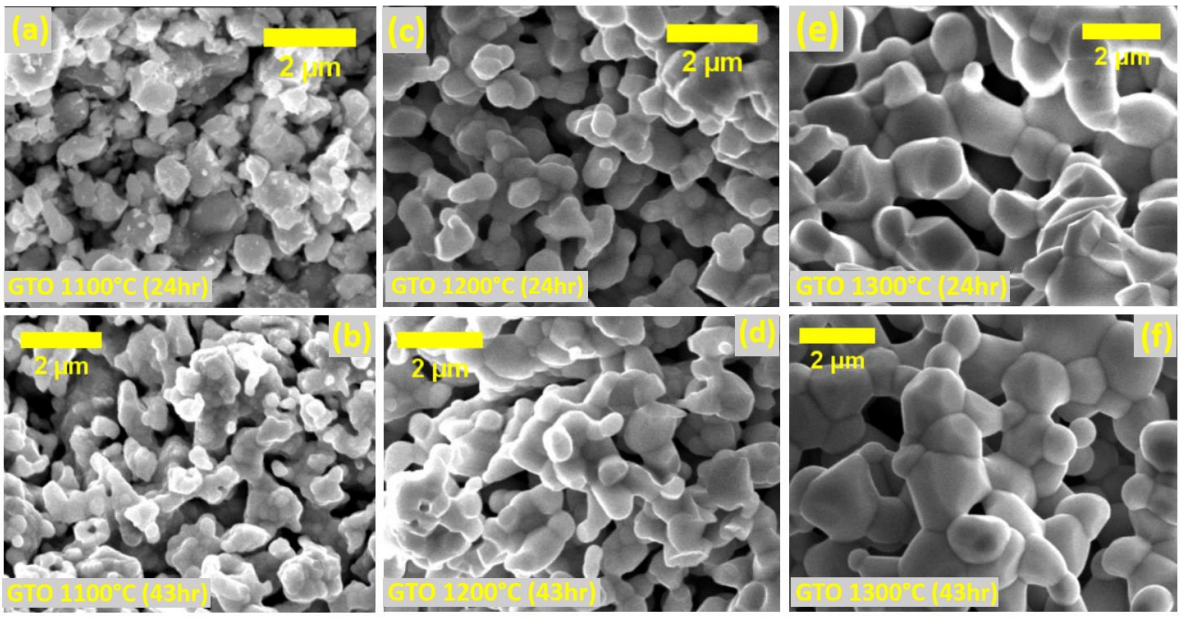

Figure 4.4. Systematic SEM micrograph of $Gd_2Ti_2O_7$ at various temperature for different annealing time

Micron sized porosity were produced at grain boundary and triple crossing due to sintering of the pellets synthesized initially, which contains accumulated crystals having wide size variation. When heating temperature raised about 1200°C, then the grain size rose, while density of pores of micron sized reduced. Pore aggregation results in an increase in pore size. Dense granules have been produced as a result of raising the annealing temperature to 1300°C. Figure 4.4. depicts micrographs of nc-$Gd_2Ti_2O_7$ specimens that have been annealed at 1100, 1200 & 1300°C respectively at 24 and 43hr, to examine the effect of different time intervals on grain development. As anticipated, grain size is enhanced as heating time increases. This further highlights how temperature effects can be felt even for different heating times. To further understand how heating time and temperature affect grain growth, grain size had been measured using SEM micrographs of each sample. It should be noticed that the SEM observed grain size is larger than the XRD estimated crystallite size. This is because grains are made up of multiple crystallites.

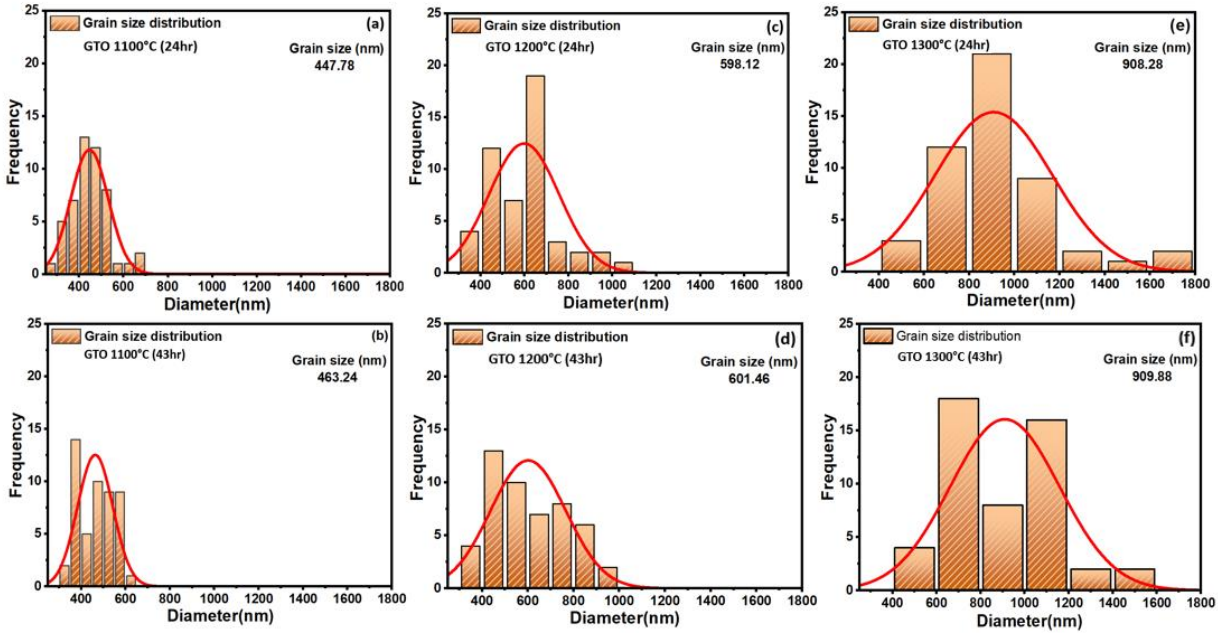

Figure 4.5. (a-f) Gaussian fitting size distribution histogram from analyzed data of SEM for whole series of $Gd_2Ti_2O_7$ at various temperature for different annealing time

CHAPTER 5

SUMMARY AND FUTURE SCOPE

5.1 SUMMARY

Series of $Gd_2Ti_2O_7$ pyrochlore oxides were formed using solid-state route. SEM micrographs are used to confirm that almost spherical particles that have agglomerated are present. XRD and Raman spectroscopy results show that a single phase pyrochlore structure has formed. $Gd_2Ti_2O_7$ shows enhancement in cation anion order with the increase in annealing time at different annealing temperatures. XRD analysis shows an increase in crystallite size and strain with increasing annealing temperature and time. There is a decrease in lattice constant with the enhancement in temperature and annealing time which is calculated using XRD data. As the annealing temperature and time are increased, the $Gd_2Ti_2O_7$ grains gradually expand. The estimated grain size for the grain growth of $Gd_2Ti_2O_7$ has been anticipated using SEM data.

5.2 FUTURE SCOPE OF WORK

In order to comprehend the influence of annealing temperature and time on atomic disorder and grain development kinetics, future work will concentrate on thin films of the

extended series of $Gd_2Ti_2O_7$. I'd want to investigate the grain disorder and growth kinetics of $Gd_2Ti_2O_7$ with Ho_2O_3 doping in the near future. To be used in a number of cutting-edge optical and electrical technologies, metal-oxides must be produced with specific microstructures. Reduced charge carrier recombination in $Gd_2Ti_2O_7$ may be the cause of its optical properties. The near future holds great potential for this material's uses and structural qualities.

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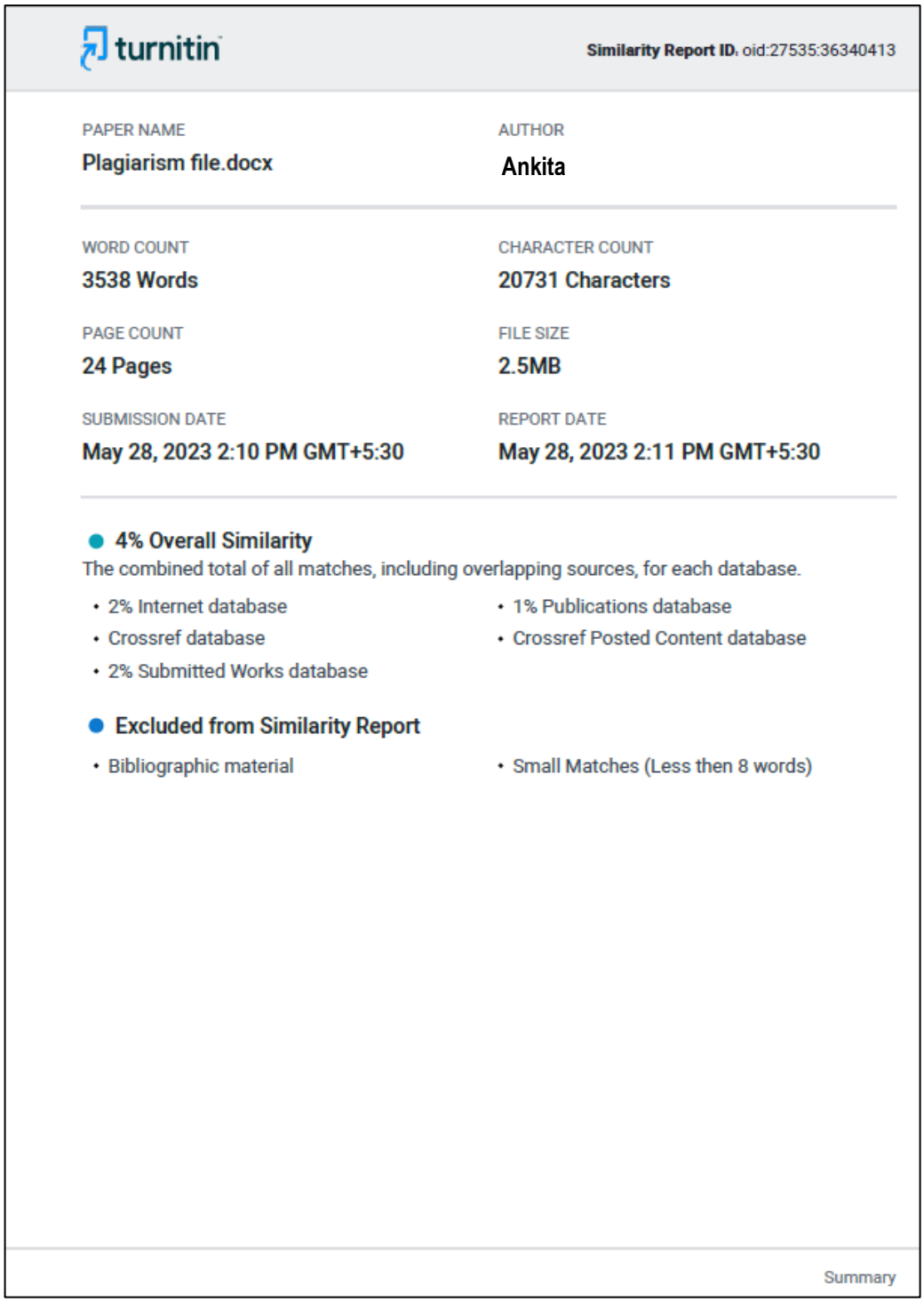

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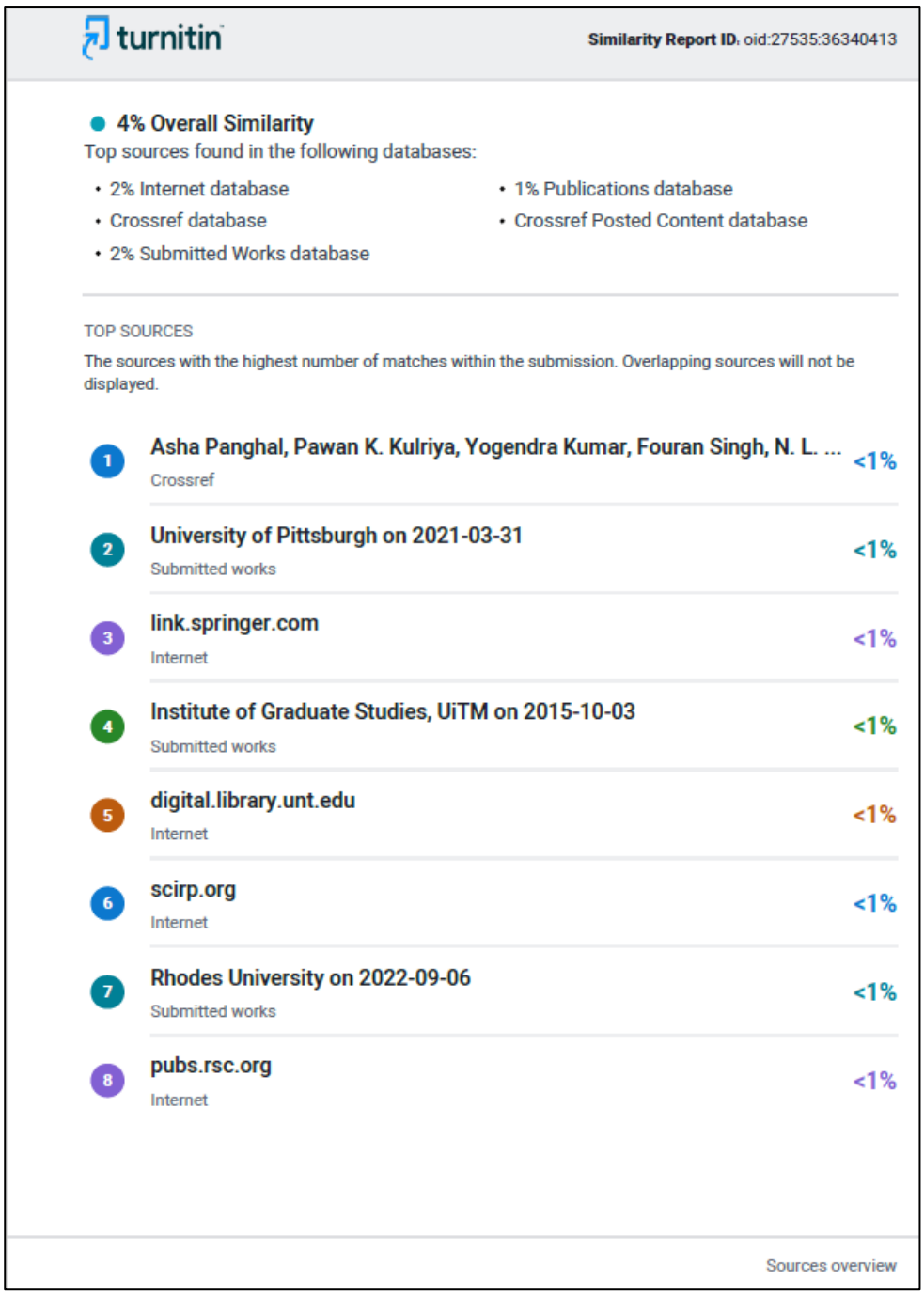

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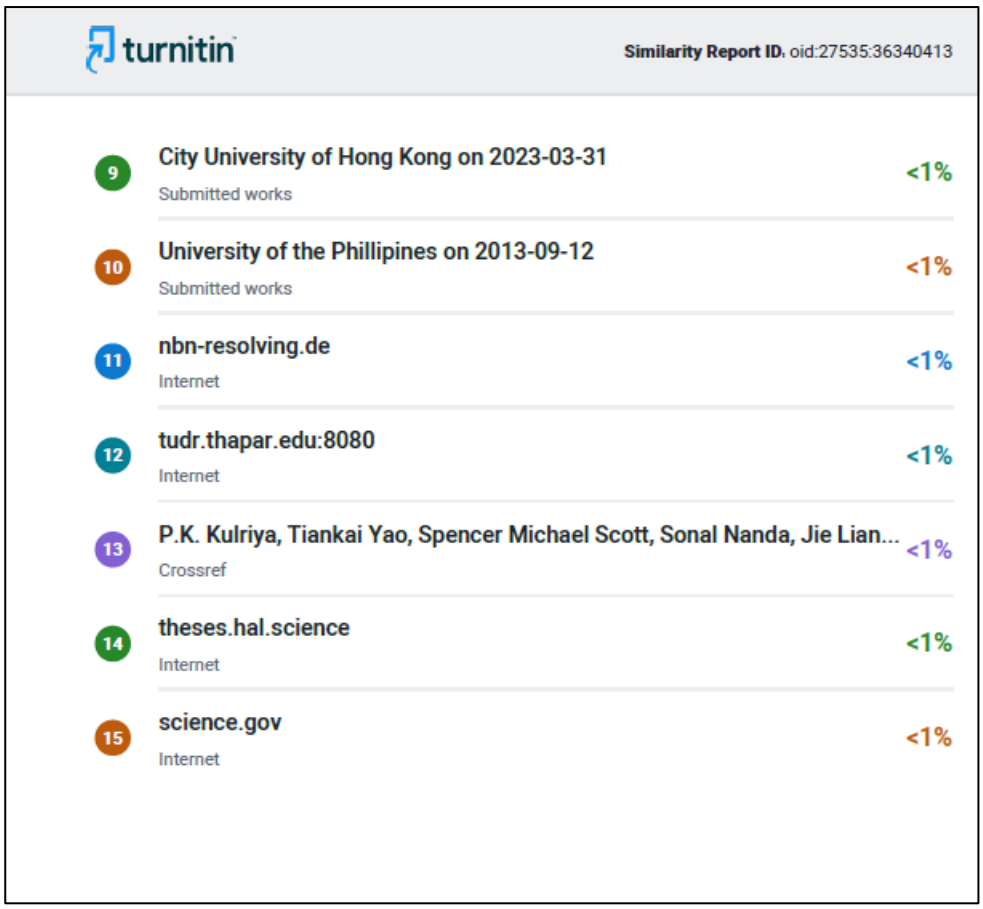

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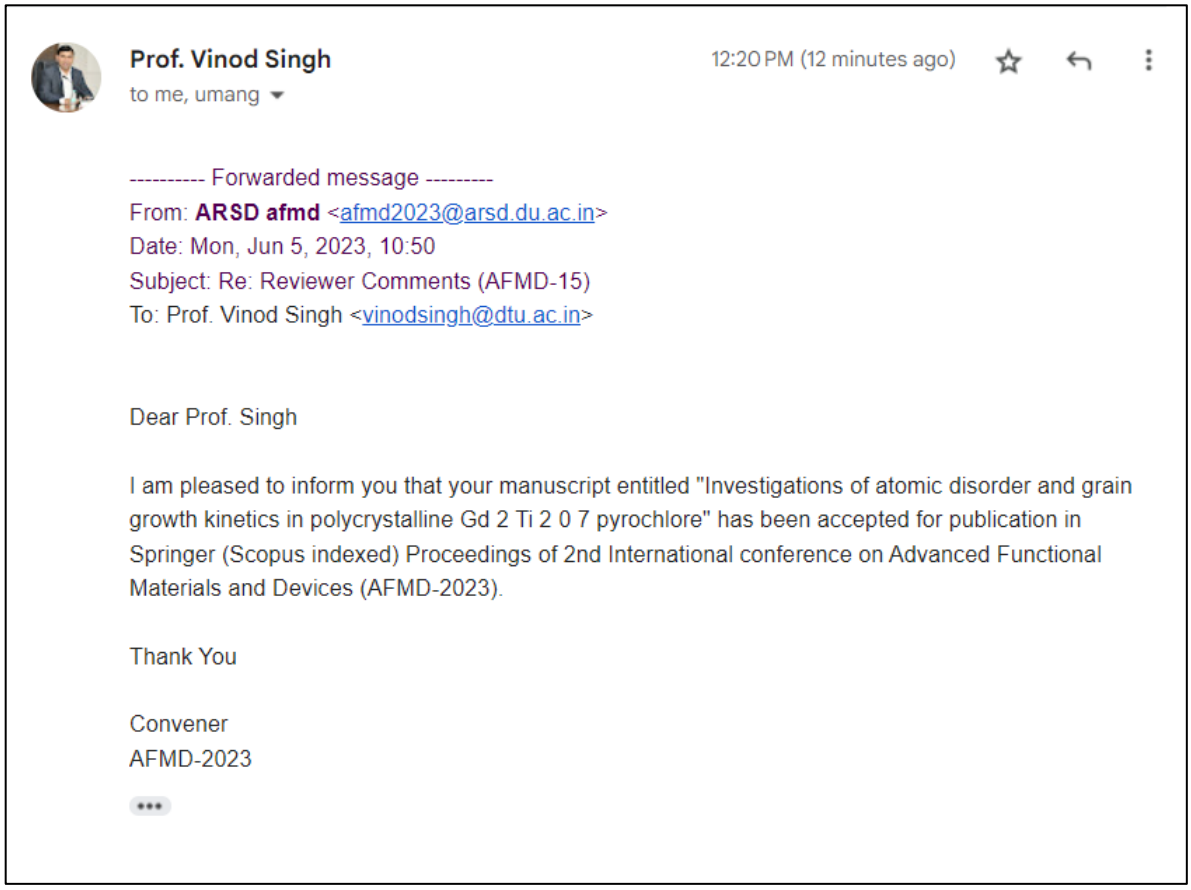

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Investigations of atomic disorder and grain growth kinetics in polycrystalline $Gd_2Ti_2O_7$ pyrochlore

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Abstract

Pyrochlores are used for a variety of purposes, including luminescence, ionic conductivity, superconductivity, high temperature thermal battery coatings, nuclear waste immobilization, electrocatalyst, automobile exhaust gas control, electrocatalyst, solid oxide fuel cell, magnetoresistance and many more. The main focus of this study was to examine how the annealing temperature & duration is influencing atomic order/disorder & growth of grains in the pyrochlore $Gd_2Ti_2O_7$. Designing pyrochlore materials for diverse energy applications may benefit from understanding how atomic order/disorder and grain development affect structural characteristics. The solid state route was used to produce $Gd_2Ti_2O_7$ via uniform heating at distinct temperature level (1100, 1200, and 1300°C) in different time periods (24h & 43h). X-ray diffraction (XRD), Raman spectroscopy, and Scanning electron microscopy (SEM) characterization techniques were performed in order to study both structural & microstructural characteristics associated with $Gd_2Ti_2O_7$. With a rise in heating temperature and time, there is a greater degree of cation-anion order. The production of bigger grains was preferred over coarsening of small grains by curvature. Hence, $Gd_2Ti_2O_7$ grains gradually expand as the heating period and temperature are raised. According to XRD and Raman spectroscopy, grain expansion largely influences the system's periodic ordering through a relaxation through a of the microstrain and the rise in crystallite size. Therefore, pure phasic GTO has been successfully created using the solid-state reaction method, which was then followed by numerous grinding and heating protocols, and it can now be applied in a variety of fields.

Keywords: Gadolinium titanium oxide, XRD, Raman Spectroscopy, UV-Visible Spectroscopy

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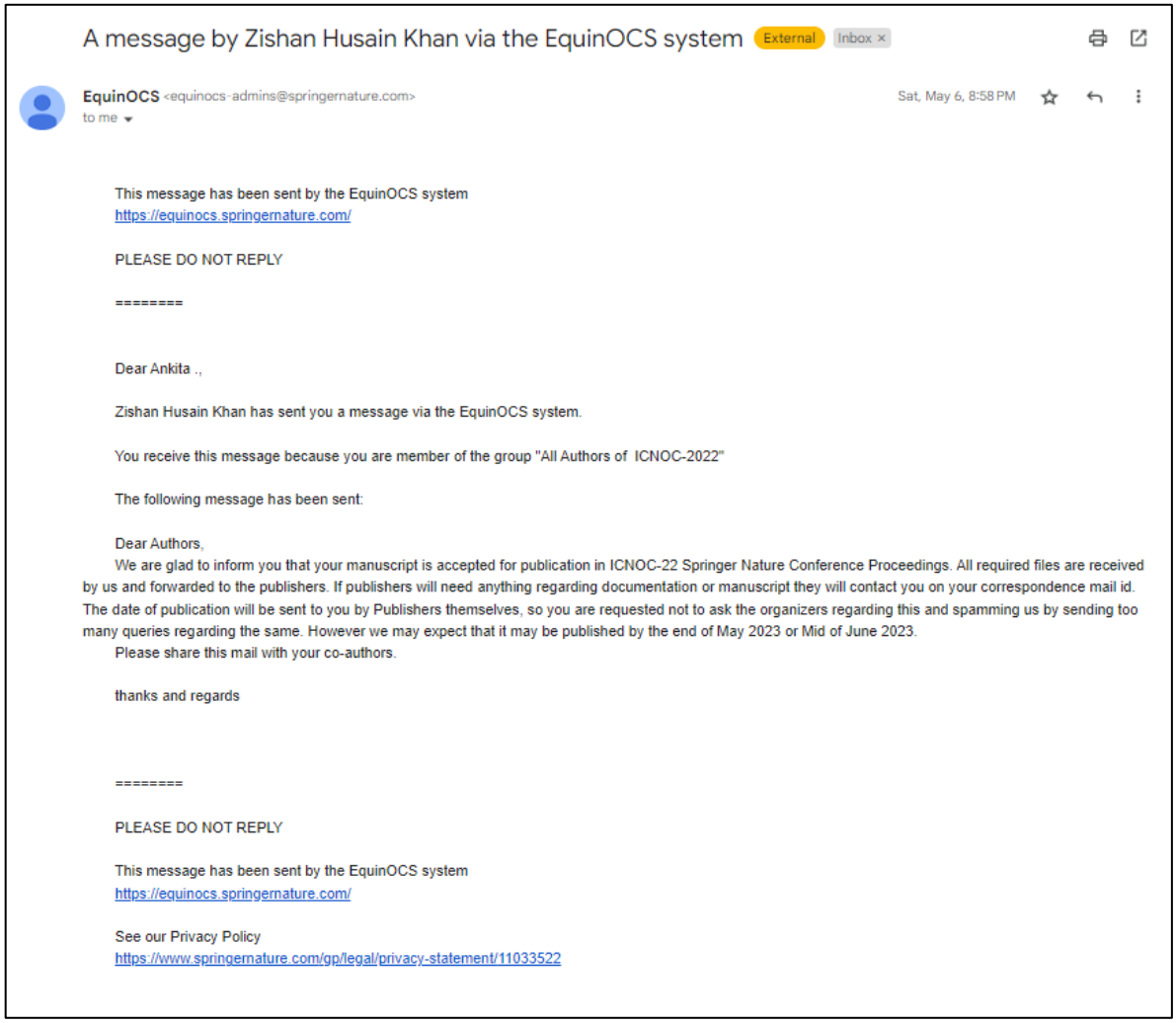

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STRUCTURAL AND OPTICAL PROPERTIES OF REDUCED GRAPHENE OXIDE

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Abstract

A wide range of doped materials, including fluorescence, optical fibres, lasers, and heterojunction PV devices, have many uses for carbon-based materials due to their intriguing structural and optical characteristics. Graphene has a special character of high electron transfer rate, this attribute leads to structural modifications, enhancing the optical properties of various substances. Here, using a variety of characterisation approaches, we have evaluated the methods used to create graphene-based nanoparticles and emphasizedtheir structural (X-ray diffraction (XRD), Raman spectroscopy and scanning electron microscopy (SEM)) and optical properties (UV- visible spectroscopy). The structural and optical qualities of diverse materials are improved with an increase in the concentration of reduced graphene oxide (rGO). The diffraction peak of rGO in the XRD diffraction pattern was virtually centered at $2\theta = 26°$, indicating the crystalline character of rGO. Additionally, as rGO concentration grows, existing grain boundaries in FESEM characterization increases as a result of electron-hole recombination, and these GO nanoparticles also intensify the G and D bands in Raman spectra. It is obvious that altering the oxidation level of graphene, which can be demonstrated using the UV-Visible spectroscopic characterisation method, can result in significant control over the band gap. The increase in surface roughness of rGO doped material leads to an increase in surface area of rGO doped samples, making photon absorption easier and increasing the rate of light absorption, which is why the UV-Vis absorbance spectrum peak's intensity rises at 255nm. Because rGO can readily tune the band gap of the material, there have been a wide range of futuristic research opportunities due to the multiple applications based on its optical features.

Keywords

Reduced Graphene Oxide, XRD, Raman Spectroscopy, UV-Visible Spectroscopy

1 Introduction

Phillip Russel Wallace created a theoretical idea in the 1940s that would allow us to build single-atom carbon structures. This substance has been the focus of arduous research for more than 60 years and is regardedas having the potential to completely transform various sectors. But for many years, this theory had been disproven by numerous scientists due to its low electrical and thermal conductivity.[10] Graphene is essentially a monolayer of securely bound carbon atoms in a two-dimensional hexagonal honeycomb lattice, which is an allotrope of carbon atoms. Strong σ-bonds help connect each atom in the graphene sheet to its closest neighbours. Carbon nanotubes also exhibit this type of bonding.[44] In essence, graphene is a superior thermal and electrical conductor with intriguing optical and light-absorbing capabilities. It is lightweight, flexible, chemically inert, and it conducts electrical and thermal energy. There are several photonics uses for graphene, ranging from transparent conductors in photonic devices to high-bandwidth photodetectors, due to its special optical properties that allow it to absorb a wide range of electromagnetic radiation.[19]

In essence, graphene oxide is an oxidised form of the material that has been infused with oxygen-containing groups. It is thought to be simple to process because it disperses in water and even in other solvents. GO is commonly available in powered or coated form for substrates.[5] Any substrate may be used for the deposition of graphene oxide layers, which will eventually be transformed into conductors. Thus, GO is employed in the fabrication of transparent conductive films, such as those utilised in sensors [9], solar cells [21], and a variety of other devices. Batteries [46], capacitors [38], and solar panels [40] all use Graphene Oxide due to its large surface area. Since graphene oxide is more accessible and less expensive to produce than graphene, it may eventually be put into mass production. GO can be blended with other polymers and substances to improve the tensile strength, elasticity, conductivity, and other qualities of substances.[14] Although graphene oxide is not a good conductor, there are two methods to improve its characteristics by doping some other element or by reducing it.