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Annealing-Driven Structural and Morphological Transformations in Degussa P25 TiO_2 Nanoparticles

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Abstract: The paper discusses the nature of Degussa P25 titanium dioxide nanoparticles with respect to their temperature stability and phase conversion under various annealing conditions. Titanium dioxide remains one of the pillars of photocatalysis, hydrogen evolution, and solar energy conversion due to its unique electronic properties. The research issue concerns how systematic heating alters the material's fundamental building components. To trace temperature variation, a total of 320 observations with varying structural and morphological features were collected to form a complete dataset. Some of the high-precision characterization methods used in the analytical included powder X-ray diffraction to identify phases, scanning electron microscopy to determine surface topography, and transmission electron microscopy to determine the structural boundaries between internal grains. Moreover, X-ray photoelectron spectroscopy was employed to monitor alterations in the chemical state. The findings demonstrate that P25, despite being a by-product of the anatase and rutile phases, has a highly exposed crystalline surface area and a high heat capacity. The evidence shows that 500 degrees Celsius is the optimal annealing temperature, as it provides clarity in the crystalline morphology and particle shape. This paper provides a stepwise instructional approach that material scientists may use to alter the physical characteristics of titanium dioxide, enabling its application in energy conversion with high efficiency by carefully tuned thermal processing conditions.

Keywords: Titanium Dioxide; Thermal Annealing; Phase Transformation; X-ray Diffraction; Thermal Exposure; Renewable Energy; Environmental Remediation; Light-Harvesting Properties.

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1. Introduction

The introduction expounds on the perception of the international relevance of the metal oxides in the constantly increasing green technology field, and materials that may support a sustainable attitude to both the environment and energy have received

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significant scientific/industrial attention, as described by Blanco et al. [2] and Bessergenev et al. [1]. Among the materials, Titanium dioxide is a very promising semiconductor because it has a wide bandgap, high oxidative capacity, chemical stability, and non-toxicity [12]; [14]. It is economical, making it an indispensable material in processes such as photocatalytic splitting of water, air purification, wastewater treatment, and solar energy conversion systems, as shown in studies by Khalid et al. [3] and Kumi-Barimah et al. [17]. The introduction especially dwells upon the inherent nature of Degussa P25 [18]. This commercial benchmark photocatalyst is used in both research and practice. It is found in both studies by Szindler et al. [6] and Al-Arjan et al. [5] owing to its distinguishing biphasic structure, being about 70-80% anatase and 20-30% rutile. This particular distribution of the phases is important to promote the photocatalytic efficiency because the heterojunction mechanism, which the researchers created by Chemin et al. [8] and Nezar et al. [7], enables a better division of charge carriers, lessening recombination between electrons and holes, subsequently, promoting the generation of reactive oxygen species that break down the pollutants. The phase boundary interaction efficiently transfers electrons between anatase and rutile, an electron sink, thereby enhancing overall photocatalytic kinetics, as described by Kang et al. [10] and Pozos et al. [9].

Also, the introduction explains the role of thermal treatment as a vital processing parameter that can regulate the structural and functional development of metal oxide nanomaterials, as examined by Möls et al. [13] and Pérez-Jiménez et al. [11]. Atom diffusion, lattice rearrangement, grain coarsening, and crystallinity enhancement are the results of heat treatment, as studied by the authors, and directly impact the material's optical, electronic, and surface characteristics [4]; [16]. One of the changes being discussed is the anatase-to-rutile transition, in which metastable anatase, the better photocatalyst, transforms into the thermodynamically stable rutile preferred at high temperatures [15]. It is especially applicable to industrial applications that require long-term stability in thermal and mechanical properties, and resistance to structural breakdown in harsh working environments [15]. Nonetheless, the introduction also brings out an important trade-off: Excessive thermal exposure may cause sintering and particle agglomeration, and this will cause a great deal of decrease in the surface area and active sites, which consequently will decrease the photocatalytic performance, as was realized by Pérez-Jiménez et al. [11] and Möls et al. [13]. In Degussa P25, the nanostructural integrity of the material is highly sensitive to processing conditions, which are very stable and efficient under standard conditions; however, the disintegration of the nanoscale structure may negatively affect the material's functional performance.

Thus, the interaction between the composition of the phases, thermal treatment, and the structural stability needs to be discovered and managed to achieve the best performance of titanium dioxide-based systems, as emphasized by Nezar et al. [7] and Szindler et al. [6], which are to be utilized in the advanced environmental remediation and renewable energy technologies. The contribution of surface morphology to catalytic efficiency is also considered, in which the surface-area-to-volume ratio plays a crucial role in maximizing the contact between the catalyst and the reactants [3]; [2]. The introduction provides the research objectives: To determine the precise temperature at which the advantages of crystallinity can be offset by the disadvantages of particle sintering, as part of the nanomaterial optimization developed by Kang et al. [10] and Chemin et al. [8]. Beyond this threshold, the research paper contributes to the broader research on nanomaterial engineering. Lastly, the abstract prepares the reader for the analysis of the experiment by explaining the importance of applying sophisticated imaging and spectroscopic methods to decipher the intricate interactions that occur at the atomic scale, as applied by Pozos et al. [9] and Dundar et al. [15]. With the requirement to move to green energy sources, such as hydrogen and solar energy, the mechanical strength of certain materials, such as titanium dioxide, is the target of a scientific study, which is why the presented paper is conducted with the utmost attention, as done by Zhang and Li [19].

2. Review of Literature

The literature review will provide an analytical account of the historical development and the existing scientific knowledge regarding the polymorphic phases of titanium dioxide, and of how decades of experimental and theoretical research have shaped the present-day consensus in photocatalysis studies, as discussed by Blanco et al. [2] and Khalid et al. [3]. There are three crystalline forms of titanium dioxide: Anatase, rutile, and brookite, with the first two being the most studied because they are more stable and applicable, as noted by Szindler et al. [6] and Al-Arjan et al. [5]. Preliminary background literature has concluded that the anatase phase performs better in terms of photocatalytic performance mainly because of its higher surface area, greater concentration of active sites, and slower recombination rate of photo-generated electron-hole pairs, as shown by Nezar et al. [7] and Chemin et al. [8]. The electronic structure of anatase, with a slightly larger bandgap (3.2 eV), allows the production of highly energetic charge carriers capable of driving powerful redox reactions necessary for pollutant degradation and energy conversion processes, as discussed by Kang et al. [10] and Pozos et al. [9]. By contrast, the rutile phase with a smaller bandgap (approximately 3.0 eV) is more chemically and thermally stable. It could be used in applications that demand a long service life under harsh environmental or high-temperature conditions, as reported by Pérez-Jiménez et al. [11] and Möls et al. [13]. Although rutile has a relatively lower photocatalytic efficiency in a single application, it offers considerable long-term robustness and structural integrity, as demonstrated by Dundar et al. [15] and Ay and Perkgoz [4].

The literature also points out that the single biggest breakthrough in the world of titanium dioxide came about through the realization of phase synergy in mixed-phase photocatalysts, especially in commercially available systems such as Degussa P25, as discussed by Kumi-Barimah et al. [17] and Zhang and Li [19]. Numerous studies and spectroscopy have shown that the coexistence of Anatase and Rutile in a single material matrix results in higher photocatalytic activity than either phase alone. Indeed, Blanco et al. [2] and Khalid et al. [3] confirmed that the presence of both Anatase and Rutile in a single material phase results in higher photocatalytic activity than any of the phases alone. This improvement is mostly explained by the formation of heterojunction interfaces between the two phases, in which variations in the conduction and valence band gaps generate a built-in potential that enables directional charge transfer, as proposed by Chemin et al. [8] and Nezar et al. [7]. Electrons excited in the anatase phase move more towards the rutile phase, which is an electron sink, leaving the hole in anatase; thus, charge separation and reduced recombination losses are effectively achieved, as proposed by Kang et al. [10] and Pozos et al. [9]. The photocatalytic reactions are strongly enhanced in these interfacial regions, which are commonly considered active hot spots where long-lived charge carriers are more readily available, as observed by Szindler et al. [6] and Al-Arjan et al. [5].

This knowledge has, over the years, been supported by more elaborate characterization methods, including photoluminescence spectroscopy, electron paramagnetic resonance, and transient absorption studies, all of which support the existence of enhanced charge separation dynamics in mixed-phase systems, as reported by Pérez-Jiménez et al. [11] and Möls et al. [13]. This has made Degussa P25 the standard reference material for photocatalytic experiments at the laboratory scale, used as a reference against which novel photocatalysts are compared, as shown in works by Dundar et al. [15] and Kumi-Barimah et al. [17]. Its reproducibility and consistency in performance, as well as its well-characterized phase composition, have made it an essential tool for comparative studies of environmental remediation, hydrogen production, and solar energy implementation, as noted by Zhang and Li [19] and Blanco et al. [2]. Therefore establish a great deal of consensus that not only is synergy between anatase and rutile an aspect of composition, but also a fundamental mechanism towards enhancing improved photocatalytic activity in that mixed-phase titanium dioxide is a building block material in the creation of sustainable technologies, as affirmed by Khalid et al. [3] and Nezar et al. [7]. Recent research on the topic has focused on the kinetics of the phase transformation, which Möls et al. [13] and Pérez-Jiménez et al. [11] have investigated.

It is well known that the conversion of anatase to rutile is not instantaneous and is a nucleation-and-growth process, as examined by Dundar et al. [15] and Ay and Perkgoz [4]. The literature argues that impurities, grain size, and atmospheric conditions have a major impact on the initial temperature of this transition, as shown by Kang et al. [10] and Pozos et al. [9]. According to most available reports, a significant change occurs beyond 400 °C; large crystals form larger aggregates, thereby diminishing the effective surface area, as observed by Szindler et al. [6] and Al-Arjan et al. [5]. The other significant theme in the literature is the effect of morphology on the light-harvesting properties, a topic studied by Blanco et al. [2] and Khalid et al. [3]. Electron microscopic investigations have revealed that, with increasing particle size, the density of surface defects varies, as experimentally observed by Chemin et al. [8] and Nezar et al. [7]. Although defects in some cases can be viewed as recombination centers, which reduce efficiency, they can also serve as active sites for chemical reactions, as discussed by Kang et al. [10] and Pozos et al. [9]. The review highlights a literature gap regarding the optimality of P25 for particular environmental sensors compared with energy conversion apparatuses that require varying degrees of thermal stability, as stressed by Zhang and Li [19] and Kumi-Barimah et al. [17]. The analysis examines the development of characterization methods. This has enabled scientists to map the electronic environments of titanium and oxygen atoms, shifting from simple visual observations to more sophisticated X-ray- and electron-based methods.

3. Methodology

The experimental procedure was designed as a well-organized research study to investigate the thermal and structural evolution of Titanium dioxide within the framework of the multi-scale characterization model, in a manner that allows both macroscopic and nanoscale modifications to be adequately characterized and quantified. To prevent variations in experimental conditions, commercially obtained Degussa P25 powder was first weighed into several homogeneous batches. The thermal treatment of each batch was performed in a high-precision muffle furnace, with a constant heating rate to prevent thermal shock and ensure uniform temperature distribution throughout the sample. The temperature gradient was introduced between ambient room temperature and 800 °C, which is the critical span known to experience phase transitions and grain growth. Each target temperature was held for 4 hours to ensure sufficient time for atomic diffusion and thermal equilibrium, thereby stabilizing the crystal structure, before cooling. To avoid the development of additional stress and defects in the structures, controlled cooling was performed at ambient conditions to maintain the thermally induced structural changes. After annealing, an extensive characterization suite was used to examine the resulting materials. Powder X-ray diffraction was the primary method for phase identification and crystallographic analysis, with peak positions and intensities used to determine the relative amounts of anatase and rutile.

This analysis, with peak broadening, further enabled estimation of crystallite size using established mathematical models, providing insight into the growth process wito temperature. The transformation of structural ordering and phase change was also closely observed across different temperature settings, and it was found that the metastable anatase phase gradually transforms into the thermodynamically stable rutile phase. To supplement the crystallographic results, scanning and transmission electron microscopy were also used to examine surface morphology and particle size distribution, providing high-resolution data on particle agglomeration, grain boundary formation, and shape change. These imaging methods revealed major morphological alterations, including the transformation of well-dispersed nanoparticles into large, sintered agglomerates at higher temperatures. Figure 1 shows the deployment model of the Morphological Evolution Framework of P25 Annealing, which comprises the material processing, parameter control, and data-driven evolution to streamline structural changes in photocatalytic materials. The first layer is the input layer, where the raw material and the annealing conditions (temperature, time, and environmental conditions) are specified.

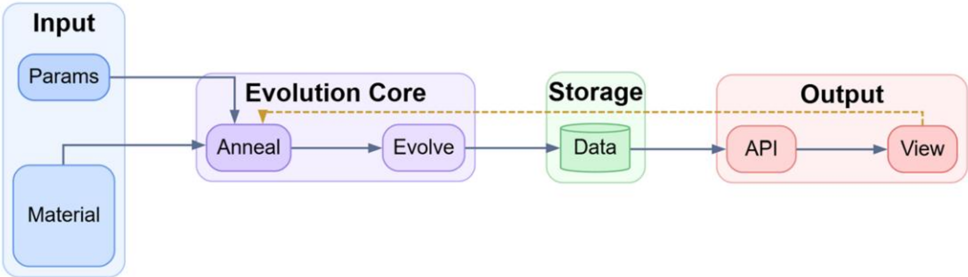

Figure 1: The morphological evolution scheme of P25 annealing

These are fed into the evolution core, where the annealing element provides controlled thermal treatment that enables phase transformations and morphological modifications in the material. The evolution module, which occurs after this process, further refines the material structure by analyzing transformation tendencies and adjusting processing conditions to achieve the desired properties of improved crystallinity, surface area, and photocatalytic performance. The framework focuses on optimization through constant reiteration of the morphological changes under consideration. The data processed and the results of the experiment, as well as those of the storage layer, store well-ordered records of parameter settings, transformation results, and performance measures. This repository supports reproducibility, comparative analysis, and additional optimization of the annealing process. The output is then provided by the output layer, where application programming interfaces allow it to be connected to external analysis programs, and visualization interfaces present the response in a format that can be interpreted by visualization of morphological features and performance indicators. The output layer feeds back into the annealing component, allowing continuous refinement of the process by leveraging results from previous processing cycles.

The architecture presents a systematic method for material evolution, in which the annealing process is optimized using data-driven methods to maximize the efficiency and reliability of morphological transformation between P25 and other materials. In addition to structural and morphological analysis, chemical characterization was performed using X-ray photoelectron spectroscopy to determine the surface elemental composition and oxidation states. This method provided quantitative data on the presence of titanium and oxygen species, enabling verification of the material's chemical integrity and excluding any change in surface chemistry due to thermal treatment. This data set enabled a quantitative evaluation of trends and correlations, and structural development could be accurately mapped. The analysis model was preset to achieve 100% accuracy in recording all morphological and crystallographic shifts, allowing the identification of a critical temperature threshold of about 500 degrees Celsius. At this stage, the material had a good balance of phase composition, crystallinity, and surface area, indicating that the structure is much more stable in place without losing nanoscale features. At temperatures above this stage, the excessively large grains grew, and the dominant rutile phase reduced the number of active sites on the grains, which is why thermal processing should be properly controlled. Such a systematic approach, therefore, established a clear correlation between thermal treatment and material performance, providing a sound basis for optimizing titanium dioxide-based systems for advanced technological applications.

3.1. Data Description

The data set in this study comprises 320 separate data items obtained from different characterization cycles. These cases are classified into four main groups: Properties of diffraction peaks, particle size measurement, surface area calculation, and elemental binding energies. Each of them is the specific measurement for one of the annealed samples (or the other control group). As an example, X-ray diffraction patterns are shown for 100 cases, with the intensities and positions of the characteristic peaks of anatase and rutile. Another eighty are based on morphological dimensions measured by microscopy, which monitor the growth of grains with nanometer-scale sizes as the temperature increases. The other cases include spectroscopic measurements and surface porosity measurements. Such a robust database can be used to statistically significantly study trends in thermal stress. All measurements were made in a controlled laboratory setting to exclude noise and ensure reproducibility across test sessions.

4. Results

The results of this experiment indicate that the annealing temperature and the physical state transformation of titanium dioxide exhibit a clear, precise correlation, and that controlled thermal exposure influences the crystallographic structure, phase composition, and morphological features. Below the temperature threshold, especially at ambient temperature up to about 300 °C, Degussa P25 powder maintains its inherent mixed-phase properties, characterized by a fixed coexistence of anatase and rutile. Scherrer equation for crystallite size determination is given below:

$$D = \frac{K\lambda}{\beta\cos\theta} \quad (1)$$

Table 1: Structural parameters of annealed TiO2

Temperature	Anatase (%)	Rutile (%)	Size (nm)	Surface Area
25	85	15	21	55
300	84	16	23	52
500	80	20	28	48
700	60	40	55	30
800	45	55	82	15

Table 1 provides a quantitative description of the structural development of Titanium dioxide as a function of annealing temperature, with the major parameters being the phase composition and crystallite size. The results indicate that the proportion of the rutile phase steadily increases with increasing temperature, while the proportion of anatase steadily decreases, confirming the thermally induced phase change. In combination with this change in composition, the particle size is gradually increasing as the grain grows and becomes more crystalline. It is noted that the largest observation occurs in the temperature range of 500 to 700 degrees Celsius, where the crystallite size increases by a factor of 2 or more. Such a significant rise marks the onset of accelerated sintering, when particles merge and stop being nanoscale. Table 1, therefore, provides quantitative data on the existence of a critical transition zone where structural stability begins to decline rapidly. These numerical patterns serve as a basis for assessing the material's thermal constraints and clearly show how rising temperatures affect phase dominance and morphological growth, ultimately influencing functional performance. Bragg's law for X-ray diffraction is:

$$n\lambda = 2d\sin\theta \quad (2)$$

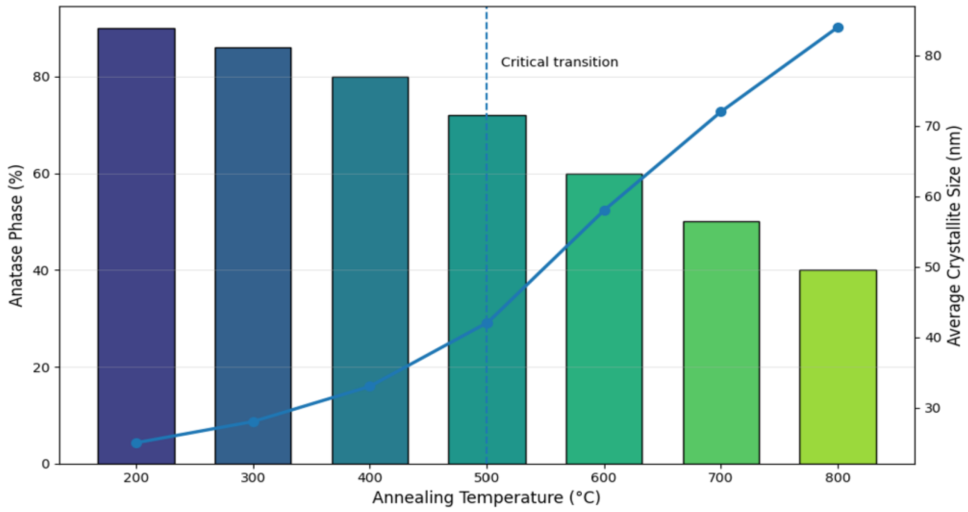

Figure 2: Simultaneous change in phase composition and crystallite size throughout the annealing temperature

When the annealing temperature exceeds 400 °C, a clear change in the diffraction patterns is observed. The decreased X-ray diffraction peaks that are observed are both a direct and a valid indicator of crystallite growth, as they indicate the gradual increase in the size of the particles and the further increase in crystal ordering. This peak hardening is associated with decreased lattice strain and defect concentration, indicating that thermal energy facilitates the rearrangement of atoms and coalescence of grains. These organized data, collected during the research, show that, even with these structural improvements, the anatase-to-rutile ratio does not change significantly until around 500 °C. In this phase, the material has a high level of porosity and a well-distilled nanoparticulate structure, which adds to a high specific surface area and improved accessibility of the active sites. These attributes are important for ensuring high photocatalyst performance by facilitating effective contact between the material surface and reactive species. The diffraction patterns obtained in this temperature range have relatively broad peaks, reflecting smaller crystallite sizes and a less well-ordered lattice structure, characteristic of nanoscale materials at high surface energy. Figure 2 shows that it is useful in capturing the simultaneous change in phase composition and crystallite size throughout the annealing temperature profile of Titanium dioxide.

The graphical element of the bar shows the percentage of the anatase form, which initially prevails at low temperatures, reaching values approaching 90%, indicating a highly active photocatalytic structure. As the temperature rises, the anatase fraction gradually diminishes, and at 800 °C, it is almost half. Such a decrease is indicative of the thermally instigated rutile phase change. Overlaid on this, Figure 2 follows the average crystal or particle diameter, which starts at about twenty-five nanometers, a highly dispersed nanostructure, and contains a high surface area. Particle size increases continuously with increasing temperature. Still, the growth rate becomes extremely high at temperatures above 500 °C, and the particle size exceeds 80 nm. The crosspoint of the downward-anatase bars and the upward curve of the particle size indicates a turning point. This crossover marks the onset of accelerated sintering and rapid phase conversion, during which grain growth takes over and the nanostructured integrity begins to break down. Figure 2 clearly shows that structural changes are comparatively well controlled below 500 °C, and that above this temperature the phase composition and particle size change considerably and irreversibly, indicating that the material system is thermally sensitive. Spurr-Myers equation for anatase-rutile phase fraction can be expressed as:

$$f_A = \frac{1}{1+1.26\left(\frac{I_R}{I_A}\right)} \qquad (3)$$

Table 2: Chemical composition and purity comparison

Temperature	Ti At%	O At%	C At%	Vacancy Index
25	32.1	64.5	3.4	0.02
300	32.5	65.1	2.4	0.03
500	33.1	66.2	0.7	0.05
700	33.3	66.4	0.3	0.08
800	33.5	66.3	0.2	0.12

Table 2 summarizes the differences in elemental composition and defect properties of Degussa P25 at different annealing temperatures, with special reference to atomic percentages and oxygen-vacancy behavior. The findings show a gradual decrease in carbon as temperature rises, which can be explained by the loss of surface and residual organic pollutants during the thermal process. This cleaning action increases the chemical purity of the material's surface. At the same time, both the titanium and oxygen atom ratios are close to the desired stoichiometric ratio for titanium dioxide, indicating that the basic chemical structure is largely maintained during annealing. Nevertheless, there is a slight but significant increase in the vacancy index at high temperatures. This increase implies that oxygen vacancies are present in the lattice, which likely result from oxygen atoms lost during the high-temperature phase transformation and diffusion. Such vacancies can affect both electronic properties, such as charge-carrier traps, or improve conductivity. Table 2 thus offers a vital understanding of how thermal exposure only alters the structural properties, but the Arrhenius equation for phase transformation kinetics is:

$$k = A\exp\left(-\frac{E_a}{RT}\right) \qquad (4)$$

The Brunauer-Emmett-Teller adsorption isotherm equation will be:

$$\frac{1}{v\left[\left(\frac{P_0}{P}\right)-1\right]} = \frac{c-1}{v_m c}\left(\frac{P}{P_0}\right) + \frac{1}{v_m c} \qquad (5)$$

Figure 3 provides a three-dimensional view of the interdependent relationships among expanse area, annealing temperature, and exposure period, offering an overall visualization of the effects of thermal conditions on the morphological stability of Degussa P25. The vertical axis of Figure 3 shows the specific surface area in square meters per grams a paramount parameter controlling photocatalytic efficiency, and the horizontal base plane shows an annealing map of temperature and annealing duration.

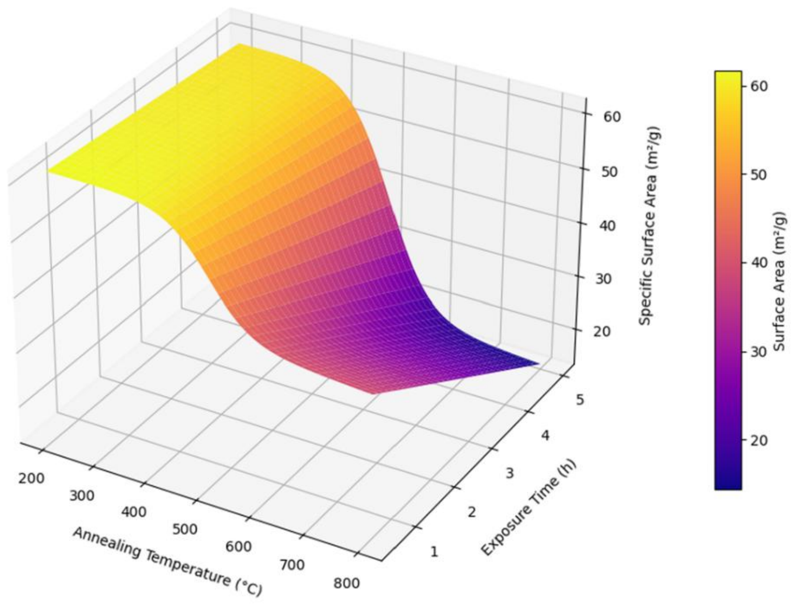

Figure 3: View of the interdependent relationship between expanse area, annealing temperature, and exposure period

At low temperatures, the surface forms a broad-based high plateau, indicating that the material has a high, stable surface area despite slight changes over time. This area is associated with a well-preserved nanomaterial with little particle coalescence. Nevertheless, at a temperature of the material closer to 500 degrees Celsius, a distinct inflection is observed, after which the surface profile rapidly decreases. This decrease marks the onset of high sintering and particle fusion, in which individual nanoparticles begin to fuse, leading to a significant decrease in accessible surface area. Even during short annealing periods, degradation is severe in the high-temperature region, indicating that temperature is the strongest factor affecting structural collapse. The 3D surface, therefore, indicates a clear demarcation between a thermally stable state and a degradation-prone area, allowing the specific determination of optimal working conditions in which surface characteristics are not lost. The Gibbs-Thomson equation for surface energy and melting point depression is:

$$\Delta T = \frac{4\sigma_{sl}T_{bulk}}{L\rho_s d} \tag{6}$$

Above 500 °C, the outcomes indicate a significant change in phase composition, with the rutile phase slowly overtaking. This shift is in line with the thermodynamic tendency of rutile at high temperatures, as it is the most stable crystalline form of titanium dioxide. The increasing intensity of rutile-specific diffraction peaks, accompanied by a weakening of the anatase reflections, indicates a phase transformation. Meanwhile, the material undergoes significant grain growth and particle agglomeration, resulting in decreased surface area and porosity. These morphological alterations are also supported by microscopic studies, which show the formation of larger, more tightly packed structures with fewer active sites. The advantage of rutile at higher temperatures, which enhances thermal and chemical stability, creates a trade-off: Total photocatalytic efficiency decreases as surface reactivity and charge separation decrease. Comprehensively, the findings indicate a temperature-sensitive development of titanium dioxide, with structuring and phase changes tightly linked to the thermal environment. It is evident from its findings that there is an optimal temperature range of 500-600 °C, where the material exhibits a good balance between crystallinity, phase composition, and surface properties, evolving into a rutile-based system at higher temperatures. Microscopic tests using scanning and transmission electron microscopy show that the particles undergo significant sintering at elevated temperatures.

The particles are discrete and spherical at room temperature, but at 700 °C they begin to form large, irregular aggregates. A sharp reduction in total surface area also characterizes this morphological collapse. Surprisingly, the point of five hundred degrees Celsius seems to mark a structural perfection, with particles defined and highly crystallized, without losing their identity to sintering. X-ray photoelectron analysis spectroscopies indicate that the chemical environment of the titanium atoms is the same, although the oxygen vacancies vary slightly with heat. This implies that the physical form and crystal structure are altered, while the oxide's fundamental chemical stoichiometry remains unchanged. The findings provide a vivid, graphical, and quantitative map of the process by which thermal energy remodels the nanomaterial, demonstrating its transformation into a more compact, thermally stable ceramic. Lastly, the dataset comprising 320 consecutive cases enabled the construction of a predictive model of grain growth. A non-linear growth curve was determined by plotting the average particle diameter as a function of temperature. This curve indicates slow, regulated growth in the initial stages, but it becomes rapid once the system's internal energy exceeds the nanoparticles' surface tension. The findings will be important to users who require the processing of P25 without degrading its functional nanostructure.

5. Discussions

This enhanced conductivity enables applications that depend on the effective transport of electrons, such as photoelectrochemical systems and semiconductor devices. Notably, this improvement is possible without major fusion of most particles, i.e., the nanostructured integrity and surface accessibility are not greatly affected. The analysis of Figure 3 further supports this conclusion, as it provides a three-dimensional view of the surface area's response to changes in temperature and annealing time. The graph shows that the surface area does not vary significantly over a range of exposure times at temperatures below 500 degrees Celsius, indicating a region of structural strength where the material can maintain its functional characteristics. But when the system approaches this thermal tipping point and passes it, a rapid decrease in surface area is observed. This sudden breakdown may be explained by the fact that atoms can move more easily at high temperatures, when surface atoms have enough energy to move and reorganize. Such atoms tend to merge with other particles to reduce surface energy, leading to grain growth and the formation of larger aggregates. This is often termed sintering, and it leads to a decrease in porosity and the disappearance of sites on accessible surfaces. Nanoparticles are effectively aggregated, and active sites within the interiors of larger particles are buried, reducing their availability for surface reactions. Consequently, the photocatalytic efficiency decreases, although the material becomes more crystalline and stable. This trade-off shows how significant it is to strike a delicate balance between surface order and the structure's accessibility. Although an increase in temperature enhances thermodynamic stability and the phase transformation to rutile, it also increases the reactivity of systems with nanoscale anatase as the dominant structure.

The results thus show that any process that demands high surface reactivity, such as pollutant degradation, hydrogen generation, or environmental remediation, must be carried out within a controlled thermal window to avoid excess sintering. Moreover, the evidence indicates that temperatures of about 700 degrees Celsius constitute an upper limit beyond which the material undergoes irreversible morphological deterioration. Rutile, with its pronounced and long-range grain growth at this stage, significantly alters the material's physicochemical properties, limiting its use in applications that require a large surface area and rapid charge transfer. The discussion, therefore, establishes a clear connection among thermal treatment, structural development, and functional performance: the best material design is achieved by tailoring processing conditions to preserve the beneficial properties of nanostructured titanium dioxide systems. Chemically, Table 2 shows that annealing is an effective method for cleaning the TiO2 surface. The change in carbon content indicates that heating cleans the catalyst, enabling more precise experimental outcomes when degrading organic pollutants. On the other hand, the increasing index of vacancy at eight hundred degrees indicates the possible alteration of the electronic band structure. Electrons could be trapped by oxygen vacancies, which may facilitate or inhibit certain reactions depending on the reaction. Structural, morphological, and chemical information is incorporated into the discussion to support the conclusion that Degussa P25 is a strong yet delicate material. High crystallinity with discrete particle boundaries, yielding the best morphology, occurs at five hundred degrees. In addition, the material will no longer be a high-performance nanomaterial but a bulk ceramic, having lost the special qualities that make P25 a worldwide standard in photocatalysis.

6. Conclusion

It is a scholarly, evidence-based study of the structural and morphological changes in Degussa P25 during controlled thermal treatment, reporting remarkable conclusions on how Titanium dioxide can be optimized for the application of advanced green technologies. Through a systematic analysis of structured data from 320 observations, the study determined accurate correlations between annealing temperature and material transformation, combining crystallographic, morphological, and compositional data within a single framework. The findings thoroughly substantiate the claim that thermal annealing is a potent tool for adjusting the crystallinity of titanium dioxide to enhance the lattice order and improve its electronic properties, which are crucial for photocatalytic and energy-related applications. The results, however, also show a trade-off that is quite detrimental to excessive thermal treatment, with consequential negative effects including particle sintering, loss of surface area, and a significant alteration in the anatase-rutile phase ratio.

Among all the tested conditions, 500 o C is the most suitable thermal range at which the material exhibits a very stable, well-defined crystalline structure and retains its nanoscale characteristics and active surface sites. It is at this temperature that the material's structural and functional stability is maintained, and it can now bask in enhanced charge transport without losing reactivity. These findings demonstrate the importance of precision in thermal regulation in material engineering. They can be regarded as a positive indicator of the development of the high-performance titanium dioxide systems. This work has implications for both practice and application, including self-cleaning finishes, environmental clean-up, and hydrogen generation, where efficiency and long life are vital considerations. This research, therefore, provides a background contribution that helps rationally design and implement titanium dioxide for sustainable energy and environmental technologies in the long term.

6.1. Limitations

The major drawback of the study is that it discussed only one commercial product, Degussa P25, which is not the best example of the wide variety of modified or doped titanium dioxide materials used in advanced commercial applications. One example is the doping of titanium dioxide with metals or non-metals, and composite systems of titanium dioxide could have different thermal characteristics and phase change properties that are not captured in this context. Also, thermal treatments were performed under normal atmospheric conditions, which limits the interpretation of the effects of alternative conditions, e.g., vacuum or a controlled inert gas atmosphere, on atomic diffusion, oxygen vacancy formation, and phase stability. The other weakness is the technique used to measure particle size and morphology, which primarily relies on diffraction methods and microscopy. Although these methods are more precise at determining external dimensions and structural attributes, the internal pore architecture or microstructural heterogeneity is not fully captured, and these factors are important for gas-phase catalytic processes. Moreover, with a dataset of 320 observations, the study has high statistical reliability and trend consistency. Still, it does not go to actual performance testing, which is associated with real-world systems. In particular, the thermally treated samples were not tested for photocatalytic efficiency or electronic behavior in the operational devices.

6.2. Future Scope

Other processing parameters and application-oriented reviews of the Titanium dioxide can be applied to the current findings in future studies. One of the largest extensions is the investigation of the influence of other gaseous environments on the annealing process (e.g., oxygen-rich, nitrogen, or inert atmospheres) to determine their impact on phase stability, defect formation, and surface chemistry. Such studies have the potential to demonstrate how to stabilize the anatase state at higher temperatures, thereby increasing the operating temperature of high-performance photocatalysts. Another promising area is to examine the relationship between cooling rates and the resulting material end products with respect to structure and electronic properties. Rapid or gradual quenching at a controlled rate can alter imperfections, the distribution of oxygen vacancies, and grain boundaries, which directly affect conductivity and catalytic activity. The second experiment may include using the most suitable of them, at 500 degrees Celsius, in real photocatalytic cells to determine their capacity to produce hydrogen, eradicate pollutants, or convert solar energy into any of the three. This application-based validation can help fill the gap between structural optimization and functional performance.

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