JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **17** No 3, 03027(5pp) (2025)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **17** № 3, 03027(5cc) (2025)

OPEN ACCESS

REGULAR ARTICLE

Dynamic Optimization of Non-Equilibrium Processes in Nanostructures for High-Performance Applications

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(Received 15 April 2025; revised manuscript received 16 June 2025; published online 27 June 2025)

Dynamic optimization of non-equilibrium processes in nanostructures is critical for enhancing their functionality in high-performance applications, including nanoelectronics and energy devices. This research investigates the impact of controlled non-equilibrium synthesis on the structural, chemical, and electrical properties of nanostructured materials, focusing on titanium dioxide (TiO_2) and zinc oxide (ZnO) nanostructured films. These nanostructures are synthesized using chemical vapor deposition (CVD) and electrodeposition, where deposition parameters are dynamically tuned to optimize crystallinity, surface morphology, and electronic behavior. CVD deposits uniform, high-purity TiO_2, and ZnO films by controlling gas-phase precursor reactions on a heated substrate, ensuring well-defined crystallinity and surface morphology. Electrodeposition is utilized to synthesize nanostructured films in an aqueous electrolyte by electrochemically reducing metal precursors, allowing for tunable thickness, porosity, and grain size. The resulting films are characterized using Brunauer-Emmett-Teller (BET) surface area analysis, X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR) to assess textural properties, phase purity, and chemical interactions. This research demonstrates how precise control of non-equilibrium states during synthesis can optimize nanostructure properties. It highlights the effectiveness of dynamic optimization in non-equilibrium synthesis, and paves for their integration into high-performance nanostructured devices.

Keywords: Titanium Dioxide (TiO_2), Zinc Oxide (ZnO), Non-Equilibrium Processes, Nanostructures, X-ray diffraction (XRD).

DOI: 10.21272/jnep.17(3).03027 PACS numbers: 61.05.C –, 77.84.Bw

1. INTRODUCTION

Nanostructures have transformed various technological areas because they contain exclusive physical, chemical, and mechanical properties. Nanoscale materials show distinct characteristics when compared to their bulk material form due to dimensions measured in nanometers (Gigault et al., 2021). The successful application in a multitude field of nanostructures results from their ability to operate outside equilibrium states. Non-equilibrium processes comprise dynamic and time-dependent phenomena that force systems to exit the thermodynamic equilibrium state while producing unique structural, electrical and thermal effects (Khantuleva, 2022). The comprehension and control of such processes drive the optimal development of nanostructures for high-performance applications across electronic systems energy storage, catalytic and biomedical fields (Li and Jin 2021).

The processes of non-equilibrium processes in nanostructured materials take place by phase transitions in addition to defect dynamics and electronic excitations. Systems undergo such processes following outside stimuli, such as heat and electricity as well as optical radiation and mechanical impacts that modify their structural energy distribution (Avdizhiyan et al., 2023). The catalytic activity alongside the optical properties of nanoparticles

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Cite this article as: A. Shrivastava et al., *J. Nano- Electron. Phys.* 17 No 3, 03027 (2025) https://doi.org/10.21272/jnep.17(3).03027

increases due to metastable phases produced through laser-induced heating or rapid quenching techniques. Non-equilibrium processing of nanocrystalline materials through defect and grain boundary control provides improved mechanical performance and improved ionic conductance to benefit lithium-ion batteries and fuel cells (Jamil and Fasehullah, 2021).

Nanostructures with small dimensions enhance interface reactions and surface mobility when reacting systems are away from balance. Catalytic processes depend on this phenomenon because the active interface changes shape while reactions take place to boost performance (Wu et al., 2021). Semiconductor nanostructures with non-equilibrium carrier behavior enable the development of devices with ultrafast photonics and highly efficient solar cells through fast charge separation and movement. Advances in experimental techniques, such as extremely fast spectroscopy, in situ electron microscopy, and atomistic simulation have offered more insights into non-equilibrium processes at the nanoscale (Yun et al., 2022). The focus of the exploration effect of dynamic optimization of non-equilibrium synthesis on structural, chemical, and electrical properties of TiO_2 and ZnO nanostructured films. Through controlling deposition conditions, the research aims at increasing charge transport, defect reduction, and performance improvement of nanomaterials for high-performance energy and electronic devices.

2. RELATED WORKS

Using pulsed laser deposition (PLD) for a system consisting of three phases of $BaTiO_3$ (BTO) with Au and Fe, Rutherford et al., (2022) attempts to investigate the unique characteristics of nanocomposite thin films. Nanoparticle morphology changes from separate to alloyed structures when the laser frequency was adjusted, enabling the tuning of magnetic and optical characteristics. It shows how non-equilibrium approaches might be used to develop new material systems.

The research investigated the heat transport characteristics in a non-Newtonian fluid using Ti6Al4V and AA7075 nanoparticles in a porous media with magnetic effects under local thermal non-equilibrium (LTNE) circumstances by Alsulami et al., (2023). The boundary value issue was solved using the Runge–Kutta–Fehlberg methodology and the firing method. The findings indicated that higher magnetic and porosity parameters improved thermal performance and reduced velocity. The model's simplicity and the omission of some intricate interconnections were among its drawbacks.

Shun et al., (2024) aimed to enhance hydrogen spillover by creating non-equilibrium RuNi alloy nanoparticles. To facilitate hydrogen spillover, graphene oxide was heated in air to produce ether groups and carbon defects. The results demonstrated the enhanced catalytic activity of RuNi nanoparticles in the hydrolysis of ammonia borane. The requirement for further scalability and long-term stability analysis was a drawback.

Understanding the real-time creation of ultra-thin gold layers on films of polymers for flexible electronics used through Schwartzkopf et al., (2021). The interfacial morphology and gold diffusion were tracked using situ high-rate sputter deposition with a temporal resolution of 0.5 ms. Rapid gold intermixing and unexpected cluster aspect ratio variations were shown by the results. Limitations include scalability issues and possible material-specific discoveries.

3. METHODS AND MATERIALS

The dynamically optimizing synthesis conditions during synthesizing titanium dioxide (TiO_2) and zinc oxide (ZnO) nanostructured thin films improve their structural, chemical, and electrical properties.

3.1 Target Materials Preparations

TiO_2 and ZnO, are pressed into pellets of 5-10 mm at high pressure. It was sintered at 600 °C for 4-6 hr to enhance density and crystallinity. It was used as source material for CVD and electrodeposition reactions, where it was deposited on a substrate or submerged into an electrolyte solution for the development of nanostructures.

3.2 Material Synthesis

Using specified techniques scientists create nanostructured materials to control their structure together with their properties. Heated substrates accept thin, uniform films by gas precursor methods in CVD, whereas electrodeposition produces films through electrochemical reduction of solution-based metal ions enabling control over texture, thickness and regulation.

3.2.1 CVD

A gas, caring a material to be deposited (a precursor) is introduced into a chamber. The substrate (the surface where the material is deposited) is heated to very high temperatures. The heat energy breaks up the gas molecules and they deposit a thin solid film on the substrate. Figure 1 illustrates the Chemical Vapor Deposition (CVD) process. To fabricate TiO_2 nanostructured thin films, it can use titanium tetrachloride ($TiCl_4$) gas as a precursor. When $TiCl_4$ is heated in the presence of oxygen (O_2), it produces a thin film of titanium dioxide (TiO_2) on the surface. This process ensures the film is high-purity, uniform, and well-crystallized, which is appropriate for solar cells and photocatalysis uses.

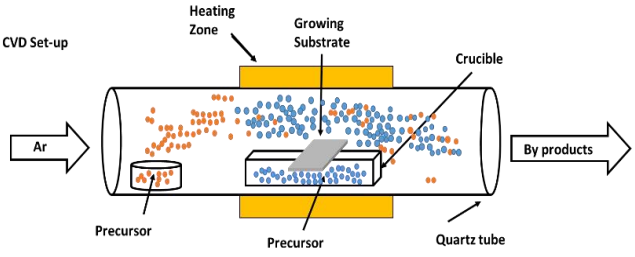

Fig. 1 – CVD process for fabricating TiO_2 nanostructured thin films

3.2.2 Electrodeposition

A dissolved metal ion is introduced as a metal precursor to a liquid electrolyte solution. A negative potential (cathode) is applied on the substrate to draw in the metal ions. Ions receive electrons (reduction reaction) and condense as a thin film on the substrate. Figure 2 illustrates the Electrodeposition process. A ZnO nanostructured film production starts with the electrolysis of zinc nitrate ($Zn(NO_3)_2$) in a water solution. The deposition of zinc ions alongside oxygen ions becomes possible through the electrical current formation of ZnO on the electrode surface. The controlled manufacturing process enables the production of devices with precise thicknesses, porosities and grain sizes, which makes it appropriate for sensors along with transparent electronic devices and energy storage technologies.

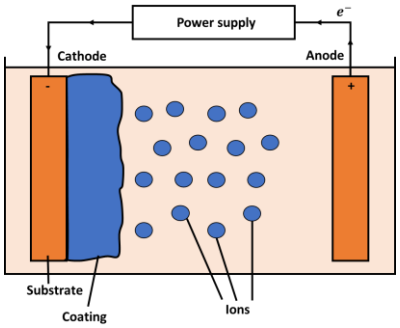

Fig. 2 – Electrodeposition process for fabricating ZnO nanostructured thin films

3.3 Optimizing Parameter

The temperature, precursor concentration, and deposition time are essential to regulate the structural and electrical properties of nanostructured TiO_2 and ZnO films. Crystallinity is regulated by temperature; for example, TiO_2 films deposited at 400-600 °C exhibit more ordered structures compared to low-temperature-deposited films. Grain size and thickness are regulated by precursor concentration; an appropriate zinc nitrate concentration (0.1-0.2 M) in electrodeposition provides uniform ZnO films, whereas high concentration results in roughness. Deposition time regulates film thickness and porosity; e.g., 30-minute electrodeposition provides well-covered, crack-free films, and longer deposition can impose cracks. By controlling these parameters to the optimal level, the nanostructures achieve enhanced stability, charge transport, and overall performance. Table 1 presents a summary of how each parameter varies to enhance the quality and performance of TiO_2 and ZnO nanostructured films.

Table 1 – Optimization parameters and their impact on the structural properties of TiO_2 and ZnO nanostructured films

Parameter	Effect	Optimal Outcome
Temperature	Controls crystallinity and grain size	400–600 °C for well-defined, defect-free crystals
Precursor Concentration	Affects film thickness and grain size	0.1 M – 0.2 M for uniform, connected grains
Deposition Time	Determines film thickness and porosity	30 minutes for balanced thickness and fewer defects

4. RESULT

Dynamic optimization in the synthesis of ZnO and TiO_2 nanostructures influences their structural, electrical, and chemical properties. The most important results are obtained through various characterization methods and electrical tests like BET, XRD, and FIRT.

Different methods of film fabrication through CVD and electrodeposition affect the EOT in TiO_2 and ZnO nanostructured films as shown in Figure 3. The EOT value of TiO_2 films reaches higher levels through CVD because the films establish thicker and more consistent layers. The EOT values of ZnO films grown through electrodeposition are lower than those obtained through electrodeposition because film thickness increases more gradually. The ability to control film thickness arises from electrodeposition by optimizing deposition time and chemical concentration. The examination indicates that these approaches generate materials of varying thickness levels, thus influencing their electronic application capabilities.

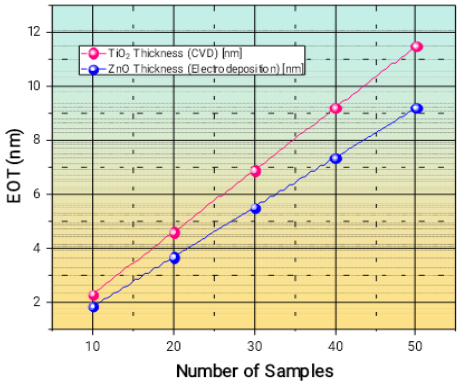

Fig. 3 – EOT of TiO_2 and ZnO nanostructured films synthesized using CVD and electrodeposition

4.1 Brunauer-Emmett-Teller (BET)

The surface area of solid or porous materials can be measured through BET theory, which reveals vital structural details about these materials. Nanostructured TiO_2 and ZnO thin films show properties, such as adsorption capacity together with catalytic activity, which is directly affected by the material's surface area.

$$\frac{1}{X\left(\left(\frac{Q_0}{Q}\right)-1\right)} = \frac{1}{X_n D} + \frac{D-1}{X_n D}\left(\frac{Q}{Q_0}\right) \quad (2)$$

Where equation (2), X_n is the weight of the film deposited that forms a monolayer of surface covering, and

X is the weight of the gas deposited at an average pressure of $\frac{Q}{Q_0}$. Since the amount of energy of adsorption in the first deposited layer is associated with the term D, BET (D) constant, its value indicates the strength of the deposit interactions.

Table 2 – BET surface area analysis for TiO_2 and ZnO nanostructured films at different heat treatment temperatures (HTT)

Sample Name	HTT (°C)	BET Surface Area (m^2/g)	Phase Composition (Anatase: Rutile)	Average Crystallites Size of Anatase (nm)
TiO_2	400	85	100:00	10
TiO_2	600	45	60:40	25
ZnO	400	50	–	–
ZnO	600	30	–	–

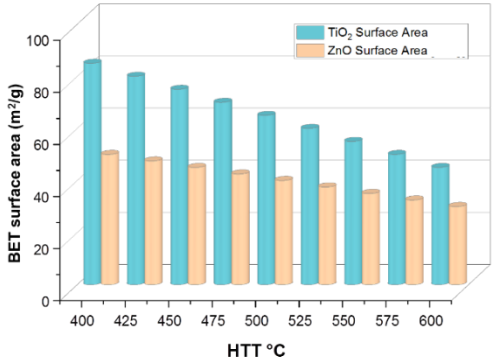

Fig. 4 – BET surface area analysis of TiO_2 and ZnO nanostructured films

Anatase and rutile are two forms of TiO_2 crystals, but ZnO does not have any such forms. ZnO comes in a naturally occurring form with a different crystal structure called the wurtzite structure that does not alter like TiO_2 when treated with heat. In addition, crystallite size is included only in TiO_2 as it indicates the variation of TiO_2 with varying temperatures. ZnO crystal structure does not change; thus, this measurement is not required in ZnO.

4.2 X-Ray Diffraction

Temperature variations influence both TiO_2 and ZnO nanostructured film crystal structures, according to X-ray diffraction (XRD) analysis. A temperature of 400 °C generates TiO_2 anatase crystals of smaller size, which transform into mixed anatase-rutile crystals at 600 °C while the crystal dimensions increase, as shown in Figure 5. The wurtzite crystal structure exists in both ZnO films, although higher operation temperatures lead to bigger crystallites, which results in less intense peaks due to structural compactness. The examination indicates how heat modifications influence crystallite dimension and phase identity, which shapes the entire material properties.

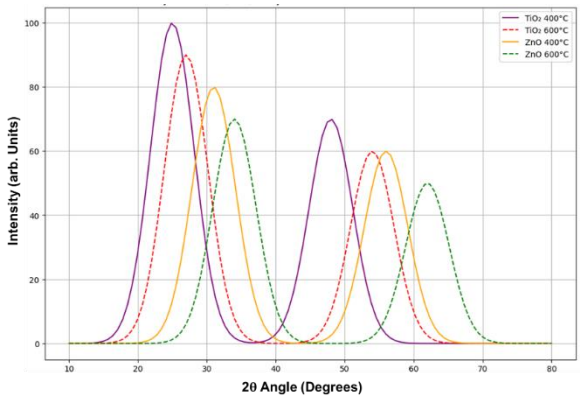

Fig. 5 – XRD analysis of TiO_2 and ZnO

Fourier-transform infrared spectroscopy (FTIR)

In contrast to traditional infrared spectroscopy methods, FTIR uses a mathematical process known as a Fourier transform to convert raw data into a readable spectrum, providing high resolution and sensitivity. Fourier-transform infrared (FTIR) spectroscopy is used to identify and analyze chemical compounds in materials, like TiO_2 and ZnO by measuring their infrared absorption across various wavelengths.

5. CONCLUSION

Structural chemical and electrical properties of TiO_2 and ZnO nanostructured films underwent analysis under dynamic optimization of non-equilibrium synthesis for high-performance applications. The production through CVD and electrodeposition required dynamic parameter control of temperature with precursor concentration and deposition time for improving film quality. The optimized synthesis parameters produced better material stability and lower defect density along with improved charge transport using current-voltage (I-V) performance. The assessment proved that dynamic optimization of non-equilibrium synthesis greatly improved the structural and electrical properties of TiO_2 and ZnO nanostructures to be integrable in high-performance nanoelectronic and energy devices. The complex control of synthesis parameters presents the main challenge in dynamically optimizing non-equilibrium nanostructures, as it reduces both reproducibility and scalability. Future research can explore advanced automation systems, machine learning algorithms, and multi-material hybrid nanostructures to enhance accuracy, scalability, and applications in nanoelectronics, energy storage, and sensors.

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Динамічна оптимізація нерівноважних процесів у наноструктурах для високопродуктивних застосувань

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Динамічна оптимізація нерівноважних процесів у наноструктурах має вирішальне значення для підвищення їхньої функціональності у високопродуктивних застосуваннях, включаючи наноелектроніку та енергетичні пристрої. Це дослідження показує вплив контрольованого нерівноважного синтезу на структурні, хімічні та електричні властивості наноструктурованих матеріалів, зосереджуючись на наноструктурованих плівках діоксиду титану (TiO_2) та оксиду цинку (ZnO). Наноструктури синтезуються за допомогою хімічного осадження з парової фази (CVD) та електроосадження, де параметри осадження динамічно налаштовуються для оптимізації кристалічності, морфології поверхні та електронної поведінки. CVD осаджує однорідні, високочисті плівки TiO_2 та ZnO, контролюючи реакції попередників у газофазній фазі на нагрітій підкладці, забезпечуючи чітко визначену кристалічність та морфологію поверхні. Електроосадження використовується для синтезу наноструктурованих плівок у водному електроліті шляхом електрохімічного відновлення металевих попередників, що дозволяє налаштовувати товщину, пористість та розмір зерна. Отримані плівки характеризуються за допомогою аналізу площі поверхні методом Брунауера-Еммета-Теллера (БЕТ), рентгенівської дифракції (XRD) та інфрачервоної спектроскопії з перетворенням Фур'є (FTIR) для оцінки текстурних властивостей, фазової чистоти та хімічних взаємодій. Це дослідження демонструє, як точний контроль нерівноважних станів під час синтезу може оптимізувати властивості наноструктур. Воно підкреслює ефективність динамічної оптимізації в нерівноважному синтезі та відкриває шляхи їх інтеграції у високопродуктивні наноструктуровані пристрої.

Ключові слова: Діоксид титану (TiO_2), Оксид цинку (ZnO), Нерівноважні процеси, Наноструктури, Рентгенівська дифракція (XRD).