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Studying the effect of solution temperature on the structural and spectral properties of nano barium oxide

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Abstract
In the current study, nano barium oxide is synthesized using the co-precipitation method with sodium hydroxide (NaOH) as the precipitating agent. The effect of solution temperature within the ranges of 25°C, 60°C, and 90°C on the structural and spectral properties is studied.
The results of the analyses show that the phase of the powders does not change with increasing solution temperature—all powders exhibited a tetragonal crystalline structure with a lattice constant of 4.209. However, it is observed that the nanoparticle grain size increases with rising temperature. The XRD analysis reveals grain sizes of 12.36 nm, 16.1 nm, and 17.4 nm at solution temperatures of 25°C, 60°C, and 90°C, respectively. The IR spectrum results also indicated an increased presence of the O-H bond at 90°C. Additionally, the UV spectrum analysis shows an increase in absorbance with the decrease in grain size and the increase in the surface area of the prepared powders.

Keywords: Nano barium oxide, co-precipitation method, solution temperature, structural properties, spectral properties.

1. Introduction
Nano barium oxide (BaO) is considered one of the important nanomaterials that has attracted significant attention in various fields, such as chemical catalysis, energy storage, and optoelectronics, due to its unique physical and chemical properties. Reducing the material to the nanoscale enhances its structural and spectral properties, resulting in new behaviors compared to its micro- and macro-scale forms [1]. The structural properties of nano barium oxide largely depend on the synthesis method used, such as chemical precipitation, thermal methods, or the sol-gel technique. Nano BaO is characterized by a distinct crystalline structure that can be studied using techniques like X-ray diffraction (XRD), and electronic microscope examinations (SEM and TEM) which reveal the particle size, distribution, and morphology [2]. Particle size significantly affects the effective surface area, making it a promising material for numerous applications. Moreover, spectral properties play an important role in understanding the behavior of nano BaO and its applications in optical and electronic fields [1, 3, 4]. The present study aims to investigate the effect of increasing the solution temperature on the grain size of nano barium oxide synthesized via the co-precipitation method, which in turn influences its structural and spectral properties.

2. Practical Aspect
2.1 Preparation of the Nano Powder
The raw materials used in the preparation of primary solutions for the production of barium oxide (BaO) using the co-precipitation method, along with their chemical formulas, purities, and manufacturers, are listed in Table (1). A solution of barium acetate hydrate ($C_4H_6BaO_4$) and deionized water is prepared Prepare a 0.5 M solution, then add 1.5 M acetic acid (CH_3COOH). Stir the mixture using a magnetic stirrer at 3000 rpm for at least 2 hours. After stirring, let the solution rest for 24 hours to ensure complete dissolution before use.
To prepare the basic solution, the raw materials of the base (as listed in Table 1) are added separately at a concentration of 1.5 M and Add deionized water. Dissolution is carried out using a magnetic stirrer following the same procedure used for preparing the barium acetate hydrate solution. All solutions are passed through a filtration process to remove impurities and potential power particles before continuing with the analysis.

The base solution is then added dropwise at of $5\frac{ml}{min}$ to the barium acetate hydrate solution, The mixture is placed on a magnetic stirrer at a rotation speed of 300 rpm, and under different temperature conditions (25°C, 60°C, and 90°C, respectively). The dropwise addition continues until the desired pH value (pH = 12) is reached, at which point the precipitation process is stopped. The resulting precipitate is washed with deionized water until neutrality is achieved (pH = 7). Then it dries at 100°C for 72 hours. After drying, the powders are placed in a calcination furnace where the temperature is raised to 600°C and maintained for 2 hours, then leave it to cool gradually.

Table 1: Chemicals used in the preparation

No	materials chemicals	Chemical formula	Purity%	Manufacturer
1	Aqueous barium acetate	$C_4H_6BaO_4$	98	Merck
2	Acetic acid	CH_3COOH	65	Merck
3	Sodium hydroxide	NaOH	99	GmbH

2.2 Characterization of nano powders

To conduct all the tests, the following steps are to be followed:

2.2.1 X-Ray Diffraction Test

The English scientist W.L. Bragg was able to establish an important mathematical relationship for determining the interplanar spacing in crystals using X-ray diffraction. He based his work on the fact that atoms within a crystal are arranged in distinct sets of planes. When a beam of X-rays strikes these planes, it is scattered in various directions within the crystal. From this scattering, the interplanar distances and Miller indices can be determined, thereby allowing the identification of the phases present in the material by applying the following equations [5-7].

$$n\lambda = 2d\sin\theta \quad (1)$$

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (2)$$

where h, k, and l are known as Miller parameters, and d is the interatomic distance.

To calculate the grain size, the Scherrer equation is used in the following form:

$$D = \frac{K\lambda}{\beta \cos\theta} \quad (3)$$

Where

θ: X-ray diffraction angle

β: Full Width at Half Maximum

K: shape factor

To calculate the grain size, the Scherrer equation is applied.

To estimate the specific surface area from the grain size, the following formula is used:

$$D = \frac{6}{S \times \rho} \quad (4)$$

Where:

S: Specific surface area ($m^2 \cdot mg^{-1}$)

ρ: Density of barium oxide, 5.7 g/cm^3

To perform this analysis, X-ray diffraction (XRD) is used, employing a Shimadzu-manufactured instrument (of Japanese origin). The target material used in the X-ray tube is copper (Cu) with a wavelength of 1.54060 Å.

2.2.2 Fourier Transform Infrared Spectroscopy (FTIR) Analysis

Infrared spectra were recorded using a Fourier transform FTIR spectrometer (Shimadzu 8400), manufactured in Japan. The analysis is conducted by mixing a portion of the sample powder with potassium bromide (KBr), then pressing the mixture into pellet form. The spectra are recorded within the wavenumber range of 400-4000 cm^{-1}.

2.2.3 UV-Visible Spectroscopy Analysis (UV-VIS)

Ultraviolet-visible (UV-Vis) spectroscopy is considered a fundamental analytical tool for characterizing the optical properties of nanomaterials, providing valuable insights into their shape, size, distribution, and aggregation behavior. In this study, UV-Vis absorption spectra were recorded using a Shimadzu UV-1800 spectrophotometer (Japan) within the wavelength range of 200-1100 nm. The nanomaterial suspensions were prepared by dispersing a specified amount of nanopowder in deionized water at a concentration of 0.01 M to ensure homogeneous dispersion. To prevent rapid particle agglomeration, the solution was subjected to ultrasonic treatment using an ultrasonic bath for 30 minutes, which enhanced colloidal stability and improved the accuracy of the spectral measurements

Discussion and Findings

3.1 X-ray diffraction

The X-ray diffraction (XRD) results for nano barium oxide are shown in Figure (1), where the recorded XRD patterns of the samples reveal the appearance of characteristic peaks at (100), (101), (111), (110), and (103) corresponding to diffraction angles of 23.7°, 24.01°, 29.72°, 35.00°, and 44.21°, respectively. These peaks are consistent with the standard card (JCDS.NO-8425-89) and confirm a tetragonal crystal structure with a lattice constant of 4.209 Å [8]. It is observed that increasing the solution temperature enhances the crystallization of the tetragonal phase, as indicated by the increase in peak intensity. This behavior is attributed to the gradual growth of crystals with increasing temperature, reaching a point where higher thermal energy promotes more particle collisions and larger grain growth. As shown in Table (2), with increasing solution temperature, the nanocrystalline grain size increases, while the specific surface area decreases. This is because elevated temperatures enhance grain growth. Compared to powders synthesized at room temperature, higher temperatures allow more time for the aggregation of numerous small grains, increasing the likelihood of interaction during the crystallization process, ultimately resulting in the formation of larger crystallites. This observation is consistent with the findings of [9].

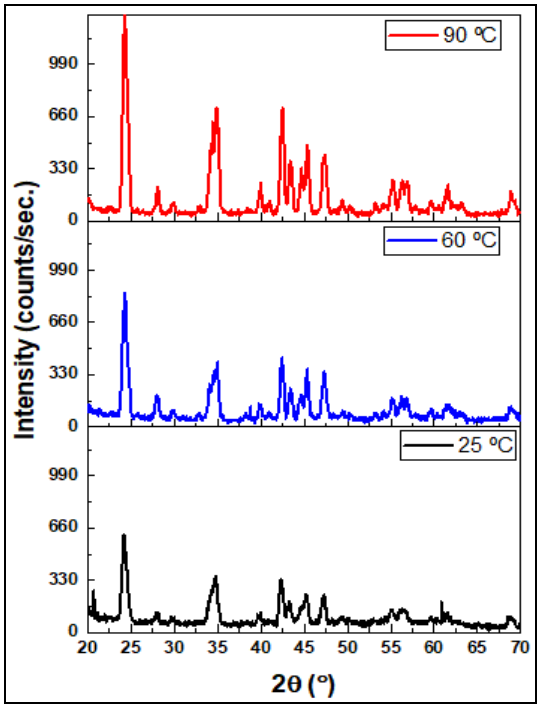

Fig 1: Shows the X-ray diffraction examination of barium oxide nanoparticles as a function of solution temperature.

Table 2: Shows X-ray diffraction parameters

Models BaO	S (m^2/mg)	D (nm)	a (Å)
25°C	8*7*.5	1*1*.3	4.209
60°C	6*4*.3	1*7.2*	4.209
90 °C	60.*20*	17.*9*	4.209

3.2 The Effect of pH on the Spectral Properties

3.2.1 FTIR (Fourier Transform Infrared) Spectrum

The FTIR analysis provides information about the vibrational modes of molecules. The FTIR spectra of the samples were recorded in the range of 4000-500 cm^{-1} at room temperature. The infrared spectrum shown in Figure (2) displays the Ba-Obond stretching bands at wavenumbers 631-592 cm^{-1}, 638-582 cm^{-1}, and 622-573 cm^{-1} for powders prepared at three different temperatures: 25°C, 60°C, and 90°C. The results revealed that increasing the temperature led to a reduction in the nanoparticle grain size, which was clearly reflected by a shift of the vibrational bands toward lower wavenumbers. This behavior is attributed to the increase in specific surface area resulting from the reduced particle size, which enhances the interaction between photons and the particle surface. Consequently, higher photon absorption occurs, leading to an increase in molecular vibrational energy and, hence, an enhancement in the intensity of the observed spectral bands. These results are consistent with those reported by [10].

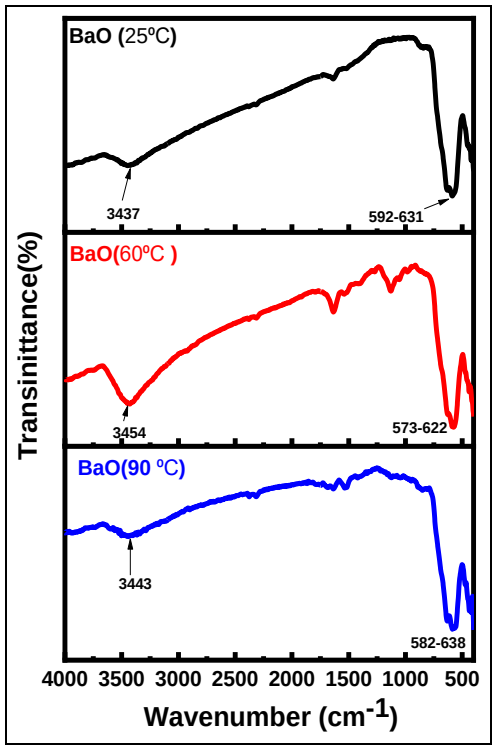

Fig 2: FTIR spectrum of barium oxide nanoparticles as a function of solution temperature.

3.2.2 UV-Visible (UV-VIS) Spectroscopy

Figure (3) shows the relationship between the absorption in the UV-VIS spectrum and the varying nano-crystalline grain sizes resulting from different solution temperatures. It is observed that as the grain size decreases, the absorption values increase. This effect is associated with the enlargement of surface area that occurs as the grain size diminishes, which provides a larger interaction surface between the photons and the BaO powder. Generally, for powders prepared at different solution temperatures, the absorption edge appears below 300 nm, which is consistent with the findings reported in [11].

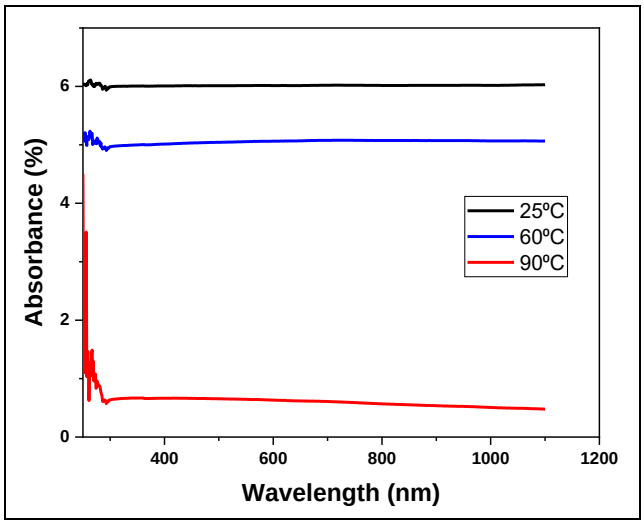

Fig 3: Shows the UV-VIS spectrum of barium oxide nanoparticles

3. Conclusions

- The results of the current investigation indicate that higher solution temperatures promote grain growth in the synthesized BaO powders.
- The intensity of the Ba-O bonds increases with decreasing nano-crystalline grain size of BaO.
- With the reduction in grain size, the absorption values increase across various regions of the visible spectrum.

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