# Investigation of Optical Properties of Barium Oxide (BaO) Thin Films Deposited by Chemical Bath Technique.

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## ABSTRACT

Thin films of barium oxide (BaO) were deposited on glass substrates using a chemical bath deposition technique from aqueous solutions of barium chloride and potassium hydroxide. The film properties studied include optical transmission, optical constants, dielectric constants, optical conductivity, and band gaps. The films in this study produced fairly high transmission (>86% between 400 and 800). Band gaps of 3.45eV for direct transition and 1.60eV for indirect transition were obtained. Such films could be used as transparent conducting oxides for window layers in solar cell fabrications. The films showed poor absorbance in the UV–VIS–NIR regions; hence, they also have potential applications as thermal control coatings for cold climates and as antireflection coatings.

(Key words: Chemical bath deposition, BeO, thermal coatings, thin films, antireflection)

## INTRODUCTION

Various techniques have been employed for thin film deposition including chemical deposition, RF sputtering, pulse laser, molecular beam epitaxy, chemical vapor deposition, and spray pyrolysis. Most of these techniques are expensive and require high vacuum and controlled formation conditions [1]. The chemical bath deposition technique for the creation of thin films from aqueous solution is a promising technique because of its simplicity and economics.

In the last ten decades, this technique has become part of a group of new, intensively studied thin film deposition methods for the synthesis of various functional coatings [2-3] which are mostly sulphide thin films; in particular cadmium sulphide [4-6]. These coatings are being used to develop thin films for photothermal and photovoltaic conversions, decorative and protective coatings, and imaging techniques [5-8]. The chemical bath deposition technique has previously been used for oxide films [4,10].

This paper reports on the optical properties of barium oxide thin films deposited using a chemical bath deposition technique. The optical properties investigated include the absorbance (A), transmittance (T), and reflectance (R), which were used to calculate other properties such as refractive index (n), extinction coefficient (k), dielectric constant ($\varepsilon$), and optical conductivity ($\sigma$). These optical properties and the band gap of the films were deduced from equations within the literature [4, 11-13] while the thicknesses were obtained by using the optical method [14].

## EXPERIMENTAL DETAIL

The deposition of the barium oxide thin films on glass slides at room temperature was achieved using a chemical bath consisting of barium chloride, potassium hydroxide, and distilled water. The substrates (glass slides) were previous degreased in nitric acid for 48 hours, cleaned with detergent in cold water, rinsed with distilled water, and allowed to air dry.

The nitric acid treatment caused the oxidation of the halide ions in the glass slides (halide glass) used as substrates, thereby introducing functional groups called nucleation and/or epitaxial centers, which formed the basis for the thin film growth.

The reaction baths for the deposition of BaO thin films contained alkaline solutions of barium salt and potassium hydroxide in cold water. The reaction baths were made up of given volumes of $BaCl_2•2H_2O$ and KOH solutions added into 50ml beakers in that order. The solutions were stirred thoroughly using glass rods at each stage to obtain a homogenous mixture of the solutions. The reaction baths were made up to 40ml with distilled water and allowed to stand for 6 to 24 hour dip times.

The reaction baths were tested for their pH values and were found to be in the alkaline range before the substrates were introduced into the solutions. The reaction is a hydrolysis reaction [4] occurring at room temperature with KOH acting as both a complexing agent and a pH stabilizer in the alkaline medium.

The basic reaction involved is as follows :

$$BaCl_2 + 3KOH + H_2O \rightleftharpoons 2KCl_2 + 2H_2O + BaO + KOH$$

After the films were deposited, they were rinsed with distilled water and allowed air dry.

The spectral absorbance and transmittance characteristics of the films were obtained using a PYE UNICAM SP8-100UV spectrophotometer in the UV-VIS-NIR regions.

## RESULTS AND DISCUSSION

The spectral absorbance, transmittance, and reflectance of barium oxide films prepared at 300k are displayed in Figure 1.

The sample of the film grown in this work exhibits poor absorbance, high transmittance (between 73% and 96%), and low reflectance (between 2% and 14%) in the UV-VIS-NIR regions. The film produced a high visible transmission (>86%). The property of high transmittance throughout UV-VIS-NIR region makes this film a suitable material for both cold climate thermal control window coatings and antireflection coatings. The variation of n with hν for samples of BaO is shown in Figure 2.

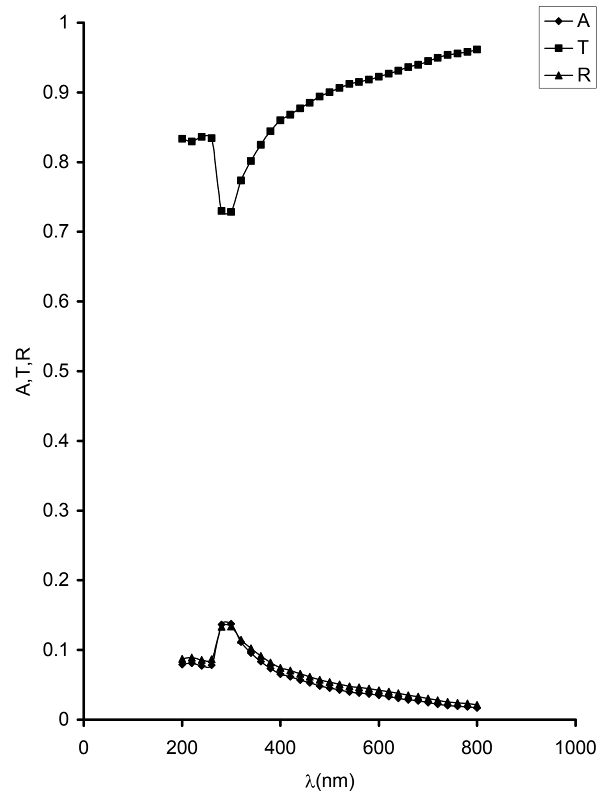


Fig. 1: Spectral Absorbance/Transmittance/Reflectance of BaO Film prepared at 300k.

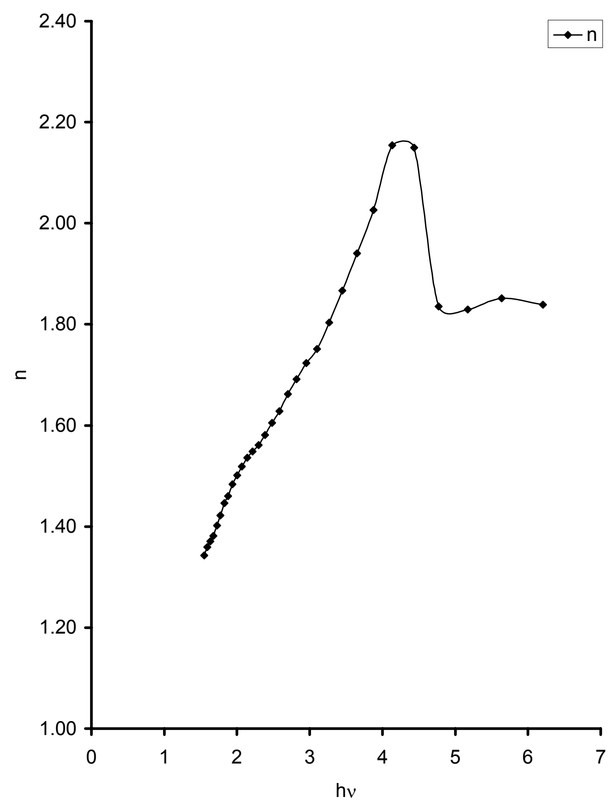


Fig. 2: Plots of Refractive Index (n) against Photon Energy for BaO Sample.

It was observed that n reached a peak value of 2.15 at a photon energy level of 4.14eV. After the fundamental absorption, n decreased with increasing wavelength towards the NIR region.

The variation of k with hν for samples of BaO is shown in Figure 3.

The k peak value for the sample occurred at 7.56 x $10^{-3}$ with a photon energy of 4.14eV.

The BaO thin films prepared in this work were observed to be semiconductors since the maximum value in the refractive index (n) occurred at energy ranges near where the maximum change in k occurred [15]. This can be observed in Figures 2 and 3.

The plots of $\varepsilon_r$ against hν are displayed in Figure 4.

The thin film sample produced a $\varepsilon_r$ peak value of 4.64 at photon energy level of 4.14eV. The plots of $\varepsilon_i$ against hν are displayed in Figure 5.

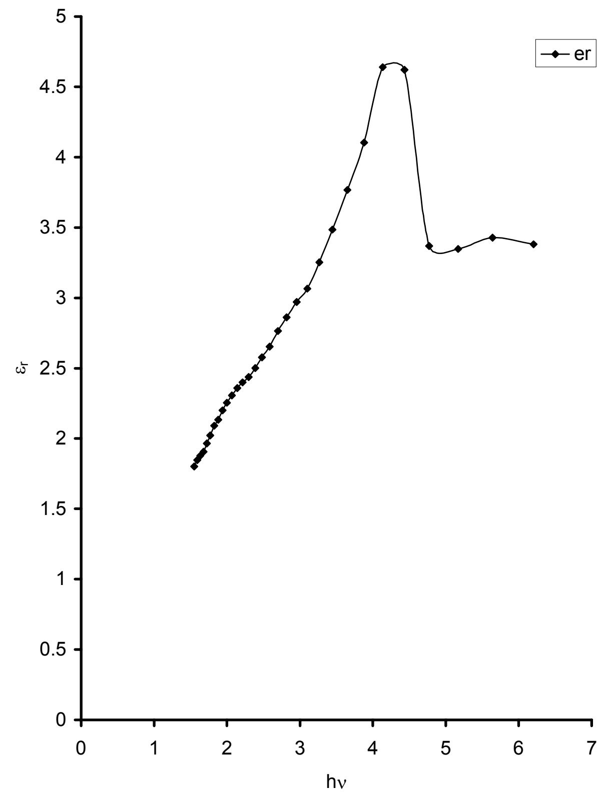


Fig. 4: Plots of Real Dielectric Constant ($\varepsilon_r$) against Photon Energy for BaO Sample.

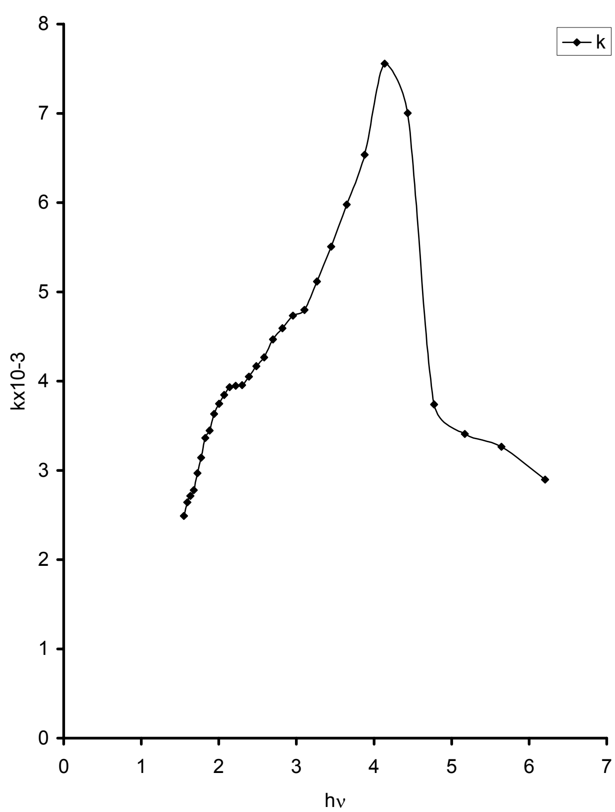


Fig. 3: Plots of Extinction Coefficient (k) against Photon Energy for BaO Sample.

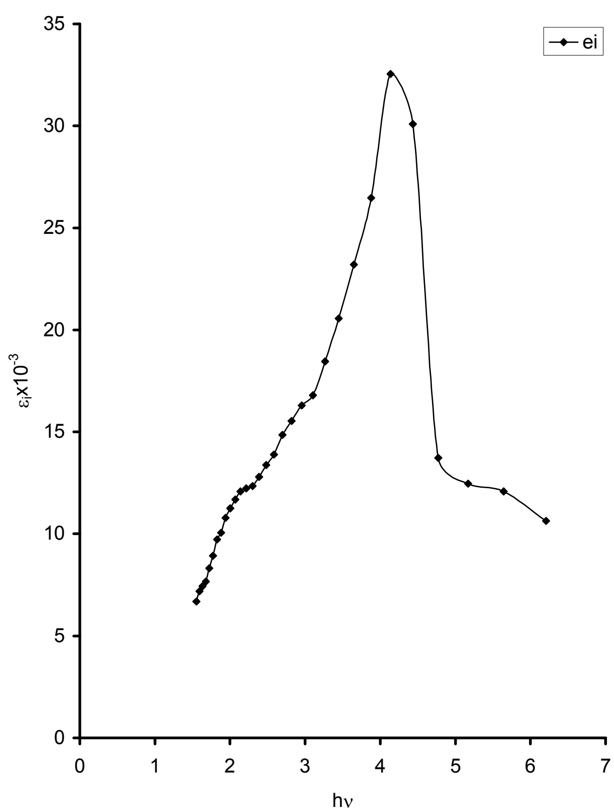


Fig. 5: Plots of Imaginary Dielectric Constant ($\varepsilon_i$) against Photon Energy for BaO Sample.

The sample film produced a $\varepsilon_i$ peak value of $3.25 \times 10^{-2}$. The shapes of the spectral curves of n and k (Figures 2 and 3), and $\varepsilon_r$ and $\varepsilon_i$ (Figures 4 and 5) show a striking similarity.

The plots of optical conductivity $\sigma_o$ against $h\nu$ are shown in Figure 6. The film produced a peak value of $0.16 \times 10^{14} S^{-1}$ at 4.14eV which decreased with decreasing photon energy.

The plot of $(\alpha h\nu)^2$ against $h\nu$ for the BaO film is shown in Figure 7. This reveals a band gap of 3.45eV. Unaogu and Okeke [16] have reported that a high visible transmission and a large band gap is required for use in the window layers of solar cells. Therefore the high visible transmission of this film together with the large band gap makes it a good material for the fabrication of a window layer in solar cells.

The plot of $(\alpha h\nu)^{1/2}$ against $h\nu$ for the BaO film is shown in Figure 8. It reveals an indirect band gap of 1.60eV. The values for complex refractive index, dielectric constant, and optical conductivity increased from the minimum values in low energy regions to peak values at 4.14eV in the higher energy regions and then decreased to low values in the same regions.

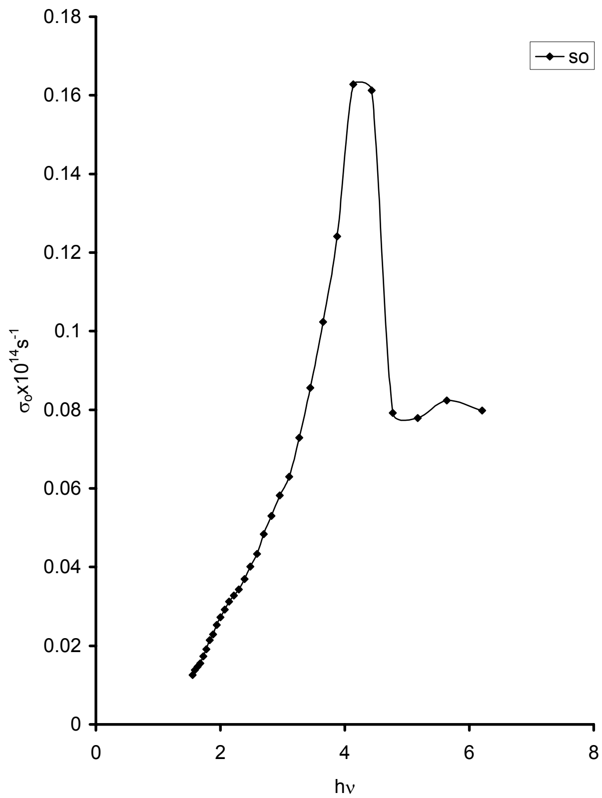


Fig. 6: Plot of Optical Conductivity, $\sigma_o$ against Photon Energy for BaO Sample.

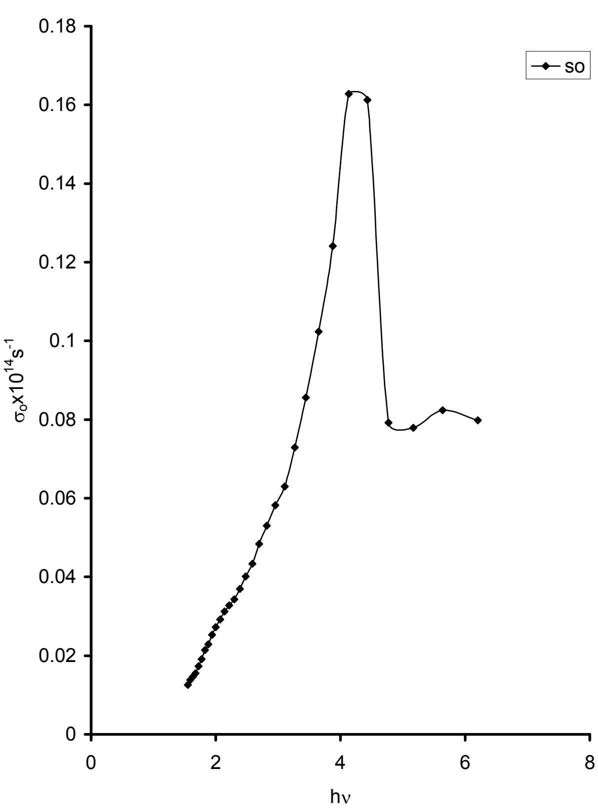


Fig. 6: Plot of Optical Conductivity, $\sigma_o$ against Photon Energy for BaO Sample.

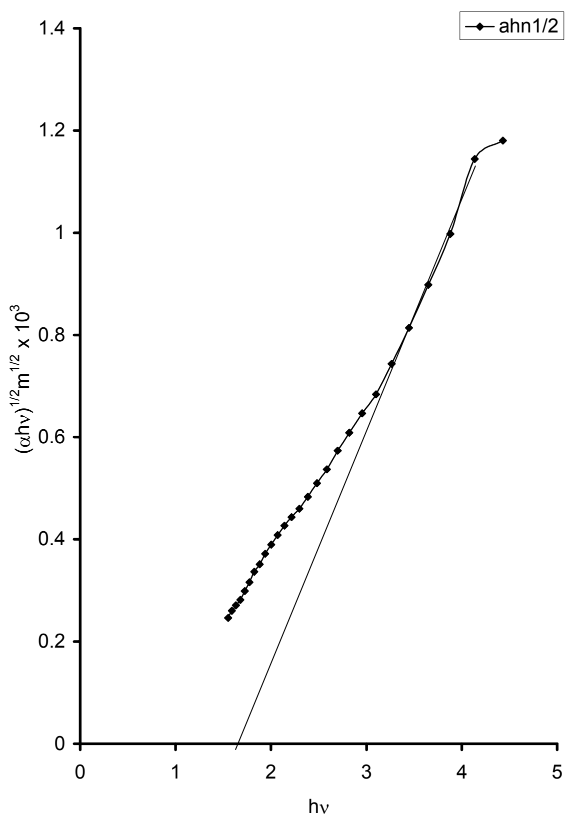


Fig.8: Plots of $(\alpha h\nu)^{1/2}$ against Photon Energy for BaO Sample.

## CONCLUSIONS

BaO thin films were successfully deposited in an alkaline medium using the chemical bath deposition technique. The films produced in this study were found to have high transmittance in the range between 73% and 96% in the UV-VIS-NIR regions; hence, they have potential for use as both thermal control window coatings in cold climates and antireflection coatings. The large band gap (3.45eV) and high visible transmission (>86%) also make the films suitable for use in the window layer of solar cells.

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