

A Study of the Optical Bandgap Energy and Urbach Energy Tail of Two White A4 Copy Paper Samples

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Abstract

Two white A4 copy paper samples Q-Connect and Laser Copy were tested for the fiber component of their pulps using the optical microscope and were determined as chemical pulps. UV-VIS data revealed the values of Urbach energies of 498.2meV and 498.1meV of the two copy paper samples respectively, when the thickness of both samples was $d=1\text{mm}$. The value of indirect bandgap energy was calculated to be 1.16984469010026eV for Q-Connect copy paper sample, and 1.1698449010027eV respectively, with the Laser Copy paper sample. The Urbach energy of the A4 copy paper sample Q-Connect was calculated to be 333.7meV when its thickness was $d=0.101\text{mm}$ whereas the Urbach energy of the A4 copy paper sample Laser Copy was calculated to be 330.2meV when its thickness was $d=0.094\text{mm}$. A decrease in Urbach energy with a decrease in thickness from $101\mu\text{m}$ to $94\mu\text{m}$, and an increase in energy band gap, were observed for the two copy paper samples, respectively.

Keywords: Cellulose; White A4 copy paper sample; Optical bandgap; Absorption spectra; Kubelka-Munk K/S value; Urbach energy (E_u); Band gap energy (E_g); Thickness

Introduction

Paper samples are interesting materials for applications in optoelectronics. Many workers have investigated the optical properties of other materials, stones, thin films, doped thin films, coated glass substrates, and have studied the relation between bandgap energy E_g and thickness and the tailing in the band gap (E_u) [1,2]. The optical properties are useful in studying the electronic band structure, absorption characteristics, and the disorder present in the materials. Urbach has proposed an empirical rule for the optical absorption coefficient $\alpha(\omega)$ associated with electronic transition from the valence to the conduction band tail in disordered solids [3]. The relations are examined between E_g (band gap energy) and thickness and the tailing in the E_g [4]. The increase of band gap energy E_g with film thickness is attributed to the improvement of the crystallinity of the material studied when it becomes thicker [5].

In this work a fiber furnish analysis is carried out under the optical microscope and it is used to determine the fiber component of the pulps of two white A4 copy paper samples quantitatively which were found to be chemical pulps. Then, reflectance measurements are carried out over the spectral range 400-700nm and are processed to extract the spectroscopic and band gap properties of the two white A4 copy paper samples [1,2]. In the present work the thickness dependence of the band gap E_g and Urbach energy tail (E_u) for the two A4 copy paper samples is reported.

Experimental

The microscope, a projection optical microscope SDL S.N. 232431, 220V, 60W, S1, was used with a round screen and no binoculars, and with a magnification of $\times 10/0.2$ to $\times 20/0.4$. Optical properties of the two A4 copy papers were investigated using a UV-Vis spectrophotometer, a CM-3630, BCMTS M Type 40605, S.N. 43029, Touch Screen-M V2.0 Frank-PTI spectrophotometer equipped with an integrating sphere, at room temperature (293K-298K). Important optical parameters like E_g and E_u were calculated by analyzing the reflectance spectra obtained at normal incidence geometry and diffused reflectance spectra were collected for both the samples in the wavelength range of 400-700nm [6]. The thickness of the two copy paper samples was measured using a digital precision micrometer TMI (Testing Machines INC) Model No 49-61-01-0002, S.N. 33421-01 with range 0-1.270mm. The thickness of the two A4 paper samples was measured in the range $100 \pm 10 \mu\text{m}$ and with $\pm 5.5 \mu\text{m}$ uncertainty. As we set the thickness of the paper samples with more significant digits, during the course of this work, we could calculate the Urbach energy more accurately, and we could separate the Urbach energies of the two A4 copy paper samples better.

Results and Discussion

The K/S ratio of the first A4 copy paper sample, Q-Connect, was found to be $K/S=46.63024934$ and the reflectance ISO brightness used was measured to be 95.25% whereas those for Laser copy were 46.67024494 and 95.33% respectively. The ISO brightness measured was the numerical value of the reflectance of the two A4 copy paper samples at 457nm, blue light reflectance. The value of absorption coefficient at a particular wavelength [7] was the ratio of absorption to sample thickness and was represented as α ,

$$\alpha = \frac{A}{d} \quad (1)$$

where α was the absorption coefficient, A was the absorption and d was the thickness of the sample, here $d=1\text{mm}$.

For the calculation of Urbach energy (E_u) the following equation [8] was used,

$$\alpha = \alpha_0 \exp(\frac{hv}{E_u}) \quad (2)$$

where α was the absorption coefficient, α_0 was a constant, and hv was the photon energy. The slope of the logarithm [9,10] of $\ln(\alpha)$ versus hv plot in the lower photon energy region was used for the calculation of E_u (Urbach energy) of the two copy paper samples.

For the calculation of direct and indirect band gap energies the following equation applied,

$$\alpha hv = K(hv - E_g)^x \quad (3)$$

where E_g was the band gap energy and was direct or indirect depending on the value of x. Also, α was proportional to the Kubelka-Munk function $F(R)$ given as follows,

$$(F(R)) = \frac{K}{S} = \frac{(1-R)^2}{2R} \quad (4)$$

where $F(R)$ was the Kubelka-Munk function, R was the reflectance, K was the absorption, and S was the scattering from the samples, and was used for the calculation of Urbach energy and the band gap energy.

The slope of the $\ln(\alpha)$ versus hv plot in the lower photon energy region was used for the calculation of E_u (Urbach energy) of each A4 copy paper sample [11]. The Urbach energy for copy paper Q-Connect was calculated by the slope of the best fit line through the vertical segment of the plot of Figure 1. The slope was calculated to be 2.340036622eV and the Urbach energy of 498.2meV for copy paper sample Q-Connect. UV-V is data revealed the value of Urbach energy of 498.2meV and the value of indirect bandgap energy of 1.16984469010026eV (Figure 2) for copy paper sample Q-Connect. Also, the value of Urbach energy was estimated to be 498.1meV (Figure 3) and the value of indirect bandgap energy of 1.1698449010027eV (Figure 4) for copy paper sample Laser Copy [12]. The thickness of both samples was taken as $d=1\text{mm}$.

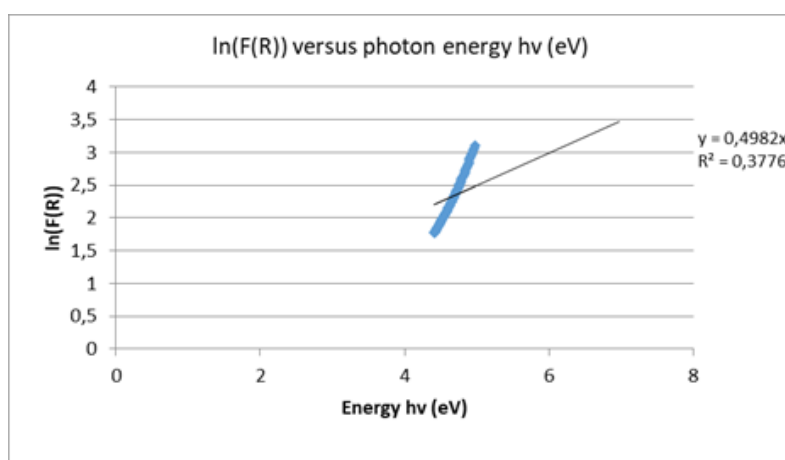


Figure 1: Plot of $\ln(F(R))$ versus photon energy hv for the calculation of Urbach energy of the first copy paper sample Q-Connect where $(F(R)) = \frac{K}{S} = \frac{(1-R)^2}{2R}$ where K was the absorption or coefficient of reflectivity and S was the coefficient of light scattering, and R was the observed reflectivity for monochromatic light.

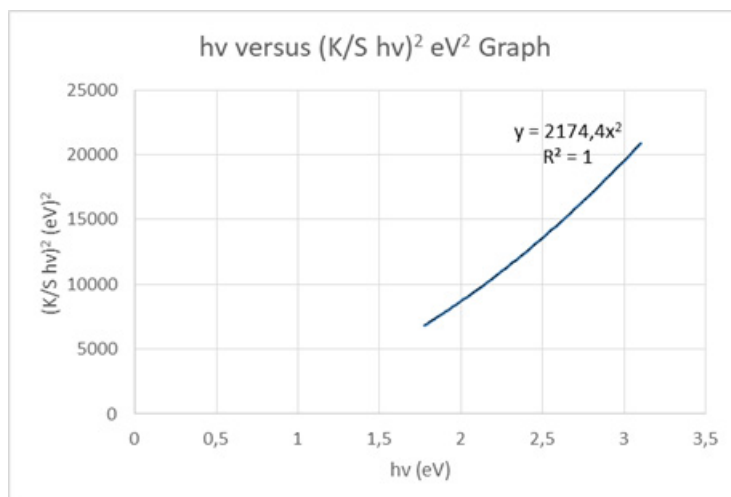


Figure 2: $(K/S hv)^2$ versus hv graph of the cellulosic chromophores i.e., C=O group and double bonds, in the first copy paper sample, Q-Connect consisting of 100% cellulose, for the calculation of band gap energy for permitted indirect transitions $n=2$.

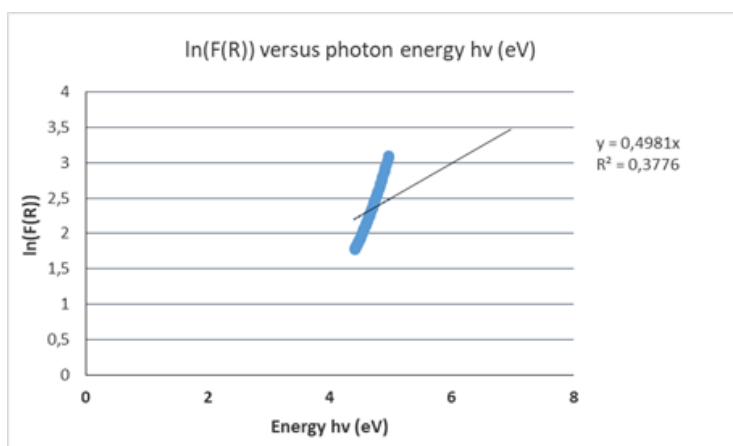


Figure 3: Plot of $\ln(F(R))$ versus photon energy hv for the calculation of Urbach energy of the second A4 copy paper sample Laser Copy.

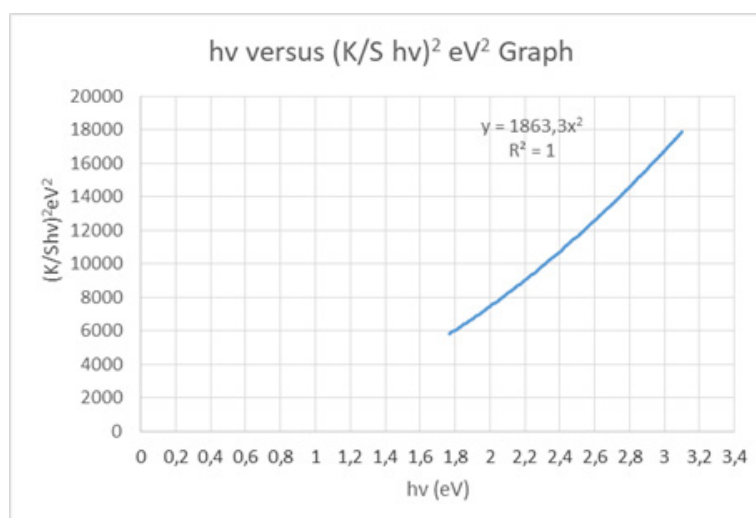


Figure 4: $(K/S hv)^2$ versus hv graph of the cellulosic chromophores i.e., C=O group and double bonds, in the second copy paper sample, Laser copy consisting of 100% cellulose, for the calculation of band gap energy for permitted indirect transitions $n=2$.

The structural disorder due to the presence of impurities in the chemical pulp of the two copy paper samples, at room temperature, was attributed to the low values of Urbach energies and high values in band gaps [13]. The thickness of the two paper samples was also measured as per ISO 534 [14]. The thickness of the Q-Connect A4 paper sample was measured to be 101 μ m and that of Laser Copy A4 paper sample 94 μ m. Thus, a decrease in Urbach energy with decrease in thickness and an increase in energy band gap with a decrease in thickness was observed for the two A4 copy paper samples at room temperature [13]. The Urbach energy varied

inversely to the band gap [15,16].

The slope of the $\ln(\alpha)$ versus $h\nu$ plot in the lower photon energy region was used again for the calculation of E_u (Urbach energy) of each A4 copy paper sample when the thickness of the sample was now $d=0.1$ mm. The Urbach energy for copy paper Q-Connect was calculated by the slope of the best fit line through the vertical segment of the plot of Figure 5. The slope was calculated to be 2.340036622eV and the Urbach energy of 333.2meV for both A4 copy paper sample Q-Connect, and A4 copy paper sample Laser Copy.

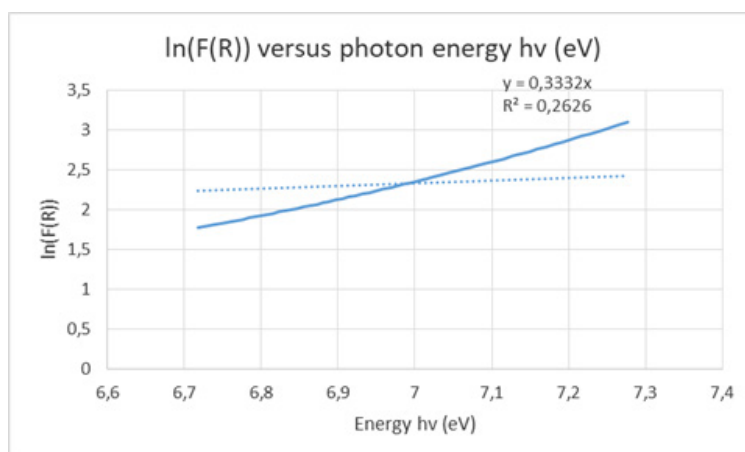


Figure 5: Plot of $\ln(F(R))$ versus photon energy $h\nu$ for the calculation of Urbach energy of the first A4 copy paper sample Q-Connect where $(F(R)) = \frac{K}{S} = \frac{(1-R)^2}{2R}$ where K was the absorption or coefficient of reflectivity and S was the coefficient of light scattering, and R was the observed reflectivity for monochromatic light, when the thickness of the sample was $d=0.1$ mm.

Also, the slope of the $\ln(\alpha)$ versus $h\nu$ plot in the lower photon energy region was used again for the calculation of E_u (Urbach energy) of A4 copy paper sample Q-Connect when the thickness of the sample was $d=0.101$ mm and, also of the A4 copy paper sample Laser Copy when its thickness was $d=0.094$ mm. The Urbach energy for copy paper Q-Connect was calculated by the slope of the best fit line through the vertical segment of the plot of Figure 6 and also for

the copy paper Laser Copy through the vertical segment of the plot of Figure 7 (Table 1). The slope was calculated to be 2.340036622eV and the Urbach energy of 333.7meV for A4 copy paper sample Q-Connect. Also, the slope was calculated to be 2.340036622eV and the Urbach energy of 330.2meV for A4 copy paper sample Laser Copy as listed in Table 1.

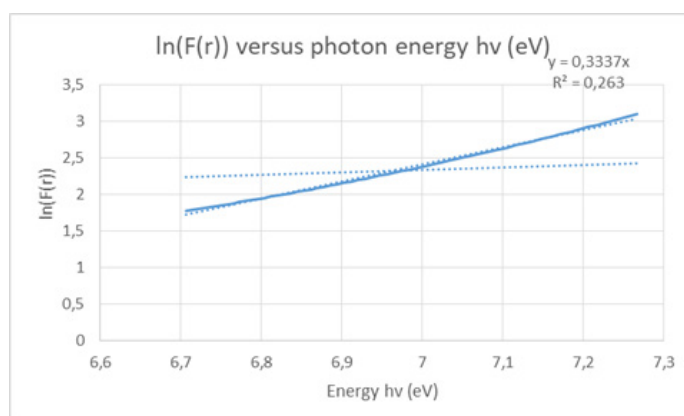


Figure 6: Plot of $\ln(F(r))$ versus photon energy $h\nu$ for the calculation of Urbach energy of the first A4 copy paper sample Q-Connect where $(F(r)) = \frac{K}{S} = \frac{(1-R)^2}{2R}$ where K was the absorption or coefficient of reflectivity and S was the coefficient of light scattering, and R was the observed reflectivity for monochromatic light, when the thickness of the sample was $d=0.101$ mm.

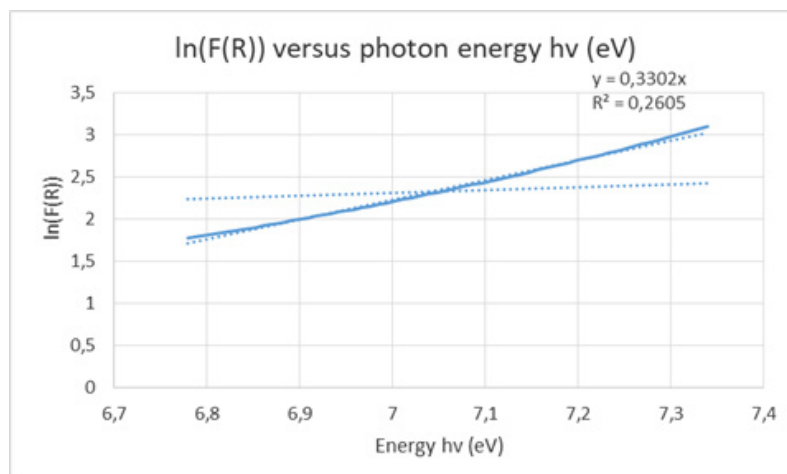


Figure 7: Plot of $\ln(F(R))$ versus photon energy $h\nu$ for the calculation of Urbach energy of the second A4 copy paper sample Laser Copy where $(F(R)) = \frac{K}{S} = \frac{(1-R)^2}{2R}$ where K was the absorption or coefficient of reflectivity and S was the coefficient of light scattering, and R was the observed reflectivity for monochromatic light, when the thickness of the sample was $d=0.094\text{mm}$.

Table 1: Urbach energies (meV) and thicknesses (mm) of the two A4 copy paper samples.

A4 Copy Paper Sample	Thickness (mm)	Urbach Energy (meV)
Q-Connect	1.000±0.0055	498.2
Laser Copy	1.000±0.0055	498.1
Q-Connect	0.100±0.0055	333.2
Laser Copy	0.100±0.0055	333.2
Q-Connect	0.101±0.0055	333.7
Laser Copy	0.094±0.0055	330.2

Conclusion

In this work UV-VIS spectroscopy was performed to calculate the Urbach energies and indirect band gap energies of two A4 white copy paper samples. The indirect band gap energy involved interaction of photon with an electron in the valence band which subsequently got excited into the conduction band, across the fundamental band gap. In the case of the indirect transition, interaction with lattice vibration also took place. Thus, the appearance of optical band gap in thin A4 copy paper samples was affected by the microstructure, like the presence of defects. Urbach energy tailing was estimated into the band gap in each paper sample. Urbach energy tail (E_u) has been estimated to account for the optical disorder of the two paper samples [17,18]. The width of Urbach tail decreased on going from the thicker to the thinner copy paper sample which meant that from order to disorder. Thus, the present work contributes to understanding that the energy tails can be optimized to engineer the optical band gap for various applications in the field of thin film devices, and therefore of thin copy paper samples.

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