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B-spline Regression Modeling of Strontium Titanate Data in Transmittance Properties with Rutenium Oxide Doping Concentration

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Abstract

Strontium titanate ($SrTiO_3$) doped with ruthenium oxide (RuO_2) 6% was characterized by the transmittance properties using UV-Vis (Ultraviolet-Visible) spectrophotometer. The application of transmittance properties to electronic devices has different wavelengths. Therefore the wavelength influence of transmittance will be segmented. The model that is feasible to use in this aspect is spline regression. This study used b-spline regression to measure each wavelength segment to the percentage of transmittance strontium titanate materials with various contributions of RuO_2. Then it compares the B-spline regression model on strontium titanate with various comparisons of RuO_2. Based on the estimated yield curve obtained for $SrTiO_3$ material, it can be recommended the maximum percentage of transmittance from a part of the regression curve obtained at wavelength of 755,067 nm. While the minimum percentage of transmittance reached at wavelength of 435,787 nm. In $SrTiO_3$+RuO_2 2%, the rising wavelength of one nm will cause each segmentation to rise by 4.2%, 8.2% and 3.9% respectively.

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Then the wavelength fired through the material of $SrTiO_3$+RuO_2 4% 432.44 nm up to 438,776 nm when the wave rises by one nm it will cause transmittance displacement of 0.374%. In addition, the percentage increase in segmentation was 0.095%, 0.0578% and 0.0089% respectively. The estimated curve of $SrTiO_3$+RuO_2 6% material is the most maximum percentage of transmittance obtained from the calculation of regression curve at 744,935 nm wavelength with percentage transmittance value of 63,015%. While the minimum percentage of transmittance reached at wavelength of 436.755 nm with percentage transmittance value of 37.287%.

Keywords: B-spline regression; RuO_2; $SrTiO_3$;Transmittance.

1. Introduction

Strontium titanate ($SrTiO_3$) is one of the ferroelectric materials which has spontaneous polarization properties. In the thin strontium titanate layer then doped with 6% Ruthenium Oxide (RuO_2) to reduce the cost without changing the properties made into ferroelectric thin films, then characterized using a UV-Vis (Ultraviolet-Visible) spectrophotometer. UV-Vis (Ultraviolet-Visible) spectrophotometer is a tool to measure the optical properties of a material. The use of UV-Vis (Ultraviolet-Visible) Spectrophotometer by firing light at a certain wavelength produces a percentage of the optical properties of transmittance or part of the light that is transmitted. So we need to know the effect of wavelength on the nature of transmittance. Electronic devices that apply the nature of transmittance are microwaves, rice cookers, irons, radios, etc. The application of transmittance properties to electronic devices has different wavelengths. Therefore, the approach to the effect of wavelength on the percentage of transmittance will be segmented. The model that is feasible to use in this aspect is spline regression. Spline regression is one of the nonparametric regression approaches suggested by reference [12]. Spline is one type of polynomial model that has segmented properties. The segmented nature provides more flexibility than ordinary polynomials, making it possible to adjust effectively to the local characteristics of a function or data. The basic functions used in the spline regression approach are truncated power base and B-spline [9]. Truncated power bases have weaknesses that can be reflected in almost singular matrices, making normal equations difficult to solve. While the B-Spline base is a basis that can overcome these weaknesses [5]. Research on ferroelectric materials with a nonparamteric regression approach has been carried out. Reference [2] conducted a study of truncated spline regression modeling to estimate the regression curve. This study concludes that estimating the X-Ray Diffraction strontium titanate data regression curve using the truncated spline regression produces a good predictive regression curve. In the estimation of $SrTiO_3$ and $SrTiO_3$ + RuO_2 material, the best spline regression model is estimated to be linear spline regression model with the approach of 42 point knots and 37 point knots. Based on these considerations, the authors would like to apply ferroelectric material, namely strontium titanate from experiments The Department of Physics, Bogor Agricultural Institute uses a B-spline nonparametric regression method with the aim of knowing the effect of each segment of light wavelength on the percentage of transmittance. Besides that, it compares the B-spline regression model on strontium titanate materials with various concentrations of RuO_2.

2. Materials and methods

The data used in this study are secondary data from the experimental results of the Department of Physics, Bogor Agricultural Institute 2018. Data were obtained using a UV-Vis spectrophotometer. The $SrTiO_3$ material used was pure $SrTiO_3$ and doped with concentrations of ruthenium oxidation 6% ($SrTiO_3$ + RuO_2 6%). The response variable in this study are the percentage of pure transmittance of SrTiO3 (Y_1) and $SrTiO_3$ + RuO_2 6% (Y_2). The explanatory variable in this study is the wavelength (X).

The steps of analysis in this study are described as follows:

1. Data exploration

   Explored by looking at the data plots to see a general picture of the pattern of the relationship between pure transmittance data of SrTiO3 and concentrations of RuO_2 6%.

2. Selection of the number and location of point knots

   The number of knots specified is small, because of the simplicity of the model and the location of the knot points in this study determined by using the freeknotsplines package in the R program, then the GCV values are calculated for each combination of point knots and at a certain order. The GCV formula as follows :

$$GCV(u) = \frac{MSE(u)}{\left(\frac{1}{n} tr\,[\boldsymbol{I}-\boldsymbol{A}(\boldsymbol{u})]\right)^2} \quad (1)$$

   with I is the identity matrix, u is the point of knots (u1, u2, ..., uk), A (u) = B (u) (B (u) 'B (u))$^{-1}$B (u)', n is the number observation, and MSE is the mean squared error.The order used in this study is order 1 (linear) and order 2 (quadratic).

3. Determination of optimal knot points

   The optimal point of knots is obtained by looking at changes in the GCV values that are most different from the previous GCV values. The number and location of the optimal knot points for order 1 (linear) and order 2 (quadratic) are different for $SrTiO_3$ materials and $SrTiO_3$ + RuO_2 6%.

4. Parameter estimator

   Estimating the B-spline regression parameter using the laest squares method. The estimator of B-spline regression parameters is obtained by the following equation :

$$\hat{\beta} = \left(B^T(u)B(u)\right)^{-1}(B^T(u)Y) \quad (2)$$

   WithY is response variable,$B(u) = (B_{j,m}(x_i))$ and

$$B_{j,m}(X) = \frac{X - u_j}{u_{j+m-1} - u_j} B_{j,m-1}(X) + \frac{u_{j+m} - X}{u_{j+m} - u_{j+1}} B_{j+1,m-1}(X)$$

5. Selection of the best B-spline regression model

Selecting a linear or quadratic B-spline regression model based on the smallest MSE criteria and the largest R^2 with the following equation:

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \quad (3)$$

$$R^2 = \frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \quad (4)$$

with n is the number of observations, $\hat{y}_i$ is the estimated value of the response in i-th observation, y_i is the actual value of the i-th response, $\bar{y}$ is the average value of the actual response.

6. Comparison of materials

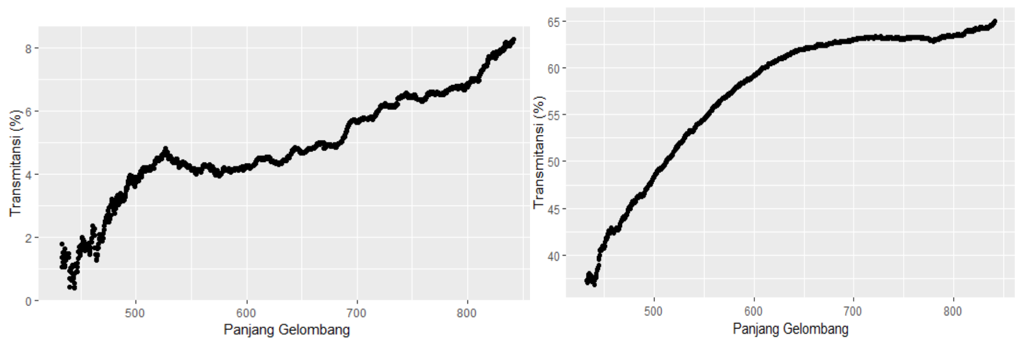
Comparison is done by studying each segment which affects the percentage transmittance of pure $SrTiO_3$ and $SrTiO_3$ doped with RuO_2 6%.

Steps 2 through 5 are carried out forlinear and quadratic B-spline regression models.

3. Results and Discussion

3.1 Exploration Data

Scatter plots are used to show patterns of relationships between response variables and explanatory variables. The following is scatter plot between the explanatory variable (X) and the response variable (Y).



(a) $SrTiO_3$ (b) $SrTiO_3 + RuO_2$ 6%

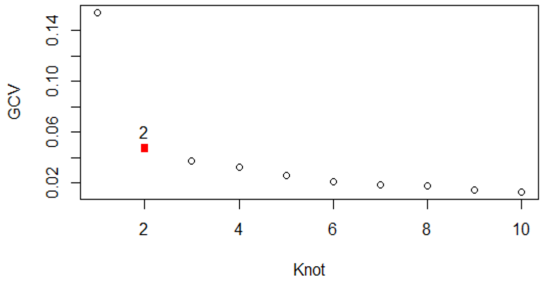
Figure 1: scatter plot between the explanatory variable and the response variable

Based on Figure 1, the percentage of pure transmittance of $SrTiO_3$ material and at RuO_2 concentrations of 6% tends to have a positive relationship with the wavelength. This shows the greater the wavelength, the greater the percentage of transmittance. However, at certain wavelengths the percentage transmittance does not always increase when the wavelength increases.

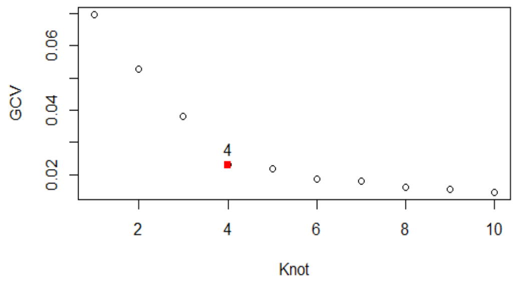
3.2 Selection of the number and location of point knots

Determining the number and location of knot points is the first step taken to form a B-spline regression model. The location or position of the knot point can be determined in several ways, namely by dividing the distance between knots as large, dividing the number of observations as much (quantile knots) and using the freeknotsplines package in program R. The third way is to determine the location or position of the knots the most effective way, because the algorithm works by testing all X explanatory variables as candidate point knots. This algorithm was introduced by reference [10]. Determining the location of knots for linear order and different quadratic orders for each SrTiO3 material.

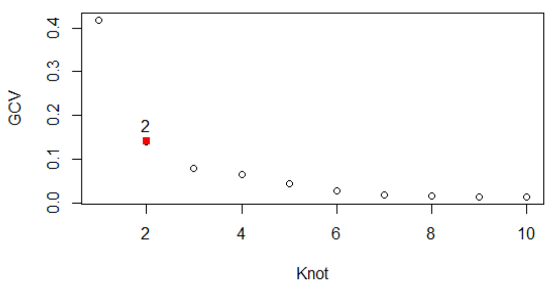
Figure 2 shows the movement of GCV values for the number and location of knots using the freeknotsplines package in program R. Figures 2 (a) and 2 (b) show the movement of GCV values on SrTiO3 materials with linear and quadratic ordo. Figures 2 (c) and 2 (d) show the movement of GCV values in SrTiO3 + RuO2 6% with linear and quadratic ordo.



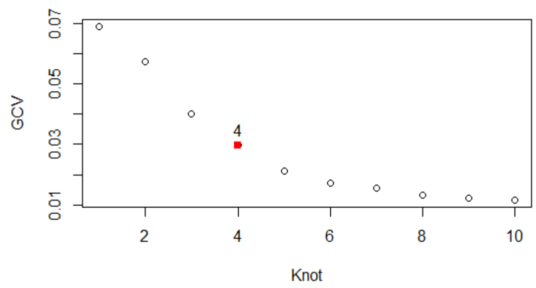
(a) $SrTiO_3$ Linier



(b) $SrTiO_3$ Kuadratik



(c) $SrTiO_3 + RuO_2$ 6% Linier



(d) $SrTiO_3 + RuO_2$ 6% Kuadratik

Figure 2: Determination of the number and location of point knots

In determining the number and location of optimal knots, GCV values are different from the previous GCV values. In Figure 2, it can be seen that there is a GCV value that is quite different from the previous GCV value. So that it can be determined the determination of the number and location of knot points used in the formation of linear and quadratic B-spline regression models for $SrTiO_3$ materials with various concentrations of RuO_2 up to 10 knots.

3.3 Determination of optimal knot points

The optimal point of knots is the point of knots used in making B-spline bases. The point of the knot used is the knot point which has a GCV value whose value is far different from the previous GCV value. This is done for the simplicity of the model called the parsimony model. The results of the calculation of GCV values on each material and model can be seen in table 1.

Table 1: Optimal GCV values for each material and model

Material	Ordo	Knot	GCV
$SrTiO_3$	linear	2	0.042
	quadratic	4	0.023
$SrTiO_3 + RuO_2$ 6%	linear	2	0.141
	quadratic	4	0.029

Based on table 1, it can be seen that the optimal number of knots in $SrTiO_3$ material for linear models is 2 knots with GCV values of 0.042 and for quadratic models as much as 4 knots with GCV values of 0.023. Whereas in the material of $SrTiO_3 + RuO_2$ 6% the optimal number of knots for the linear model is 2 knots with GCV values of 0.141 and for quadratic models as much as 4 knots with GCV values of 0.029.

3.4 Selection of the best B-spline regression model

After determining the number and location of the optimal knot points and estimated parameters, the next step is to select the best B-spline regression model. The selection of the best B-spline regression model is based on the criteria of the smallest MSE value and the largest R^2 value by comparing linear and quadratic models on each $SrTiO_3$ material and doped with concentrations of RuO_2 6%. The results of calculating the MSE and R^2 values can be seen in table 2 below.

Table 2: The value of MSE and R^2 for each material and model

Material	Ordo	MSE	R^2
$SrTiO_3$	linear	0.046	0.983
	quadratic	0.023	0.992
$SrTiO_3 + RuO_2$ 6%	linier	0.139	0.997
	quadratic	0.029	0.999

In table 2 it can be seen that the best model for $SrTiO_3$ material is a quadratic ordowith an approach of 4 point knots. This model has the smallest MSE value of 0.023 and the highest R^2 value is 0.992, when compared with the linear model of SrTiO3 material. While the best model for the material SrTiO3 + RuO2 6% is a quadratic model with an approach of 4 point knots. This model has the smallest MSE value of 0.029 and the highest R^2 value is 0.999, when compared to the linear model of $SrTiO_3 + RuO_2$ 6%.

3.5 Comparison of materials

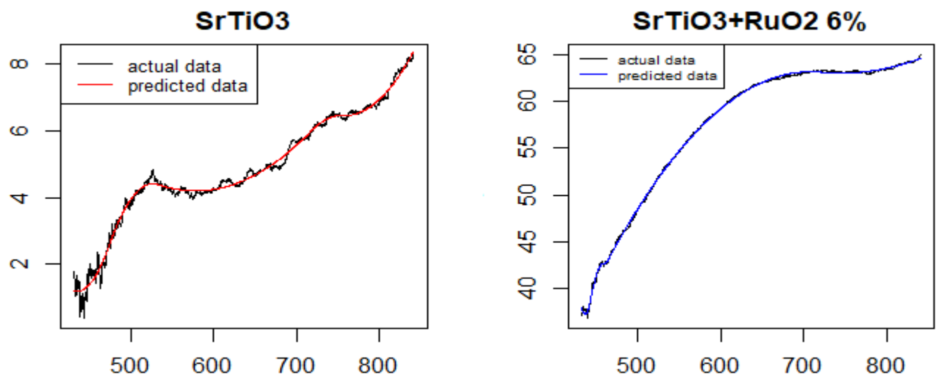


Figure 3: Estimated curve of $SrTiO_3$ and $SrTiO_3 + RuO_2$ 6%

In Figure 3 displays each of the predicted curves and actual data for the materials of SrTiO3 at various concentrations of RuO2. The ingredients of SrTiO3 and SrTiO3 + RuO2 6% were estimated using quadratic B-spline regression. The estimated yield curve for SrTiO3 and $srTiO_3$+RuO_2 6% is almost close to the actual data.

Table 3: Comparison of each segmentation for $SrTiO_3$ and $SrTiO_3 + RuO_2$ 6%

Material	Segmentation	Curva Shape	Min. Lokal	Maks. Lokal	Min. Global	Maks. Global
	$432.44 \leq x < 474.19$	Sunken	433.428 1.172	- -		
	$474.19 \leq x < 533.39$	Convex	- -	545.911 4.711		
$SrTiO_3$	$533.39 \leq x < 717.42$	Sunken	572.881 4.180	- -	x = 433.428 y = 1.172	x = 754.478 y = 6.467
	$717.42 \leq x < 756.59$	Convex	- -	754.478 6.467		
	$756.59 \leq x < 841.29$	Sunken	758.406 6.440	- -		
	$432.44 \leq x < 444.07$	Sunken	436.575 37.395	- -		
	$444.07 \leq x < 459.34$	Convex	- -	464.265 43.118		
$SrTiO_3 + RuO_2$ 6%	$459.34 \leq x < 464.58$	Convex	- -	462.682 42.857	x = 436.575 y = 37.395	x = 705.572 y = 63.055
	$464.58 \leq x < 720.68$	Convex	- -	705.572 63.055		
	$720.68 \leq x < 841.29$	Sunken	758.587 63.069	- -		

With the model criteria produced by $SrTiO_3$ material it can be recommended that the maximum maximum percentage of transmittance between the five regression line pieces is achieved at a wavelength of 754,478 nm with a transmittance value of 6.467%.

While the minimum percentage of transmittance is reached at a wavelength of 433.428 nm with a transmittance value of 1.172%.

The model criteria produced by 6% $SrTiO_3$ + RuO_2 material can be recommended that the maximum maximum percentage of transmittance between the five regression line pieces is achieved at a wavelength of 705.572 nm with a percentage transmittance value of 63.055%.

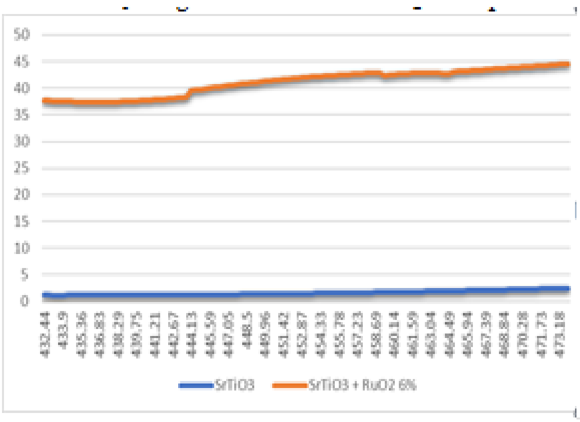
While the minimum percentage of transmittance is reached at a wavelength of 436,575 nm with a percentage transmittance value of 37,395%.

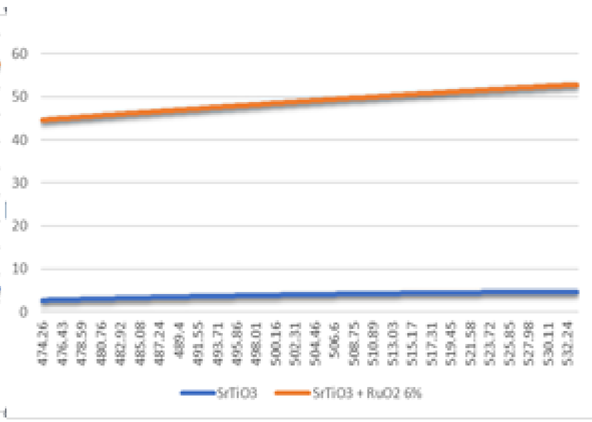
Table 4: Comparison of R^2 for each segmentation for $SrTiO_3$ and $SrTiO_3$ + RuO_2 6%

Material	Segmentation	R^2
	$432.44 \leq x < 474.19$	0.586
	$474.19 \leq x < 533.39$	0.951
$SrTiO_3$	$533.39 \leq x < 717.42$	0.953
	$717.42 \leq x < 756.59$	0.781
	$756.59 \leq x < 841.29$	0.974
	$432.44 \leq x < 444.07$	0.354
	$444.07 \leq x < 459.34$	0.943
$SrTiO_3$ + RuO_2 6%	$459.34 \leq x < 464.58$	0.724
	$464.58 \leq x < 720.68$	0.999
	$720.68 \leq x < 841.29$	0.945

The wavelength segment formed can be studied further by making a regression curve. The five segments in pure $SrTiO_3$ material were used as a comparison, this is because the pure $SrTiO_3$ material became a reference among the $SrTiO_3$ ingredients with RuO_2 receptacle. Comparison of the five segments can be seen in the Figure 4 below

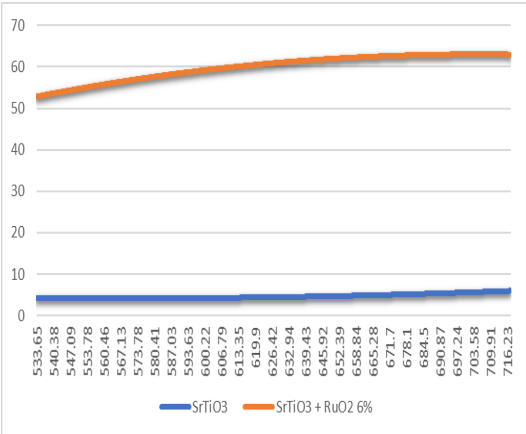
Based on figure 4 can be seen from the five segments, the material of $SrTiO_3$ + RuO_2 6% has the highest percentage transmittance value while $SrTiO_3$ has the lowest percentage transmittance value

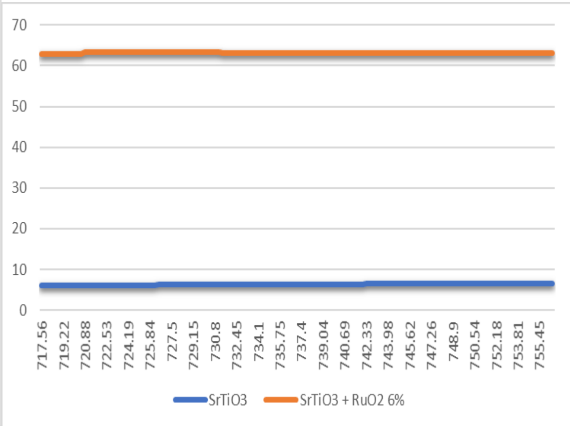




(a)First segment

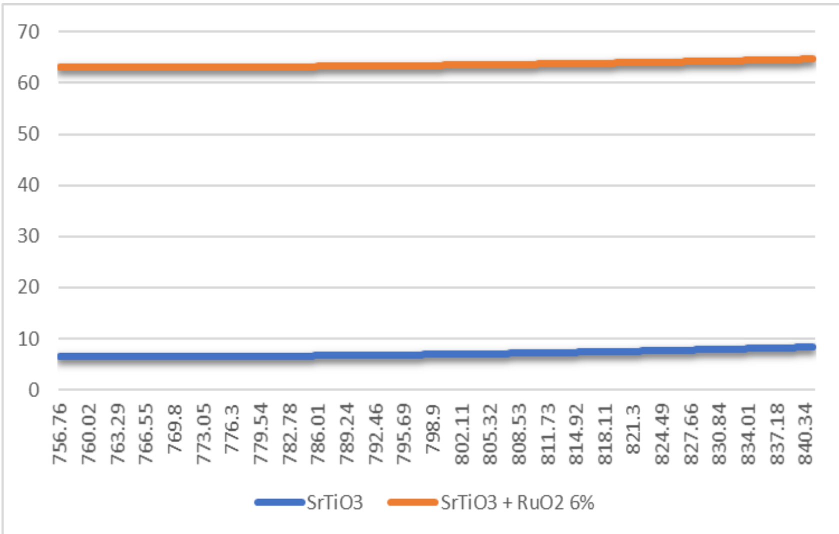
(b) Second segment





(c) Third segment

(d) Fourth segment



(e) Fifth segment

Figure 4: Segment One

4. Conclusion

Based on the estimated yield curve obtained for $SrTiO_3$ material, it can be recommended that the maximum maximum percentage of transmittance between the five regression line pieces is reached at a wavelength of 754,478 nm with percentage transmittance value of 6.467%. While the minimum percentage of transmittance is reached at a wavelength of 433.428 nm. Whereas for the $SrTiO_3$ + RuO_2 6% material the estimated yield curve is the most maximum percentage of transmittance between the five regression line pieces achieved at a wavelength of 705,572 nm with a percentage transmittance value of 63.055%. While the minimum percentage of transmittance is reached at a wavelength of 436,575 nm with a transmittance percentage value of 37,395%.

5. Recommendations

For the next researcher, it is expected to be able to add tests to see the response or the results of the percentage of transmittance obtained on each test and can also apply to other optical properties such as absorption and reflectance.

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