Analyze the relationship between wavelength, refractive index and extinction coefficient separately

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Abstract: *We can know that the change of wavelength is always increasing, but the change of refractive index increases and decreases. We first analyze the relationship between wavelength, refractive index and extinction coefficient separately, and then conduct multiple regression modeling for wavelength, refractive index, wavelength, and extinction coefficient. According to this situation, we establish a multiple regression model to obtain the implicit function relationship between wavelength, refractive index, and extinction coefficient. By substituting the data, we get that the refractive index of a 50 nm thick tungsten in 0.3-5 µ m is 144.354. We model the relationship between the emission spectra of multilayer structures and material properties. Based on the composite structure emission spectrum model based on the transfer matrix method (TMM), we substitute the data of silica and tungsten, and we can clearly see the emission spectra of the composite structure formed by tungsten (50 nm) and silicon dioxide (50 nm) in the range of 0.3-5 microns.*

Keywords: *multiple regression analysis modeling, transfer matrix (TMM)*

1. Introduction

We can know that the change of wavelength is always increasing, but the change of refractive index increases and decreases. We first analyze the relationship between wavelength, refractive index and extinction coefficient separately, and then conduct multiple regression analysis and modeling for wavelength, refractive index, wavelength and extinction coefficient. According to this situation, we establish a multiple regression model to obtain the implicit function relationship between wavelength, refractive index and extinction coefficient. By substituting the data, we get that the refractive index of a 50 nm thick tungsten in 0.3-5 µ m is 144.354.

The title requires us to express the relationship between the emission spectra of multilayer structures and material properties (refractive index and thickness), and calculate the emission spectra of the composite structure formed by tungsten (50 nm) and silica (50 nm) (as shown in the figure) within 0.3-5 microns. We model the relationship between the emission spectra of multilayer structures and material properties. Based on the composite structure emission spectrum model based on the transfer matrix methAod (TMM), we substitute the data of silica and tungsten, and we can clearly see the emission spectra of the composite structure formed by tungsten (50 nm) and silica (50 nm) within 0.3-5 microns.

2. Symbol and Assumptions

Table 1: Symbolic meaning

Symbol		Symbolic meaning
	y	Observable random variable
	ε_i	random error
	β	Coefficient of regression equation
	a	Significance level
	p	freedom
		Thermoelectric conversion efficiency
	y'	
f		Nonlinear relation
		The weights of connecting neurons in the network
	ω	
	E	Connecting the threshold of each neuron
	M	training sample
	Z	Comprehensive thermoelectric conversion efficiency
		Actual output value
y_{ij}		

3. Problem restatement

Please describe the relationship between the emission spectra of single-layer structure and material properties (refractive index and thickness) and calculate the emission spectra. A 50 nm thick tungsten (as shown in the figure below) is between 0.3-5 microns.

Please express the relationship between the emission spectra of the multilayer structure and the material properties (refractive index, thickness), and calculate that the emission spectra of the composite structure formed by tungsten (50 nm) and silica (50 nm) (as shown in the figure) are within 0.3-5 microns.

4. Establishment and solution of model

Based on the above analysis of the problem, the following will start to establish the mathematical model and explain the establishment process, and then use the mathematical model to solve the problem.

4.1 Relationship between wavelength and refractive index, wavelength, and extinction coefficient

We can know from the topic that the change of wavelength is always increasing, but the change of refractive index increases and decreases. After analysis, we use a function to express it. First, analyze the relationship between wavelength, refractive index, and extinction coefficient separately, and use software to make the relationship between them.

Two fitting functions can be obtained here, namely, wavelength and refractive index, wavelength, and extinction coefficient. According to this situation, we establish a multiple regression model to obtain the binary function relationship between wavelength, refractive index, and extinction coefficient.
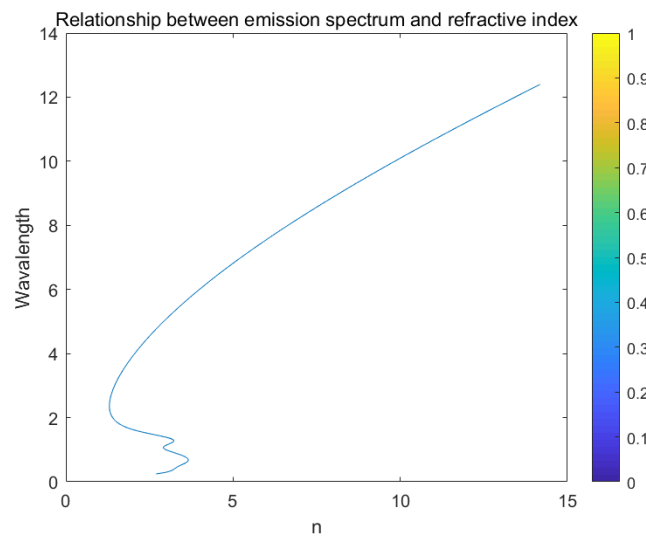

Figure 1: Relationship between emission spectrum and reactive index

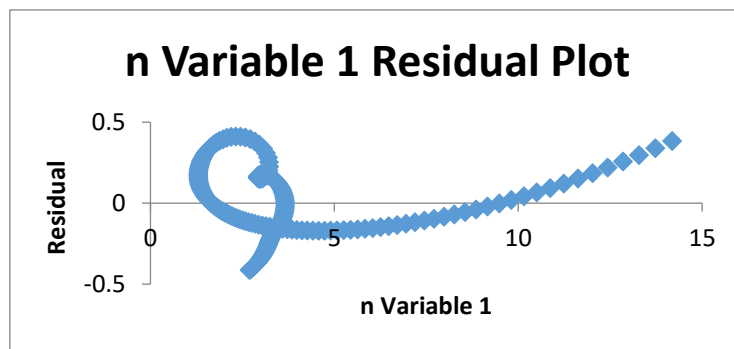Make the residual analysis diagram, including:

Figure 2: Residual plot of wavelength and refractive index

The following is the fitting function diagram of wavelength and extinction coefficient:
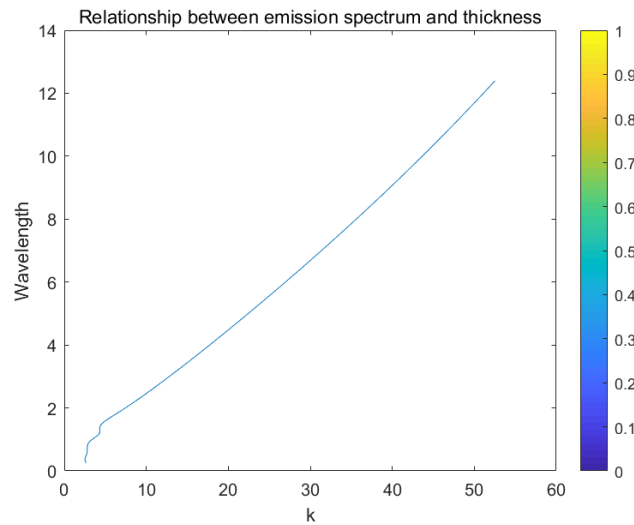

Figure 3: Relationship between emission spectrum and thickness

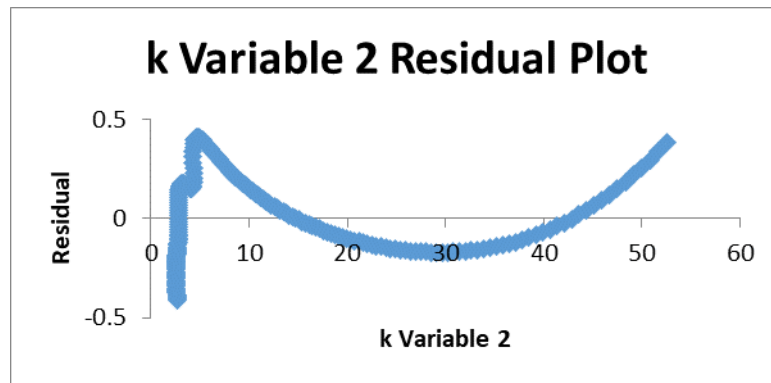Similarly, we make the residual analysis diagram, including:

Figure 4: The residual analysis diagram

Next, let's standardize.

4.2 Standardized treatment、Fundamentals of data sheets、sample space

In this chapter, we are all involved in sample points $\times$ Data table of variable type. If there are m variables $(x_1, x_2, \dots, x_{im})$, $i = 1, 2, \dots, n$

Then the data table x can be written as an n $\times$ M-dimensional matrix.

$$X = (X_{ij})_{n \times m} = \begin{bmatrix} e_1^T \\ \vdots \\ e_n^T \end{bmatrix} \tag{1}$$

Where $e_i = (X_{i1}, X_{i2}, \dots, X_{im})^T \in R^m, i = 1, 2, \dots, n, e_i$ is called the ith sample point.The mean value of the sample is

$$\bar{x} = (\bar{x}_1, \bar{x}_2, \dots, \bar{x}_m), \bar{x}_j = \frac{1}{n} \sum_{i=1}^{n} x_{ij}, j = 1, 2, \dots, m \tag{2}$$

The sample covariance matrix and sample correlation coefficient matrix are

$$S = (s_{ij})_{m \times m} = \frac{1}{n-1} \sum_{k=1}^{n} (e_k - \bar{x})(e_k - \bar{x})^T \tag{3}$$

$$R = (r_{ij})_{m \times m} = \left(\frac{s_{ij}}{\sqrt{s_{ii}s_{jj}}} \right) \tag{4}$$

$$s_{ij} = \frac{1}{n-1} \sum_{k=1}^{n} (x_{ki} - \bar{x}_i)(x_{kj} - \bar{x}_j) \tag{5}$$

Dimensionless processing of data

In practical problems, the measurement units of different variables are often different. To eliminate the dimensional effect of variables,To make each variable have the same expressiveness, the dimensionless method commonly used in data analysis is to add different variables .The so-called compression processing is performed even if the variance of each variable becomes 1, i.e.

$$x_{ij} = \frac{x_{ij}}{s_j} \tag{6}$$

$amongs_j = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} (x_{ki} - \bar{x}_i)^2}$

There can also be other dimensionless methods, such as

$$x_{ij} = \frac{x_{ij}}{\max_{i}\{x_{ij}\}}, \quad x_{ij} = \frac{x_{ij}}{\min_{i}\{x_{ij}\}} \tag{7}$$

$$x_{ij} = \frac{x_{ij}}{\bar{x}_j}, \quad x_{ij} = \frac{x_{ij}}{\max_{i}\{x_{ij}\} - \min_{i}\{x_{ij}\}} \tag{8}$$

After processing, we do multiple regression analysis to fit, and get the relationship between wavelength, refractive index and extinction coefficient.

4.3 Modeling steps of multiple linear regression model

Currently:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_1 x_{i1} + \cdots + \beta_1 x_{i1} + \varepsilon_i, (i = 1,2,3,\ldots,n)$$

Where y is an observable random variable, $\beta_0, \beta_1, \beta_2, \ldots, \beta_n$ is $(n + 1)$ unknown parameters, $(x_1, x_2, x_3, \ldots, x_n)$ and y are n groups of observations of n times, $x_{i1}, x_{i2}, x_{i3}, \ldots, x_{in}, y_i)$, ε_i is a random error and meets the following assumptions

(1) Normality hypothesis: obey the mean value of 0 and the variance of σ^2 positive distribution.

(2) Unbiased assumption: ε_i The conditional expectation of I is 0.

(3) Independence assumption: ε_i are independent of each other and meet $Cov(\varepsilon_i, \varepsilon_j) = 0, (i \neq j)$

(4) Covariance assumption: ε_i all variances are the same.

Here, set ε_i=0.

Multiple linear regression equation is obtained by using the existing observation data $\beta_0, \beta_1, \beta_2, \ldots, \beta_n$ Estimate of $\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_n$ is the multiple linear regression equation.

Order:

$$Y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$X = \begin{pmatrix} 1 & x_{11} & x_{11} & \cdots & x_{11} \\ 1 & x_{21} & x_{11} & \vdots & x_{11} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{11} & \cdots & x_{11} \end{pmatrix}$$

$$\beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{m-1} \end{pmatrix}$$

Expressed in matrix form, that is:

$$Y = X\beta$$

Estimation of regression equation coefficients by least square method β:

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

Test of multiple linear regression model

The multiple linear regression analysis model is established by spss22.0. After obtaining the model, it is necessary to test whether the analysis model meets the modeling requirements. The test methods are mainly divided into correlation coefficient test, F test and t test.

Specifically:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_n x_{in} + \varepsilon_i, (i = 1,2,3, \dots n)$$

Hypothesis H_0: $\beta = \beta_0 = \beta_1 = \beta_2 = \cdots = \beta_n = 0$

Hypothesis H_1: $\beta_i (i = 1,2,3, \dots, n)$ incomplete 0

If h is assumed H_0: $\beta = \beta_0 = \beta_1 = \beta_2 = \cdots = \beta_n = 0$ holds, indicating y_i and x_{in} there is no linear relationship between in, the established model is invalid.

(1) Test of correlation coefficient

$$R_2 = \frac{\sum_{i=1}^n (\hat{y}_1 - \bar{y})^2 / p}{\sum_{i=1}^n \frac{(\hat{y}_1 - \bar{y})^2}{n} - p - 1} = \frac{SSR/p}{\frac{SST}{n} - p - 1}$$

Where p and $(n - p - 1)$ are degrees of freedom, $SST = SSR + SSE$

Judgment condition: the closer the value of R^2 is to 1, the stronger the correlation between y and x. If R^2 is 0, the stronger the correlation between y and x. If R^2 is 0, there is no relationship between y and x.

(2) F test

$$F = \frac{\sum_{i=1}^n (\hat{y}_1 - \bar{y})^2 / p}{\sum_{i=1}^n \frac{(\hat{y}_1 - \bar{y})^2}{n} - p - 1} = \frac{SSR/1}{SST/(n-2)} = \frac{R^2}{1 - R^2} (n - 2) \sim F(1, n - 2)$$

After the significance level a is determined, the critical value f is obtained_ a (p,n-p-1)

Judgment conditions:

If $F > F_a(p, n - p - 1)$, then reject the original hypothesis H_0, it is considered that the multiple linear regression is generally significant at the significance level a.

If $< F_a(p, n - p - 1)$, then accept the original hypothesis H_0, it is considered that the multiple linear regression is not significant at the significance level a.

(3) T-test

$$t = \frac{\hat{\beta}_1}{\frac{\sigma}{\sqrt{\sum_{j=1}^n (x_{ij} - \bar{x}_{11})}}} \sim t(n - p - 1)$$

among,

$$\hat{\beta}_1 \sim N \left(\frac{\sigma^2}{\sqrt{\sum_{j=1}^n (x_{ij} - \bar{x}_{11})}} \right)$$

After the significance level a is determined, the critical value t is obtained $t_{\frac{a}{2}}(n - p - 1)$.

Judgment conditions:

If $|t| > t_{\frac{a}{2}}(n - p - 1)$, then reject the original hypothesis H_0, it is considered that the multiple linear regression is generally significant at the significance level a.

If $|t| < t_{\frac{a}{2}}(n - p - 1)$, then accept the original hypothesis H_0, it is considered that the multiple linear regression is not significant at the significance level a.

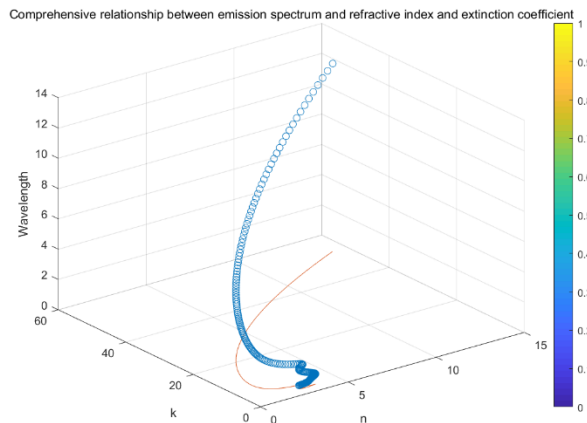We use MATLAB to draw the fitted curve, as shown in the figure:

Figure 5: Comprehensive relationship between emission spectrum and refractive index and extinction coefficient

According to the analysis, we know that the error is very small. This is an implicit function equation. The curve of the equation fits well. We substitute it. Through calculation, we get the emission spectrum. The refractive index of a 50 nm thick tungsten at 0.3-5 microns is 144.354.

4.4 Transfer Matrix Method (TMM)

This is the most widely used method for the mathematical study of wave transmission in one-dimensional structures because it allows the calculation of band diagrams, reflectivity and transmission spectra, emission spectra, guided modes and the modulization of porosity and thickness gradients.

To study the reflection and the transmission of electromagnetic radiation through a multilayer with the TMM method, we consider a one-dimensional structure consisting of alternating porous silicon layers of different refractive indices coupled to a homogeneous medium characterized by refractive index n0 at the interface. Fig. 3.1 shows this structure, where n1 and n2 are the layers refractive index, h1 and h2 are the thicknesses of the respective layers and Λ is the period of the structure (Λ= h1 +h2).
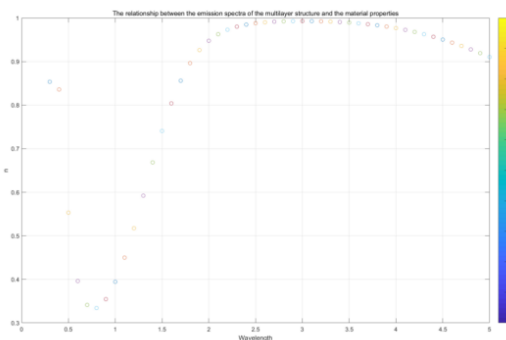

Figure 6: The relationship between the emission spectra of the multilayer structure and the material properties

From the above figure, we can clearly see the emission spectrum of the composite structure (as shown in the figure) formed by tungsten (50 nm) and silica (50 nm) in the range of 0.3-5 microns.

5. Strengths and Weakness

5.1 Strengths

Neural network indicators depend on training samples, including actual investigation data and existing evaluation. In essence, they are the synthesis of other methods. The main advantage is that the determined weight is adaptive. Compared with the weight obtained through experience in the past, it is more practical.

5.2 Weakness

Particle swarm optimization algorithm is not good for discrete optimization problems, and it is easy to fall into local optimization. Due to the limited amount of input data of BP neural network, the neural network training will cause a certain degree of deviation to the results.

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