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# A new method study of spectral measurement and prediction based on the nonlinear solution concentration of alcohol

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ABSTRACT

The configuration and the detection of solution concentration are the basic steps of scientific research. Most of solution concentrations can be obtained by indirect method. In this paper, by using the numerical relationship known between the alcohol concentration and refractive index, the relationship between the alcohol concentration and spectral transmission characteristics of the resonance peak can be calculated. The relationship between transmittance and concentration of alcohol solution can be described in a certain nonlinear mathematical expression, which is simple and inversible. Such method provides a novel way to detect alcohol solution concentration and puts forward the expression of the nonlinear correction. The linear relationship that has been using for long time is revised. And it can be reasonable to predict relative parameter that is unknown. This paper provides a new way to reasonable configuration and application for the concentration of solution.

## 1. Introduction

Solution is an important carrier of natural science researches. Its concentration is also an important metric. In scientific research, industrial and agricultural production and real life fields, the solution concentration is an important physical and chemical parameter. Solution concentration controlling is widely used in life science, agricultural science, plant production and our everyday life. Inspection of solution concentration is very important to guarantee the product quality, improve the level of scientific management etc.

At present, many detection methods of solution concentration are studied. For example, a chemical method called osmotic pressure method, a physics method called polarimeter method [1–3], and the light absorption based on the Lambert's Law, surface plasmon resonance, spectrum character method, etc. [4–6]. They all have certain advantages, but also have certain limitation. Some methods have strict conditions, and some require more perfect equipment [7,8].

When light wave propagates in the solution, its electrical parameters are different because the concentration is different. Furthermore, light acting on different solution concentration will show different transmission and reflection characteristics. We find and fit the relationship between the concentration of alcohol solution, and the transmittance at the resonant wavelengths points through numerical simulation. The relationship and can analyze and forecast different parameters, like the concentration of alcohol solution. This paper provides a new method for testing the concentration of the solution.

## 2. The theoretical model of solution concentration and the refractive index

When the light interacts with solution, different solution concentration will show different refractive index. According to the Lorentz electronic theory, assume that the atoms or molecules making up the medium of a charged particle are quasi-elastic forces to keep around their equilibrium position, and have certain inherent vibration frequency, The equation that meets the electron displacement relationship will be obtained [9].

$$\frac{d^2r}{dt^2} + \gamma\frac{dr}{dt} + \omega_0^2 r = -\frac{eE}{m} \tag{1}$$

where, $e$ is the electronic charge, $r$ is the distance that the electron departs from the equilibrium position, $\omega_0$ is electronic inherent frequency, $m$ is the mass of the electron, $E$ is the light intensity with the effects of the medium, $c$ is the speed of light in vacuums, $\gamma=10^8$ Hz is a classical radiation damping coefficient.

After a series of derivation, the relation between the solution concentration and the refractive index $n$ can be obtained as [9].

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$$y_c = \frac{4\pi\gamma\omega}{\alpha\lambda(\omega_0^2-\omega^2)}(n-1) + \frac{\pi\gamma\omega}{2\alpha\lambda(\omega_0^2-\omega^2)} \times \frac{N^2e^4}{\varepsilon_0^2 m^2} \times \frac{(\omega_0^2-\omega^2)^2-\gamma^2\omega^2}{(\omega_0^2-\omega^2+\gamma^2\omega^2)^2} \quad (2a)$$

where, $\alpha$ is a constant and independent of the concentration, $\lambda$ is the wavelength of light, $\omega$ is the light frequency, $N$ is the number of atoms per unit volume.

Eq. (2a) is the approximate relationship under certain conditions. It can be simplified to Eq. (2b) that is approximate the following form

$$y_c = an + b \quad (2b)$$

where, $a$, $b$ are relatively fixed constants under certain conditions. $n$ is the refractive index of a solution concentration. But for different solution, its value may be different.

The study shows that Eq. (2) can only be applied to a few solutions. For most of the solution, the relationship cannot show the approximate linear relationship. That is to say, Eq. (2b) cannot be well adapted to the study of concentration. Because of for most of the solution, the refractive index and solution concentration are likely to show nonlinear relationship. This paper studies the alcohol ($C_2H_5OH$) solution, which has a typical nonlinear relationship.

## 3. The transfer matrix method of one-dimensional photonic crystal (PC)

The one-dimensional photonic crystal structure model is shown in Fig. 1, where AB are composed by different materials. Its structure is $(AB)^N$. Where N is the repetition of AB. Suppose the structure of the Fig. 1 is $(AB)^NC(AB)^N$, where C represents the alcohol solution to be studied and AB is the container wall.

The light wave from the left side shots vertically to A and continues passing through B, and the whole crystal structure. The relationship between the refractive index and other parameters is theoretical analyzed as follows.

When the light wave or electromagnetic wave acts on the medium layer, the transmission coefficient can be obtained using the theory of transfer matrix method [10–13] like (3).

$$\tau = \frac{2\eta_0}{A\eta_0 + B\eta_0\eta_{N+1} + C + D\eta_{N+1}} \quad (3)$$

Here, $A$, $B$, $C$ and $D$ are four single units, $A = \cos\delta, B = -\frac{i}{\eta}\sin\delta, C = -i\eta\sin\delta$, and $D = \cos\delta$

The transmittance computational formula is

$$T = \tau\cdot\tau^* \quad (4)$$

Here, τ* is the conjugate of τ.

$$\delta = \frac{2\pi n h\cos\theta}{\lambda} \quad (5)$$

$$\eta = \sqrt{\frac{\varepsilon_0}{\mu_0}} \times \sqrt{\varepsilon_r} \times \cos\theta \quad (6)$$

where, $n$ is the refractive index for the corresponding material, $h$ is the thickness of material, $\theta$ is the incident angle of electromagnetic wave, $\varepsilon_0$ and $\mu_0$ are the permittivity and permeability of free space respectively, and $\lambda$ is the incident wavelength.

The reflection coefficient is

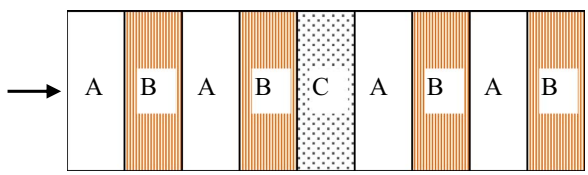


**Fig. 1.** Computational model of one-dimensional photonic crystal.

$$r_1 = \frac{A\eta_0 + B\eta_0\eta_{N+1} - C - D\eta_{N+1}}{A\eta_0 + B\eta_0\eta_{N+1} + C + D\eta_{N+1}} \quad (7)$$

The reflectance is

$$R_1 = r_1\cdot r_1^* \quad (8)$$

Here, $r_1^*$ is the conjugate of $r_1$.

Using the formulas above, the optical character of PC formed by alcohol solution concentration and the container can be analyzed. The nonlinear relation about alcohol solution can be found.

## 4. The simulation of a photonic crystal solution concentration

Assume the influence of impurities is ignored; the PC in Fig. 1 is made as a container. C layer is the bearing solution whose position is in the middle of the container. Both sides have a combination of 7 layers medium $AB$. Thus, the structure is $(AB)^NC(AB)^N$, and $N$=7.

Suppose $A$ and $B$ are $TiO_2$ and $SiO_2$ respectively. The refractive index $n_A$=2.49 and $n_B$=1.53, respectively. Now suppose common laser light *Nd:YAG* is used as the light source [14,15]. The light shots from the left side to the photonic crystal and expels from the right in Fig. 1. For this kind of laser device, wavelength of light center is $\lambda_0$=1046 nm. Now, the thicknesses of two kinds of medium are all $0.25\lambda_0$. Some pure water is filled in the cavity $C$ that is part of the photonic crystal. Its refractive index is $n_C$=1.3333. The solution concentration is equivalent to 0. Then, based on [3] and [9], different concentrations of alcohol ($C_2H_5$) solutions are put into cavity $C$. The corresponding relationship between solution concentration and refractive index is shown in Table 1.

For the measuring value of the relation between alcohol concentration in Table 1 and the refractive index, apply the correspond refractive index in the calculations of transfer matrix method. The relationship between different alcohol concentration and refractive and transmittance indices on different wavelengths is shown in Figs. 2 and 3 [16].

From Figs. 2 and 3, although the alcohol concentration is different, the reflectance or transmittance curves are almost overlapped together and seem unable to distinguish. Careful analysis found that there are certain rules theoretically in the resonant point.

There is a very narrow wave peak at $\lambda_0$=1046 mm in Figs. 2 and 3 which is the resonance wave peak. Now, its images can be made larger at Fig. 4. The relationship between $C_2H_5$ concentration and light transmittance can be obtained clearly.

Fig. 4 shows that there has importantly corresponding relationship between alcohol ($C_2H_5$) concentration and transmittance. Now, the recorded data from Fig. 4 is filled in Table 2. And for Table 1, other concentrations of numerical value are added to get a complete Table 2.

In order to find the corresponding relation, the data of Tables 1 and 2 are shown in Figs. 5 and 6. There can be seen in Fig. 5 obviously that the alcohol concentration and refractive index have nonlinear relationship. So the formula (2) is the approximate formula only and should be fined again.

From Fig. 5, it is obvious that there is a kind of nonlinear relationship between the refractive index and alcohol concentration which cannot be represented by formula (2b). Fig. 6 is the transmittance calculated using transfer matrix method (TMM) using data from the Table 1. It shows the nonlinear relationship between the transmittance and alcohol concentration.

Therefore, linear relationship will make the error large. We believe that the alcohol concentration should be predicted as nonlinear relationship provided that the conclusion in [3] is accurate.

Now, draw the data from Table 2 in Fig. 7. The points are marked with an asterisk (*). The results are also calculated with transfer matrix method (TMM) and correspond to the nonlinear relationship. At the same time, fitting is used to synthesize the data into the formula (9).

$$y_{tran} = a_1x^2 + a_2x + a_3 \quad (9)$$

Here, $a_1 = 1.8865806060604 \times 10^{-6}$