Prediction of Color of an Esthetic Restorative Material

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The color of a composite of several thicknesses with a highly chromatic background was predicted successfully from reflectance spectra of the material of a known thickness with dark and light achromatic backgrounds by applying the Kubelka-Munk theory. The infinite optical thickness of the composite increased as wavelength increased.

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Introduction.

The color of an esthetic restorative material is controlled primarily by thickness of the material and background color. Although the effects of the two factors on the reflectance spectra or color coordinates of esthetic dental materials have been reported,[1-7] the mechanism has not been clarified well enough to explain the effects quantitatively.

The reflectance of a translucent material in a simplified model has been studied theoretically by Kubelka and Munk.[8] A convenient method of prediction of luminous reflectance using Kubelka's equations[9] was reported through the study of opacity of composites;[10] however, the reported method assumed an achromatic background. In dentistry, the background color of an esthetic restoration is more or less chromatic, and the thickness of the material can vary. If the color (hue, value, and chroma) of an esthetic dental material of any thickness with any background color could be predicted precisely, shade selection could be optimized.

The purposes of this study were: (1) to obtain the optical properties of an esthetic restorative material as a function of wavelength algebraically from reflectance spectra of a sample of a known thickness with dark and light achromatic backgrounds of known reflectance spectra; (2) to predict the reflectance spectra using the obtained optical properties for samples of the same and different thicknesses with a highly chromatic background of known reflectance spectra by applying the Kubelka-Munk theory; (3) to obtain the hue, value, and chroma in the Munsell system from the predicted reflectance spectra for visual understanding; and (4) to evaluate the difference between the predicted color and the measured color.

Materials and methods.

A disk specimen of a microfilled composite* (38 mm in diameter) was formed using one of three split stainless steel rings (1, 1.5, and 2 mm in thickness) with two flat glass plates. Two min after initiation of the mix, the assembly was placed in an environment of 37 ± 1°C and 95 ± 5% relative humidity for 15 min. The specimen was then stored for 24 h in distilled water at 37 ± 1°C. Three specimens were made for each thickness.

A double-beam, ultraviolet-visible spectrophotometer† with an integrating sphere‡ was used to obtain reflectance data at every 5 nm between 405 and 700 nm for combined specular and diffuse reflectance. A transmission blank§ was used for calibration of zero reflectance. A white porcelain standard,∞ for which values of absolute reflectance were known at every 5 nm, was evaluated in a sample port (25 mm in diameter) with a barium sulfate standard in a reference port to obtain calibration coefficients at every 5 nm. There were 1080 reflectance measurements used to evaluate predicted *vs.* observed parameters.

Each of the 1-mm samples was evaluated in the sample port with the barium sulfate standard in the reference port under two conditions: (1) backed by a black tile, and (2) backed by a white porcelain tile (which was different from the porcelain standard). Also, each of the nine samples backed by a yellow tile// was evaluated in the same way. Then the data were multiplied by the corresponding calibration coefficients to obtain the reflectance values. Reflectance values of the black tile, the white porcelain, and the yellow tile backings were obtained as well.

The effects of the thickness of the material and the wavelength of the light on the reflectance values of the samples with the yellow tile background were studied. Seven levels (405, 450, 500, 550, 600, 650, and 700 nm) were chosen for the factor of wavelength. A two-way analysis of variance for a split-plot experiment[11] was used. The reflectance values were corrected slightly for statistical calculations to eliminate the effects of small variations in thickness of the samples prepared from the same ring. A correction coefficient was obtained at every 50 nm (besides 405 nm) by dividing the predicted reflectance value for the actual thickness by the predicted value for the average thickness. The observed reflectance value was then divided by the correction coefficient. In this way, variance in the data caused by variations in thickness was minimized.

Optical constants, including light reflectivity (R_∞), scattering coefficient (S), and absorption coefficient (K), were calculated algebraically at every 5 nm as described below.

Secondary optical constants (a and b) were calculated by Equations 1 and 2:

$$a = \{R(B) - R(W) - R_B + R_W - R(B)R(W)R_B + R(B)R(W)R_W + R(B)R_B R_W - R(W)R_B R_W\}/2\{R(B)R_W - R(W)R_B\} \quad \text{and} \qquad \text{(Eq. 1)}$$

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*Silar, universal shade, batch number 9A1, 3M Co., St. Paul, MN 55101

†ACTA C III UV-Visible Spectrophotometer, Beckman Instruments, Inc., Irvine, CA 92664

‡ASPH-U Integrating Sphere, Beckman Instruments, Inc., Irvine, CA 92664

§Part No. 587738, Beckman Instruments, Inc., Irvine, CA 92664

∞Standard No. D33C-2051, Hunter Associates Laboratory, Inc., Fairfax, VA 22030

//The yellow hue was considered appropriate as a background color modeling dentin or a cement base.

$$b = (a^2 - 1)^{1/2} \quad \text{(Eq. 2)}$$

where R_B is the reflectance of a dark backing (the black tile in this study); R_W is the reflectance of a light backing (the white tile); R(B) is the light reflectance of a sample with the dark backing; and R(W) is the light reflectance of the sample with the light backing.

The light reflectivity (R_∞, the light reflectance of a material of infinite thickness) is defined by Equation 3:

$$R_\infty = a - b \quad \text{(Eq. 3)}$$

The scattering coefficient (S) for a unit thickness of a material is defined by Equation 4:

$$S = (1/bX)\ \mathrm{Ar\ ctgh}[\{1 - a(R + Rg) + RRg\}/b(R - Rg)],\ \mathrm{mm}^{-1} \quad \text{(Eq. 4)}$$

where X is the thickness of the sample; Ar ctgh is an inverse hyperbolic co-tangent; and R is the light reflectance of the sample with the backing of reflectance (Rg).

The absorption coefficient (K) is defined by Equation 5:

$$K = S(a - 1),\ \mathrm{mm}^{-1} \quad \text{(Eq. 5)}$$

Besides the above optical constants, a thickness (X'_∞) at which the reflectance of the material with an ideal black background would attain the 99.9% value of its light reflectivity (R_∞) was calculated at every 5 nm from Equation 6:

$$X'_\infty = (1/bS)\ \mathrm{Ar\ ctgh}\ \{(1 - 0.999aR_\infty)/0.999bR_\infty\} \quad \text{(Eq. 6)}$$

X'_∞ can be regarded as an infinite optical thickness for monochromatic light of the corresponding wavelength.

The above optical constants were calculated for each of the 1-mm samples. Then, reflectance values of the 1-, 1.5-, and 2-mm samples with the yellow tile background were predicted at every 5 nm using the calculated optical constants from Equation 7:•

$$R = \{1 - Rg(a - b\ \mathrm{ctgh}\ bSX)\}/(a + b\ \mathrm{ctgh}\ bSX - Rg) \quad \text{(Eq. 7)}$$

The differences between the observed and predicted reflectance values of the 1.5- and 2-mm samples were studied using Welch's *t* test[12] at every 50 nm (besides 405 nm).

Tristimulus values (X, Y, and Z) relative to the 1931 CIE color-matching functions for CIE Standard Illuminant C were computed from the observed percent reflectance values of the samples and the backings as described elsewhere.[13] Furthermore, hue, value, and chroma in the Munsell color system were converted from the CIE tristimulus values as described elsewhere[13] using graphs.¶

The predicted colors of the 1-, 1.5-, and 2-mm samples with the yellow tile background were calculated in the same way. Color differences (I) between the observed and predicted colors were calculated using Nickerson's equation.[14] Then, the values of I were compared to the critical color difference (Ic) necessary to show a significant difference between two colors.[2]

Results.

Average reflectance spectra of the three 1-mm samples with the black tile and the white porcelain backgrounds are shown in Fig. 1 with the reflectance spectra of the two backings. The CIE tristimulus values and the corresponding Munsell colors are listed in Table 1.

The effects of thickness, wavelength, and their interaction on the observed reflectance values of the samples with the yellow tile background were significant ($P < 0.05$). The means of the actual thickness of the 1-, 1.5-, and 2-mm samples were 1.19, 1.69, and 2.24 mm, respectively. Means of the corrected reflectance values of the samples of each thickness with the yellow tile background at every 50 nm (besides 405 nm) are listed in Table 2. A difference larger than 0.007 between two means for samples of the same thickness was significant with 95% level of confidence, while the statistical value was 0.013 for the samples of different thickness at the same or different wavelengths. The reflectance values of the 1.19-mm-thick samples were significantly lower than those of the 1.69-mm-thick and the 2.24-mm-thick samples at 500 nm. On the other hand, the reflectance values of the 1.19-mm-thick and the 1.69-mm-thick samples were significantly higher than were those of

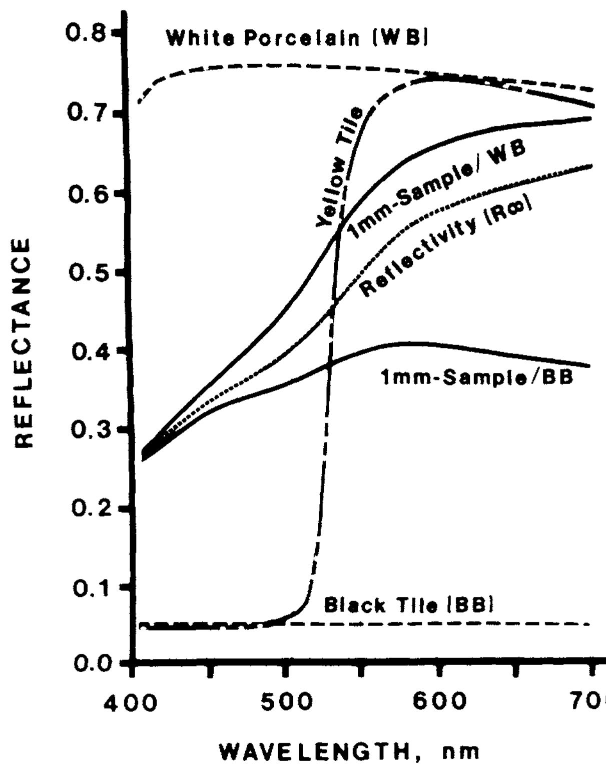

Fig. 1 – Reflectance spectra of several objects studied. The curves for the 1-mm samples show average data of three replications (actual mean thickness was 1.19 mm.).

TABLE 1
COLOR OF SEVERAL OBJECTS

Object	CIE Tristimulus Value X	Y	Z	Munsell Color
Black Tile (BB)	4.73	4.83	5.87	N-2.6
White Porcelain (WB)	73.39	75.28	38.53	N-8.95
1-mm samples/BB	37.43* (0.50)	38.85 (0.52)	37.79 (0.37)	7.5Y 6.75/1.2
1-mm samples/WB	57.42 (0.15)	58.28 (0.17)	42.77 (0.18)	2.0Y 8.05/3.5
Reflectivity of Material	50.93	50.83	39.64	0.1Y 7.6/3.2
Yellow Tile	57.43	55.80	6.28	2.4Y 7.9/13.3

*Mean values of three replications with standard deviations in parentheses.

• Equations 2, 3, 4, 5, and 7 are Kubelka's equations.[9] Equation 1 was derived from Equation 7, and Equation 6 was obtained from Equation 4.

¶ Munsell - CIE Diagrams (1931), #11-7, Munsell Color, Baltimore, MD 21218 the 2.24-mm-thick samples at 550, 600, 650, and 700 nm.

The optical properties calculated from the data of the 1-mm samples are listed in Table 3 at every 50 nm (besides 405 nm). The values of scattering coefficient (S) and absorption coefficient (K) decreased as the wavelength increased. However, the rate of decrease of K was much higher than that of S. The infinite optical thickness of the material increased as the wavelength increased. The light reflectivity (R_∞) of the material and the reflectance spectra of the yellow tile are also shown in Fig. 1. The value of R_∞ increased with increasing wavelength as the ratio of K/S decreased. The CIE tristimulus values and the Munsell colors for the aforementioned data are listed in Table 1.

The observed and predicted reflectance spectra of the samples with the yellow tile background are shown in Fig. 2. **The differences between the observed and predicted values of the 1.19-mm-thick samples were not bigger than 0.005 at any wavelength. Most of the differences between the two values for the 1.69-mm-thick and the 2.24-mm-thick samples were larger than those for the 1.19-mm-thick samples. However, each of the Welch's t_0 values, which were calculated from the corrected observed and predicted values at every 50 nm (besides 405 nm), was smaller than 2.23, and the differences were not significant.

The observed and predicted CIE tristimulus values and the corresponding Munsell colors of the three samples of different thickness are listed in Table 4 with the values of color difference (I) between the observed and predicted colors. All of the values of I were smaller than the previously determined critical value (Ic = 3.1) for restorative resins.[2]

Discussion.

In this study, as the thickness of a sample increased, an increase of reflectance was observed between 405 and 500 nm, but a decrease was observed between 550 and 700 nm (Table 2). This relationship occurs because the reflectance of a sample changes from the reflectance of the background to reflectivity of the material as the thickness of the sample increases. Also, the reflectivity of the material was larger than was the reflectance of the yellow tile up to 500 nm, but smaller beyond 550 nm (Fig. 1). The degree of this effect depends on changes in X'_∞ with wavelength.

When the overall range of visible light is considered for materials which have similar optical constants, the following phenomena are thought to take place: A sample with a white background will have a larger dominant wavelength (more reddish) than will the same sample with a black background, because the reflectance of sample is more sensitive to the reflectance of the background at longer than shorter wavelengths. This effect becomes smaller as the thickness of the sample increases, and was observed in this and other experiments.[2,3,6] For the same reason, a sample may be more chromatic with a white background than with a black background.[3] Clinically, a composite restoration with a white cement base may appear lighter, more reddish, and more saturated than that with a dark background.

The Kubelka-Munk theory was developed with several assumptions: (1) Both the light flux incident upon a colorant layer and the light flux in every direction within the layer are perfectly diffuse; (2) the layer is infinite in area

**The thicknesses of three samples prepared from the same split ring were not exactly the same. Although a mean value of the reflectances of the three samples could be different from a reflectance value of a sample of mean thickness, the two values were treated as the same because the theoretical difference was calculated to be small enough to neglect in this experiment.

TABLE 2
EFFECTS OF THICKNESS AND WAVELENGTH ON CORRECTED REFLECTANCE VALUES

Wavelength (nm)	Thickness (mm) 1.19	1.69	2.24
405	0.258*	0.261	0.261
450	0.322	0.330	0.329
500	0.355	0.374	0.375
550	0.568	0.541	0.514
600	0.663	0.640	0.612
650	0.685	0.673	0.650
700	0.683	0.683	0.663

*Mean values of three replications.

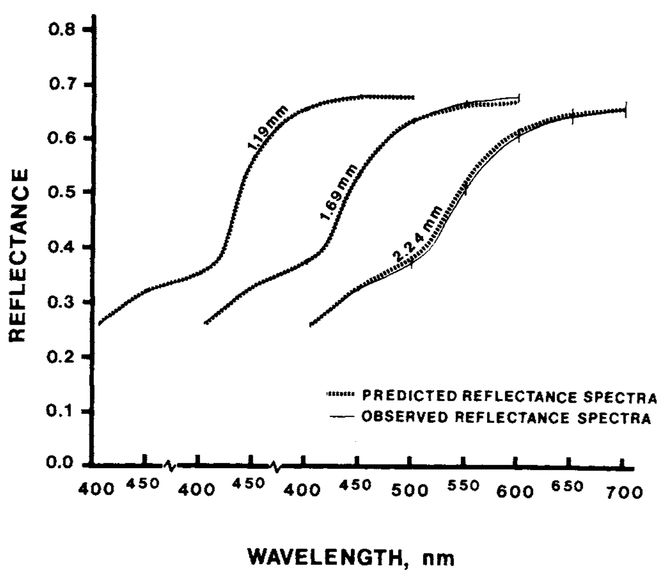

Fig. 2 – Observed and predicted reflectance spectra of a composite with a yellow tile background for three different thicknesses. Each curve is shown between 405 and 700 nm and is displaced on the x-axis for convenience. The longitudinal lines at every 50 nm for the observed reflectance spectra show the standard deviations of the corrected reflectance values, while the width of the lines for the predicted reflectance spectra closely represents the standard deviations of the predicted values.

TABLE 3
OPTICAL PROPERTIES CALCULATED FROM 1-mm SAMPLES AT SEVERAL WAVELENGTHS (nm)

Wavelengths	R_∞	S (mm^{-1})	K (mm^{-1})	X'_∞ (mm)
405	0.257 (0.003)*	1.165 (0.025)	1.250 (0.049)	1.62 (0.05)
450	0.333 (0.003)	0.968 (0.013)	0.647 (0.002)	2.63 (0.02)
500	0.393 (0.004)	0.789 (0.018)	0.370 (0.001)	3.98 (0.04)
550	0.506 (0.003)	0.707 (0.016)	0.171 (0.002)	6.36 (0.09)
600	0.584 (0.005)	0.625 (0.013)	0.093 (0.002)	9.20 (0.10)
650	0.619 (0.005)	0.565 (0.013)	0.067 (0.001)	11.40 (0.11)
700	0.640 (0.008)	0.514 (0.014)	0.052 (0.002)	13.47 (0.13)

*Mean values of three replications with standard deviations in parentheses.

TABLE 4
OBSERVED (O) *VS.* PREDICTED (P) COLOR OF A COMPOSITE WITH YELLOW TILE BACKGROUND

Thickness (mm)	Method	CIE Tristimulus Value X	Y	Z	Munsell Color		Color Difference
1.19	O	56.26	54.89	38.03	9.0YR	7.85/4.4	0.0
	P	56.01	54.66	37.91	9.0YR	7.85/4.4	
1.69	O	54.84	53.64	39.17	8.9YR	7.75/3.9	0.5
	P	54.61	53.60	39.06	9.2YR	7.75/3.9	
2.24	O	52.71	51.63	39.04	8.6YR	7.65/3.7	1.2
	P	53.46	52.72	39.45	9.2YR	7.7/3.7	

and completely homogeneous; and (3) there is no change in refractive index at the boundaries of the layer.[8] The conditions of measurement in this study did not completely satisfy the abovementioned assumptions; therefore, the optical properties obtained may not be absolute, and may not be used for prediction when the index of refraction of the material is the same as the index of refraction of the surrounding medium. Saunderson[15] has reported a method to correct the reflection losses at the boundary between air and the colorant layer whose refractive index is other than 1; however, it is difficult to satisfy the conditions required in applying Saunderson's equation to a composite material. This correction is reported to be important for lightly pigmented thick layers[16] – a condition which may not exist for esthetic restorations. Under similar experimental conditions, the obtained optical properties may be useful for the prediction of color. Clinically, the medium between the light source and restorative material is air as in this experiment. As long as the discrepancy between the predicted and actual colors is acceptable, the simple Kubelka-Munk theory is thought to be useful.

The relationship between the optical properties as a function of wavelength and the representative optical properties which have been seen in previous papers[10,17-19] will be discussed in a later paper. Future studies are desired to interpret the color phenomena actually seen clinically in relation to the optical properties.

Conclusions.

The Munsell hue, value, and chroma of a composite of several thicknesses (1.19, 1.69, and 2.24 mm) with a highly chromatic background were predicted using the optical properties calculated as a function of wavelength from reflectance spectra of the material of a known thickness with dark and light achromatic backgrounds by applying the Kubelka-Munk theory. The scattering coefficient (S) and the absorption coefficient (K) of the material tested decreased with increasing wavelength. The light reflectivity increased with increasing wavelength as the ratio of K/S decreased. The calculated infinite optical thickness increased with increasing wavelength. The values of color difference between the predicted colors and observed colors were smaller than a critical value for restorative resins necessary to show a color change significant for human eyes. The color of an esthetic restorative material which has optical properties similar to those of the material tested may be not only lighter, but also more reddish and more chromatic with a white background than with a black background.

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