Title: Optical properties of base dentin ceramics for all-ceramic restorations

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Short Title: Optical properties of dental ceramics

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Abstract

Objectives: The study was conducted to compare the optical parameters of VM7® M-shade base dentin ceramics (VITA, Germany) for all ceramic restorations to the chemical composition across the 3D-MASTER® shade system.

Methods: Three disc samples, 13 mm diameter and 1.4 mm thickness, were produced for each M-shade following the manufacturer's instructions. Each disc was ground and polished to a thickness of 1.0 mm. Spectral light transmittance and reflectance data were recorded in the visible spectrum under the standard illuminant D65 and 2° observer at 10 nm intervals by using a computer-controlled spectrophotometer. Opacity, translucency and opalescence parameters were determined for each sample.

Results: 1) Spectral transmittance and reflectance in the short-wavelength range systematically decreased with increasing chroma number (M1, M2, M3) when compared within the same value (lightness) group.

2) Spectral transmittance and reflectance decreased systematically across the whole visible spectrum with increasing value group number when compared within the same chroma group.

3) Analysis of relationship between chemical composition and various optical parameters for all the samples showed the significant contribution of ZrO_2 and

Y_2O_3 substances to optical properties of the present material.

Significance: Systematic variations in optical properties of VM7® M-shade base dentin ceramics were observed throughout the 3D-MASTER® shade system and were suggested to be caused by the fine structure of the sample which can interfere with shorter wavelengths in the visible spectrum.

Keywords: dental ceramics; optical properties; transmittance; reflectance; opacity; opalescence; color

1. Introduction

Veneering ceramics used in conjunction with high strength ceramic materials such as glass infiltrated spinell and alumina or fused alumina or zirconia materials are becoming increasingly advanced in their optical properties [1]. Dental veneering ceramics for all-ceramic restorations should allow the operator to control the optical parameters of color (hue, chroma and value) as well as the translucency. Color and translucency may be determined from the transmitted light through a material, where the light source and detector are on opposite sides of the object, or from the reflected light where the light source and detector are on the same side of the object. Differences between the transmitted and reflected light is described as opalescence where a material is preferentially transmitting different wavelengths to those that are reflected. Enamel and dentin both exhibit opalescence resulting in the transmitted light being rich in longer wavelengths (red and orange) in comparison to the reflected light [1, 2].

Modern dental ceramics also exhibit opalescence [1] and this study sets out to quantify this using the ceramics in the 3D-MASTER® shade system. These ceramics were chosen as they are arranged according to the three attributes of color and systematically change with value groups (lightness), notated 1 through 5 and chroma groups (color saturation) M1 through M3 as described previously [3]. Hue differences (color family) of L (yellow-shift) and R (red-shift) will not be considered in this study. The VM7® ceramic (VITA, Bad Sackingen, Germany) may be used as a veneering material for substructures with a coefficient of thermal expansion (CTE) of approximately 7 X 10^{-6}/K, or independently when produced on a refractory of matching CTE. This ceramic material is composed of a fine two-phase all-glass structure and does not contain a crystal phase [1].

Since the knowledge of the optical properties of dental restorative materials is very important in achieving aesthetic restorations, this study attempts to analyze optical properties of the fired VM7® base dentin ceramics. The authors suggest that the incident light entering a phase boundary between a matrix glass and the second phase glass particle is partly reflected, refracted or scattered at this boundary due to the differences in the refractive indices of both phases. To clarify this hypothesis, the study investigated the relationship between chemical compositions of the glass powders and the optical properties. The characterization of such properties will allow the materials to be selected appropriately.

2. Materials and methods

2.1. Sample preparation

Three disc shaped samples of VM7® base dentin ceramic were produced in each M-shade of the 3D-MASTER® shade system. The ceramic powder was condensed in a silicone mold to a thickness of approximately 1.8 mm and a diameter of 15 mm. The condensed ceramic samples were removed from the mold and fired according to the manufacturer's instructions. The samples were ground using a waterproof P240 silicon carbide abrasive paper until parallel sided and fired again resulting in a sample approximately 1.4 mm thick. The discs were ground to a final thickness of 1.0 mm with both faces finished with a waterproof P600 silicon carbide abrasive paper.

2.2. Recordings of spectral transmittance and reflectance and calculation of color coordinates

Spectral transmittance and reflectance data in the wavelength range of 360 to 740 nm under standard illuminant D65 and 2° observer were collected at 10 nm intervals using a computer-controlled spectrophotometer (CM-3600d, Konica Minolta Sensing, Inc., Osaka, Japan) with an integrating sphere accessory. Color coordinates, L^* (lightness), a^* (red-green chromaticity index), b^* (yellow-blue chromaticity index), C^* (chroma) and h (hue angle) were determined from the transmittance and reflectance data using a computer software (Spectra-Magic, Version 3.61, Konica Minolta Sensing, Inc., Osaka, Japan).

For each shade three measurements were obtained from three different samples. Average and standard deviation were calculated. Where reflectance measurements were carried out, the samples were placed on standard white and black backgrounds without optical coupling.

The transmittance and reflectance data at each wavelength was used to determine:

1) Average transmittance (T) = Sum of transmittance (%) at each wavelength divided by number of data points (39).

2) Average reflectance (R) = Sum of reflectance (%) at each wavelength divided by number of data points (39).

3) Opacity of a sample was calculated according to the following equation:

$$\text{Opacity (\%)} = (R_b/R_w) \times 100 \qquad (1)$$

where, R_b is the luminous reflectance of a sample with the black backing, and R_w is the luminous reflectance of a sample with the white backing [4-6].

4) Translucency parameter (TP) of a sample was calculated according to the following equation:

$$TP = [(L^*_W - L^*_B)^2 + (a^*_W - a^*_B)^2 + (b^*_W - b^*_B)^2]^{1/2} \qquad (2)$$

where, the subscript W refers to color coordinates with the white backing and the subscript B refers to those with the black backing [6-8].

5) Opalescence parameter (*OP*) of a sample was determined according to the following equation:

$$OP = [(a^*_T - a^*_R)^2 + (b^*_T - b^*_R)^2]^{1/2} \qquad (3)$$

where, the subscript T refers to the transmitted light and the subscript R refers to the reflected light from a sample with the black backing [8, 9].

6) Sum of scattering (*S*) and absorption (*A*) in percentage was calculated according to the following equation [10]:

$$S + A = 100 - (T + R_b) \qquad (4)$$

2.3. Chemical analysis

Chemical compositions of the as-received VM7® M-shade base dentin ceramic powders were analyzed by means of X-ray fluorometry using a sequential X-ray fluorescence spectrometer (XRF-1700, SHIMADZU Co., Kyoto, Japan). The analyzed compositions are accurate to 0.1%.

2.4. Data analysis

The optical parameters and chemical compositions of all the samples were tabulated and correlation coefficients, *r*, were determined to assess the relationship between glass composition and optical parameters. 95% confidence intervals for the value of *r* were calculated based on the Fisher r-to-z transformation.

3. Results

3.1. Light transmittance

Fig. 1 shows typical spectral transmittance curves for the same value 3M group samples. It can be seen that transmittance in the short wavelength range (< around 550 nm) systematically decreased with increasing chroma number (M1, M2, M3). This trend was repeatedly observed in all sets of samples with the same value group.

Fig. 2 shows typical spectral transmittance curves for the same chroma M1 group samples. With decreasing value from 1 to 5, spectral transmittance systematically decreased throughout the whole range of visible spectrum. This trend was repeatedly observed for all sets of samples with the same chroma group (M1, M2, M3).

3.2. Light reflectance

Fig. 3 shows spectral reflectance curves for the 3M group samples with the white backing. Reflectance (R_w) in the short wavelength range decreased and increased in the long wavelength range with increasing chroma number (M1, M2, M3). As a result, slope of the spectral reflectance curve near 550 nm substantially increased with increasing chroma number. This behavior was repeatedly observed in each value (lightness) group samples.

Fig. 4 shows spectral reflectance curves with the white backing for the same chroma M1 group samples. A systematic decrease in reflectance across the whole range of visible spectrum occurred with the decrease in value from 1 to 5. This behavior was also observed in other sets of the same chroma M2 and M3 group samples.

3.3. Optical parameters

Average transmittance (*T*), average reflectance with white and black backings (R_w and R_b, respectively), opacity, translucency parameter (*TP*), opalescence parameter (*OP*), sum of the scattering (*S*) and absorption (*A*), for all the fired samples are summarized in Table 1 with standard deviations in parentheses.

Opacity, translucency and opalescence parameters calculated from the color coordinates were visualized in Fig. 5 with the determined summation of scattering (*S*) and absorption (*A*) for each shade. Opacity increased with increasing chroma for the samples in the same value group 1M, 2M or 3M. However, this trend was not clear for the 4M and 5M group samples. Opacity increased with increasing value number from 1 to 5 when compared in the same chroma group. The translucency parameter (*TP*) was primarily determined by value. That is, when compared *TP* values for the same chroma group samples, *TP* decreased with increasing value number from 1 to 5. The *TP* value was not greatly affected by chroma when compared in the same value group. Opalescence parameter (*OP*) increased with increasing chroma from M1 to M3 when compared in the same value group. The *OP* value increased with increasing value number from 1 to 5 when compared in the same chroma group.

3.4. Chemical composition of ceramic powder

The chemical composition of the as-received ceramic frit analyzed by X-ray fluorometry is shown in Table 2. The compositions of all the as-received powders were similar to each other. However, as was the case for the previously investigated VM7® dentin ceramics [3], powders from higher chroma or lower value groups were slightly rich in zirconium oxide (ZrO_2) and yttrium oxide (Y_2O_3). In addition, tin oxide (SnO_2) and vanadium pentoxide (V_2O_5) also showed slightly increased contents at 4M3 and 5M group samples as highlighted in Table 2.

3.5. Relationship between optical parameters and chemical composition

Fig. 6 shows relationship between *OP* values and chemical composition for all the samples examined. The *OP* value clearly increased with increasing both ZrO_2 and Y_2O_3 concentrations. Fig. 7 shows relationship between sum of scattering (*S*) and absorption (*A*) and chemical composition for all the samples.

For the 1M, 2M, 3M group samples, the (*S* + *A*) value systematically increased with increasing ZrO_2 and Y_2O_3 concentrations. Similar tendency was also observed for the 4M and 5M group samples. However, this trend was not so clear in these high value number groups.

4. Discussion

The method used in the current study to determine the optical properties is an expansion of that previously published using an integrating sphere [3]. In this study, both transmittance and reflectance data were presented and optical parameters were determined for each. The wavelength distribution of differential coefficients of the spectral transmittance curves for the VM7® base dentin ceramics in a previous study [11] showed activity of a material at around 500nm and of a second phase at approximately 620nm, similar to that for the VM7® dentin ceramics [3].

Figs. 1 through 4 demonstrate the difference between the transmitted and reflected light from the base dentin materials and the effect on the optical parameters that are determined (Fig. 5). This is a complex system with numerous components controlling the light interaction.

Compositions of all the VM7® base dentin porcelain powders were basically analogous to those of the previously investigated VM7® dentin ceramic powders [3]. However, when looking closely at the analyzed compositions, sodium oxide (Na_2O) and ZrO_2 concentrations in the base dentin ceramics were slightly higher than those in the dentin ceramics, whereas potassium oxide (K_2O) and calcium oxide (CaO) concentrations in the base dentin ceramics were slightly lower than those in the dentin ceramics [3].

The components determining the optical properties of this series of base dentin ceramics appear to be primarily ZrO_2 and Y_2O_3, which may act to opacify the ceramic and lead to opalescence due to their scattering effect. This was demonstrated in Fig. 6 for *OP* value and in Fig. 7 for sum of scattering (*S*) and absorption (*A*). Fig. 8 shows relationship between opacity and ($S + A$) value. The opacity of this material substantially increased with increasing ($S + A$) value. This trend was more prominent in the low ($S + A$) value range.

Table 3 gives correlation coefficients, *r*, and 95% confidence intervals in parentheses between ZrO_2, Y_2O_3, sum of ZrO_2 and Y_2O_3 concentrations and each of the optical parameters for all the M-shade base dentin ceramics. The correlation coefficients for average transmittance, average reflectance with white and black backings, and translucency parameters ranged between -0.86 and -0.48 and those for opacity and opalescence parameters ranged between +0.56 and +0.85, indicating the significant contribution of ZrO_2 and Y_2O_3 substances to optical properties of the present material.

Fig. 9 shows relationship between average transmittance and sum of ZrO_2 and Y_2O_3 concentrations. It is seen that with increasing sum of ZrO_2 and Y_2O_3 concentrations from about 0.7 to 1.1, average transmittance decreased down to 15%. Further increases in the sum of ZrO_2 and Y_2O_3 concentrations did not change average transmittance substantially. This trend was also observed for other optical parameters of the present series of base dentin ceramics.

The addition of a small amount of SnO_2 to the low value and high chroma ceramics (*i.e.*, 4M3, 5M1, 5M2, 5M3) may also act as a ceramic opacifier or a ceramic pigment where it produces a milky white color [12]. However, in combination with the metallic oxide V_2O_5, it may produce a yellow color [12]. Components found throughout all ceramic powders analyzed, for example the combination of iron oxide (Fe_2O_3) and titanium oxide (TiO_2), are likely to be responsible for the underlying color of the ceramic. Minute amounts of TiO_2 (*i.e.*, 0.1%) can be used to intensify and stabilize colors; here iron oxide can be altered to produce yellow and orange rather than red [13]. Rubidium oxide (Rb_2O) is also a yellow colored but often found as an impurity in silicates.

This study has not looked at the L and R shades within the VM7® base dentin shades that represent hue shifts. Further work should focus on characterizing these materials along with the range of optical properties found in natural dentin and enamel across the shade range. The effect of dimensional change and layering of different ceramic materials would also be useful in the development of computer-aided manufacture of ceramic restorations.

5. Conclusion

The inclusion of small amounts of metal oxides into ceramic materials allows control of the opalescence quality of the material. This parameter may be determined via spectrophotometry and has the potential to be used to replicate the opalescence found in natural dentin and enamel.

Acknowledgements

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Table captions and Figure legends

	T (%) (SD)	R_w (%) (SD)	R_b (%) (SD)	Opacity (%) (SD)	*TP* (SD)	*OP* (SD)	*S+A* (using R_b)
1M1	30.98 (1.09)	59.80 (1.41)	42.70 (1.70)	69.98 (1.05)	13.19 (0.51)	5.27 (0.12)	26.32
1M2	29.43 (0.06)	58.10 (0.67)	42.10 (0.97)	71.59 (1.18)	14.24 (0.34)	6.02 (0.26)	28.47
2M1	26.74 (1.83)	53.80 (1.05)	41.70 (2.26)	77.18 (2.91)	10.57 (1.07)	5.99 (0.27)	31.56
2M2	21.78 (3.71)	53.50 (1.38)	43.10 (2.92)	80.53 (3.67)	10.49 (1.55)	8.22 (0.88)	35.12
2M3	19.60 (0.22)	52.20 (0.15)	43.60 (0.01)	84.26 (0.31)	9.39 (0.17)	9.54 (0.17)	36.80
3M1	23.49 (2.56)	49.30 (1.59)	39.50 (2.98)	80.28 (3.53)	9.10 (1.36)	6.50 (0.30)	37.01
3M2	21.89 (1.79)	51.10 (1.05)	41.80 (1.50)	82.59 (1.21)	9.44 (0.56)	7.65 (0.56)	36.31
3M3	19.10 (2.09)	49.40 (1.05)	40.90 (1.84)	84.06 (2.23)	9.68 (0.99)	10.07 (1.48)	40.00
4M1	16.99 (2.46)	40.10 (1.26)	35.30 (2.16)	88.02 (2.80)	6.06 (1.08)	8.08 (0.48)	47.71
4M2	18.06 (1.92)	41.90 (1.40)	35.30 (2.19)	86.50 (2.74)	7.70 (1.11)	9.20 (1.02)	46.64
4M3	14.82 (1.79)	42.00 (1.14)	36.50 (1.72)	90.30 (1.54)	6.59 (0.88)	12.11 (1.06)	48.68
5M1	14.80 (1.21)	37.50 (0.59)	33.40 (0.90)	91.52 (0.97)	4.60 (0.44)	8.71 (0.42)	51.80
5M2	15.20 (1.29)	35.20 (1.18)	30.30 (1.71)	89.63 (1.99)	6.08 (0.85)	9.49 (0.79)	54.50
5M3	14.55 (0.31)	35.90 (0.36)	30.80 (0.54)	90.78 (1.75)	6.11 (0.89)	12.09 (0.83)	54.65

Table 1 - Optical parameters with standard deviations in parentheses determined for all the M shade VM7® base dentin ceramics

	1M1	1M2	2M1	2M2	2M3	3M1	3M2	3M3	4M1	4M2	4M3	5M1	5M2	5M3
Lot Number	21040	21040	16900	16900	31030	10590	11680	14590	29900	23711	7468	28850	7302	7260
SiO_2	70.49	69.98	70.25	70.25	70.27	70.35	70.16	70.69	70.18	69.15	69.29	70.06	69.52	69.3
Al_2O_3	13.70	13.69	13.70	13.66	13.65	13.67	13.77	13.29	13.56	13.81	13.76	13.56	13.59	13.36
K_2O	8.80	9.10	8.92	8.92	8.80	8.94	8.87	8.77	8.86	9.48	9.25	9.10	9.09	9.00
Na_2O	4.07	4.07	4.09	4.02	4.03	4.00	4.09	4.04	4.06	4.02	4.07	3.99	4.01	4.01
CaO	2.13	2.20	2.16	2.14	2.16	2.19	2.14	2.15	2.19	2.32	2.25	2.20	2.18	2.21
ZrO_2	0.63	0.70	0.63	0.72	0.81	0.60	0.68	0.77	0.76	0.81	0.94	0.69	1.14	1.63
Y_2O_3	0.09	0.11	0.11	0.14	0.17	0.10	0.11	0.12	0.17	0.17	0.19	0.16	0.18	0.21
Fe_2O_3	0.06	0.06	0.05	0.05	0.05	0.06	0.05	0.05	0.07	0.06	0.06	0.07	0.06	0.06
Rb_2O	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04
TiO_2	0.03	-	0.03	0.03	-	0.02	0.02	0.02	0.03	0.03	0.03	0.03	0.02	0.03
PbO	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.01	0.01	0.02
SnO_2	-	0.01	-	-	-	-	0.02	0.02	0.01	0.01	0.04	0.04	0.04	0.05
V_2O_5	-	-	-	-	-	-	<0.01	0.01	0.01	0.01	0.01	<0.01	0.03	0.05
Others	bal.	bal.	bal.	bal.	bal.	bal.	bal.	bal.	bal.	bal.	bal.	bal.	bal.	bal.

Table 2 - Chemical composition in mass % of the as-received M shade VM7® base dentin ceramic powders analyzed by X-ray fluorometry

Correlation coefficient (n = 14)	T	R_w	R_b	Opacity	TP	OP	S+A (R_b)
ZrO_2	-0.59 (-0.853, -0.087)	-0.64 (-0.873, -0.166)	-0.69 (-0.893, -0.252)	0.56 (0.042, 0.840)	-0.48 (-0.805, -0.067)	0.74 (0.345, 0.912)	0.68 (0.234, 0.889)
Y_2O_3	-0.86 (-0.954, -0.606)	-0.82 (-0.941, -0.513)	-0.73 (-0.908, -0.326)	0.84 (0.559, 0.948)	-0.77 (-0.923, -0.405)	0.85 (0.582, 0.951)	0.86 (0.606, 0.954)
ZrO_2 + Y_2O_3	-0.63 (-0.869, -0.15)	-0.68 (-0.889, -0.234)	-0.71 (-0.901, -0.288)	0.61 (0.118, 0.861)	-0.53 (-0.827, 0)	0.77 (0.405, 0.923)	0.71 (0.288, 0.901)

Table 3 - Correlation coefficients, r, and 95% confidence intervals in parentheses between ZrO_2, Y_2O_3, sum of ZrO_2 and Y_2O_3 concentrations and each of the optical parameters for all the M shade VM7® base dentin ceramics

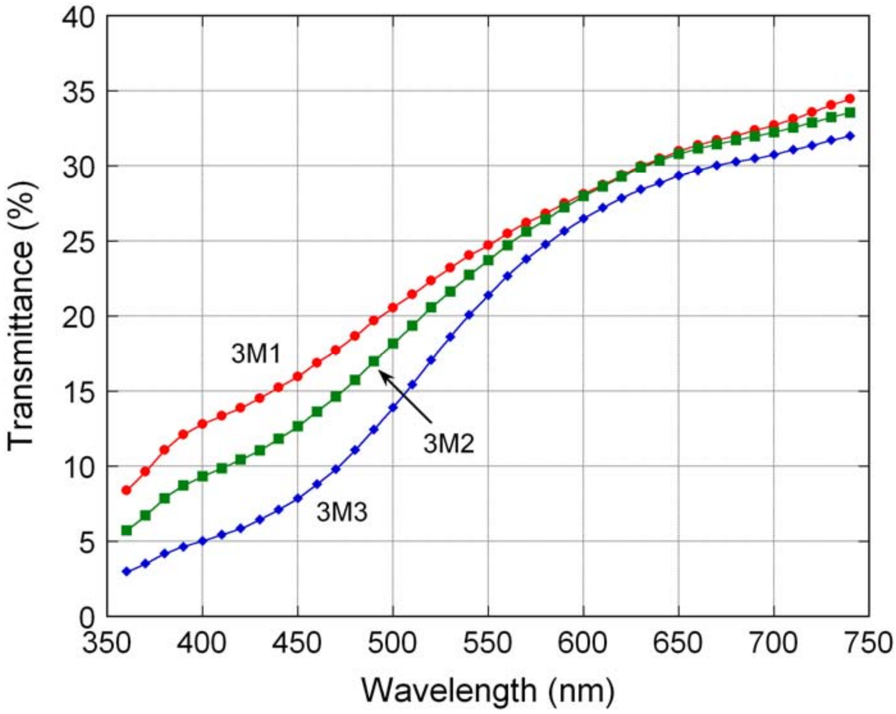

Fig. 1 - Spectral transmittance curves for the same value 3M group VM7® base dentin ceramics.

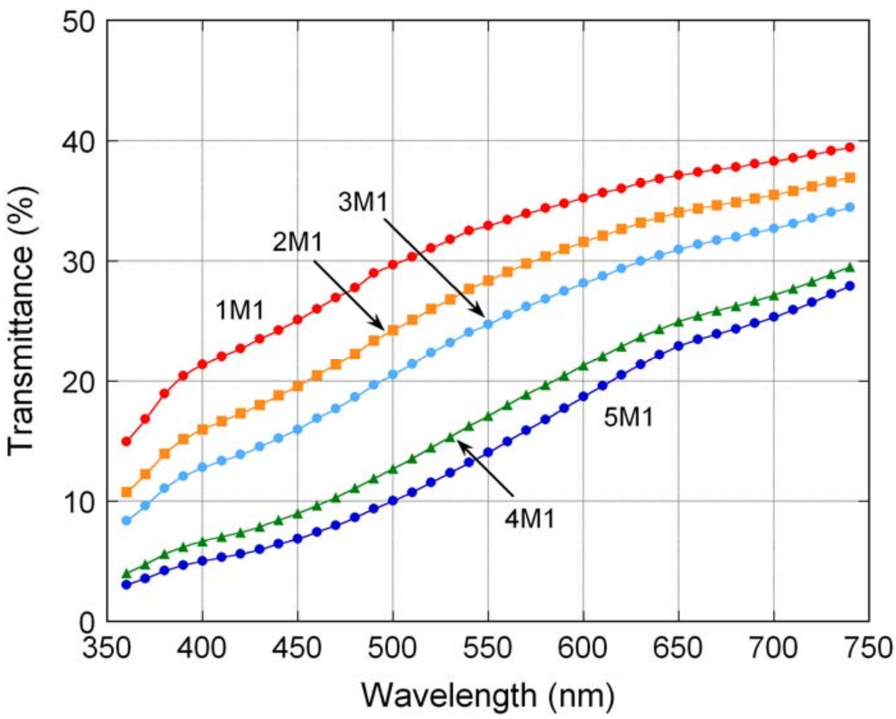

Fig. 2 - Spectral transmittance curves for the same chroma M1 group VM7® base dentin ceramics.

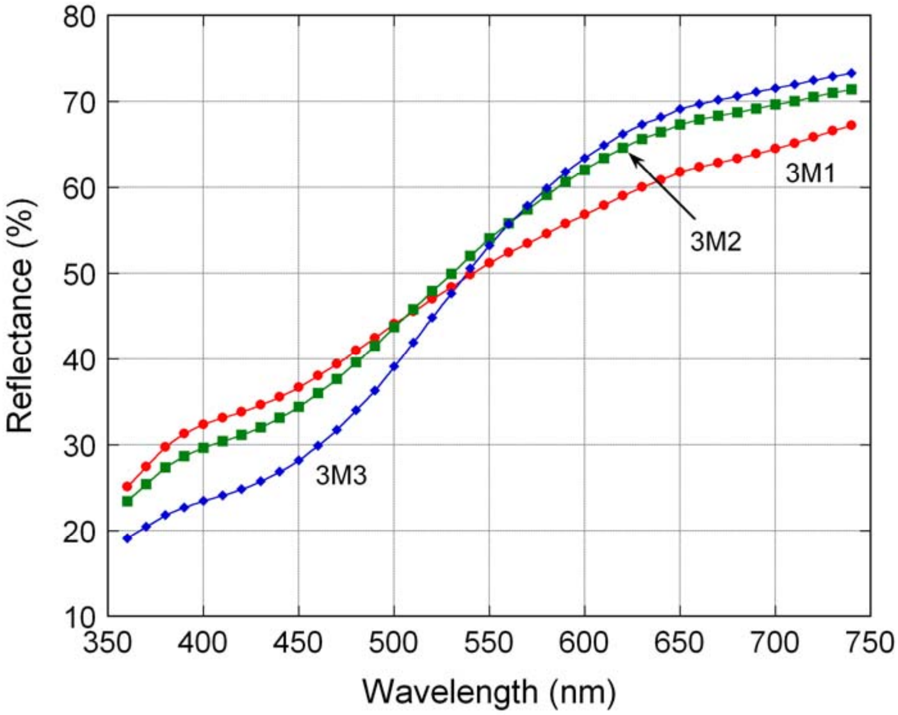

Fig. 3 - Spectral reflectance curves with the white backing for the same value 3M group VM7® base dentin ceramics.

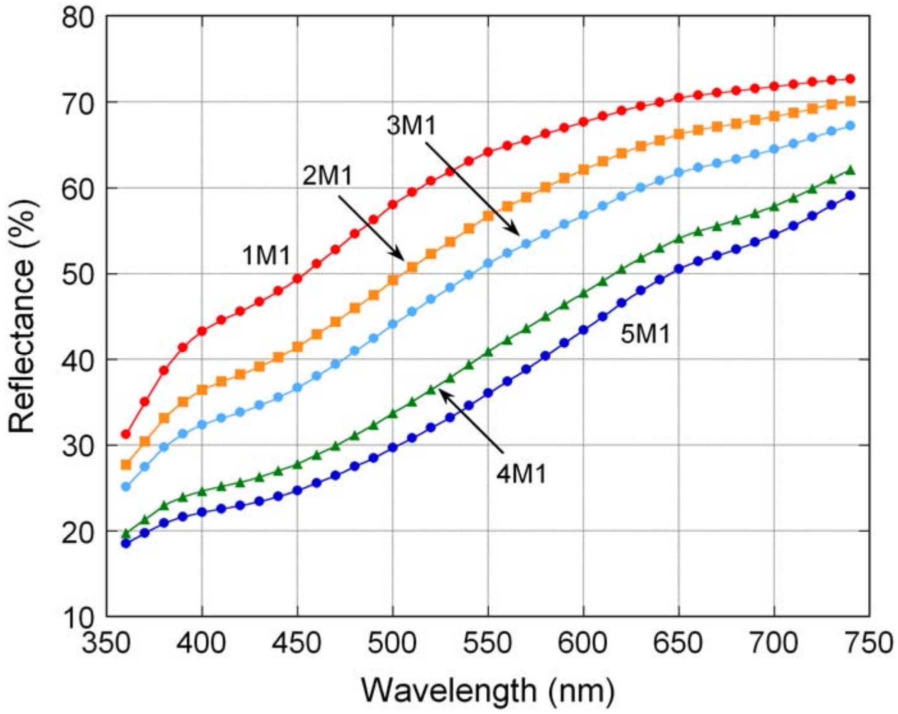

Fig. 4 - Spectral reflectance curves with the white backing for the same chroma M1 group VM7® base dentin ceramics.

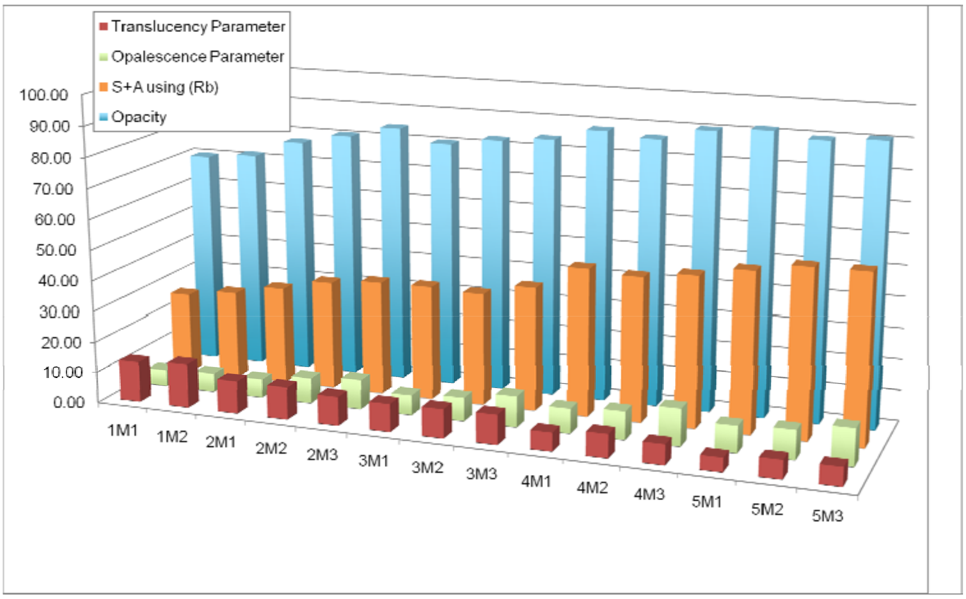

Fig. 5 - Optical parameters determined for all the M shade VM7® base dentin ceramics.

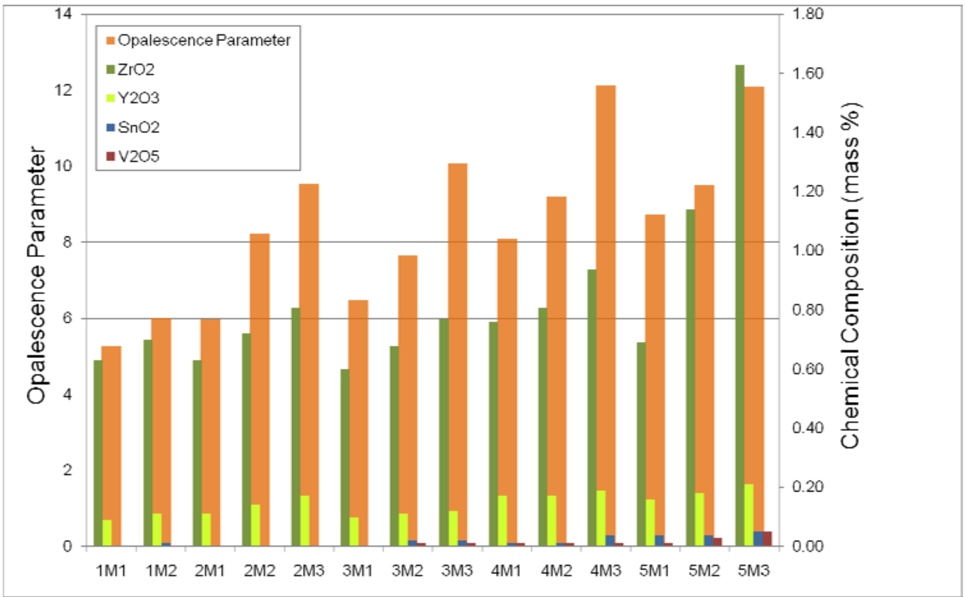

Fig. 6 - Relationship between chemical composition and opalescence parameter for all the M shade VM7® base dentin ceramics.

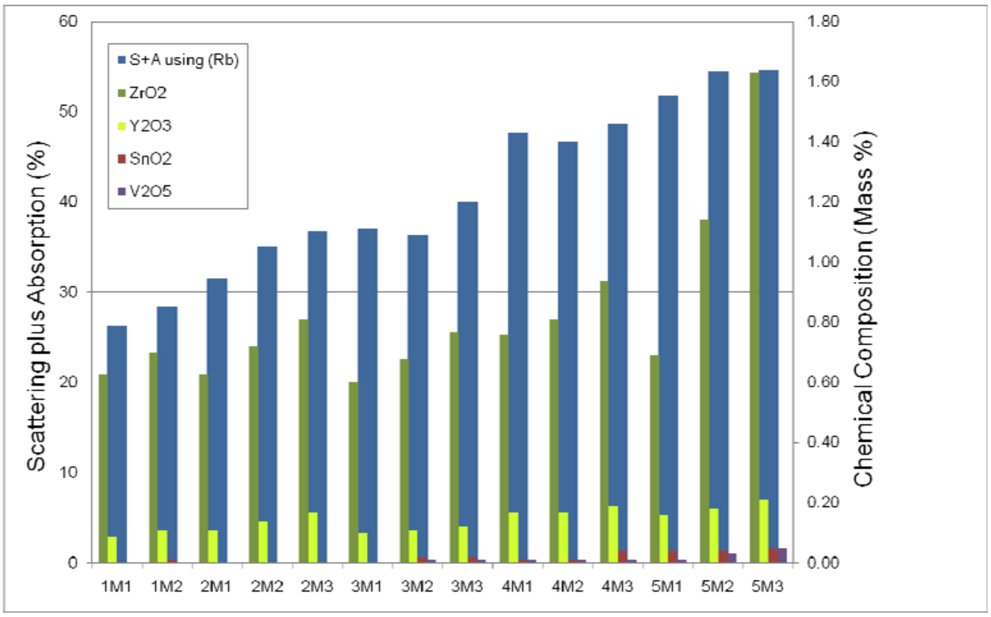

Fig. 7 - Relationship between chemical composition and sum of scattering (*S*) and absorption (*A*) for all the M shade VM7® base dentin ceramics.

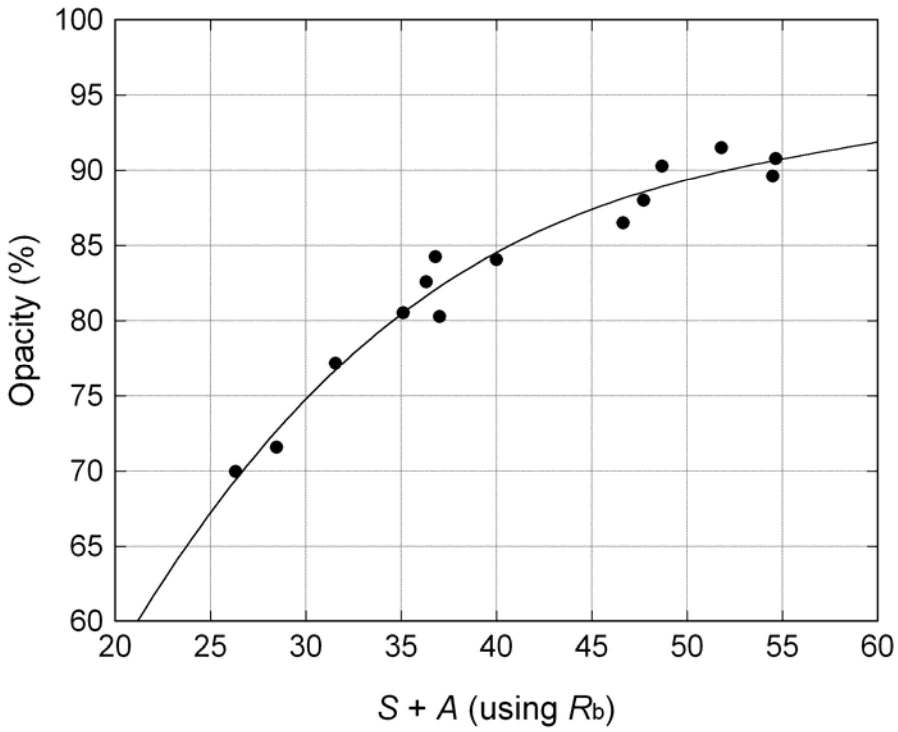

Fig. 8 - Relationship between opacity (%) and the sum of scattering (*S*) and absorption (*A*) determined by the equation (4).

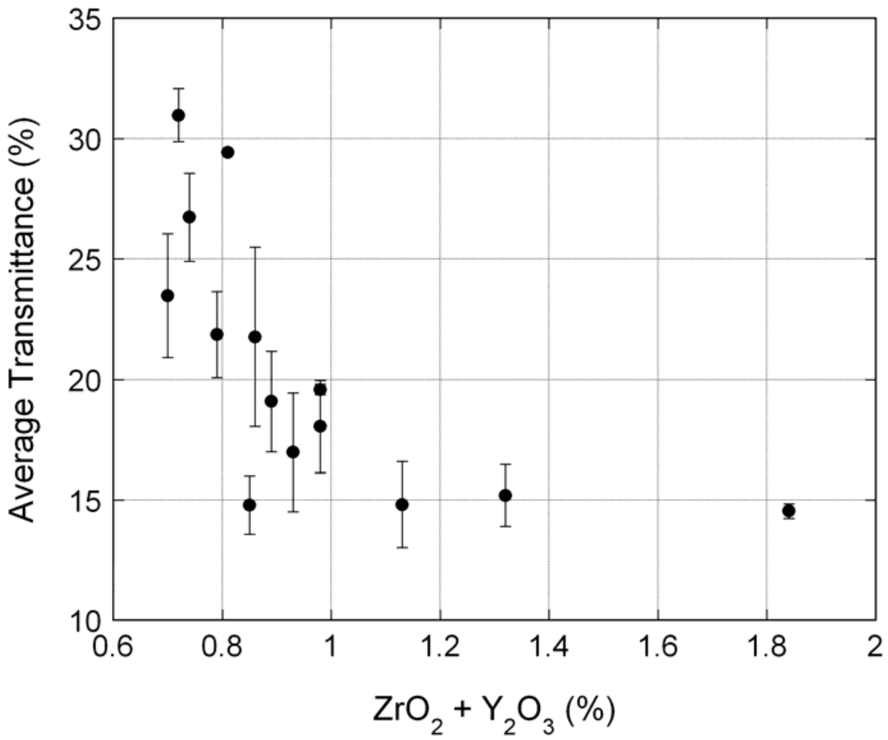

Fig. 9 - Relationship between average transmittance and the sum of ZrO_2 and Y_2O_3 concentrations for all the M shade VM7® base dentin ceramics.