Three-dimensional finite element thermal analysis of dental tissues irradiated with Er,Cr:YSGG laser

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In the present study, a finite element model of a half-sectioned molar tooth was developed in order to understand the thermal behavior of dental hard tissues (both enamel and dentin) under laser irradiation. The model was validated by comparing it with an *in vitro* experiment where a sound molar tooth was irradiated by an Er,Cr:YSGG pulsed laser. The numerical tooth model was conceived to simulate the *in vitro* experiment, reproducing the dimensions and physical conditions of the typical molar sound tooth, considering laser energy absorption and calculating the heat transfer through the dental tissues in three dimensions. The numerical assay considered the same three laser energy densities at the same wavelength (2.79 μm) used in the experiment. A thermographic camera was used to perform the *in vitro* experiment, in which an Er,Cr:YSGG laser (2.79 μm) was used to irradiate tooth samples and the infrared images obtained were stored and analyzed. The temperature increments in both the finite element model and the *in vitro* experiment were compared. The distribution of temperature inside the tooth versus time plotted for two critical points showed a relatively good agreement between the results of the experiment and model. The three dimensional model allows one to understand how the heat propagates through the dentin and enamel and to relate the amount of energy applied, width of the laser pulses, and temperature inside the tooth. © *2008 American Institute of Physics.* [DOI: 10.1063/1.2953526]

I. INTRODUCTION

Nowadays there are wide ranges of dentistry procedures that include laser applications. Lasers can be used for oral surgery, to remove both tooth sound and decayed tooth tissues, enhance tooth bleaching, and sometimes to cure restorative materials.[1,2] Depending on the case, the dentist needs different laser wavelengths and parameters, in order to use the laser continually during a period, only to irradiate the tooth with sharp pulses of light.[3]

The interactions of high-intensity laser irradiation with dental hard tissues are commonly induced by thermal action. For the clinical application of lasers, a precise irradiation parameter must be chosen in order to avoid morphological damage, such as enamel surface carbonization or cracking, which could produce structural, esthetic damages, and postoperative complaints.[4] Moreover, the energy densities used must be safe as regards pulp and periodontal tissue vitality. Therefore, several *in vitro* experiments have been conducted to evaluate the temperature rise in teeth in order to assure safe conditions for the use of lasers. Thermocouples,[5] elliptical mirror and HgCdZnTe detectors,[6] and infrared cameras[7] are widely used to measure temperature rises in pulp, periodontal tissues, and enamel surfaces. However, these experimental methods present some difficulties, such as sample standardization (considering the large variation in volume, size, and thickness of teeth), the exact duplication of the thermal load, accuracy, and cost of equipment.

The finite element method model (FEM model) seems to be a good analytical tool to model and simulate the thermal or mechanical behavior of dental structures.[8–11] In the past two decades, this mathematical model has received increasing attention in dental biomechanical studies,[8] analyzing mechanical stress,[9] thermal stress,[10] or thermal conductivity.[11]

The FEM model shown in the present study was used to simulate the effects of laser on enamel and dentin, but not on gums or inside the pulp cavity, which is filled with blood vessels and innervated tissues, since these materials are soft and highly inhomogeneous. However, the effects of laser irradiation could be difficult to simulate even on the dental hard tissues (only enamel and dentine), since the thermal characteristics of these materials may not have been well determined. Indeed, the thermal characteristics used in the models were obtained from the technical literature, but as there was considerable uncertainty about the physical properties of natural tissues, the numerical data were compared to experimental data obtained from a fast infrared thermal camera.

Therefore, the aims of this study were to simulate the heat transfer inside the dental hard tissues when irradiated with an Er:Cr:YSGG laser, and to compare the results of this simulation with the temperature measurements recorded by an infrared thermal camera in the tooth. The results of this study could be useful for predicting the physical and chemical changes in the enamel after laser irradiation, with the purpose of caries prevention.

II. MATERIALS AND METHODS

A. *In vitro* experiment

After approval by the Human Research Ethics Committee of the Energy and Nuclear Research Institute (Proj. 094/2004 CEP-IPEN), University of Sao Paulo, 12 freshly extracted human third molar teeth were selected. Each tooth was cleaned and half-sectioned longitudinally with a disk-shaped diamond saw (Isomet, Buehler, IL) under cooling. This sectioning allowed the heat transfer from enamel surface to the pulp chamber during laser irradiation to be visualized.

At the time of experiment, each sample was immobilized in optical supports with the sectioned side turned toward the lens of a thermographic camera (ThermaCam FLIR SC3000 Systems, USA), which stores infrared images and data at rates of up to 900 Hz. This experiment was performed at a room temperature of 24.6 °C, 47% air relative humidity and considering tooth emissivity as 0.91. The infrared images obtained were recorded at rates of 900 Hz. The thermographic camera was placed at a distance of 0.1 m in front of samples, and the area of interest was isolated at a focal length of 0.1 m using an internal macrolens. This apparatus made it possible to record the heat propagation from enamel surface through dentin to the pulp chamber, enabling the temperature increase in dental tissues to be evaluated at the exact moment of laser irradiation.

Laser irradiation was performed using an Er,Cr:YSGG laser (Millenium, Biolase Inc., San Clemente, CA, USA), with 2.79 μm wavelength, 140 μs pulse width, 20 Hz repetition rate, and a power output ranging from 0 to 6 W. The energy was delivered through a 430 μm spot size fiber optic system ending in a sapphire terminal of 750 μm diameter and 6 mm long (S75 tip), which resulted in 600 μm beam diameter at 1 mm distance from the irradiated surface, bathed in an adjustable air and water spray. Irradiation was performed perpendicularly to the occlusal surface of the samples with the fiber end at 1 mm distance from this surface, tangentially to the sectioned plane of the samples. Laser irradiation was performed in a single point for a standardized time of 5 s, without air-water mist.

TABLE I. Er,Cr:YSGG laser configurations used in the simulations.

Energy density (J/cm^2)	Photoabsorber	Energy per pulse (mJ)	Number of pulses	Total energy (J)
2.8	Yes	12.5	100	1.25
2.8	No	12.5	100	1.25
5.6	Yes	25	100	2.5
5.6	No	25	100	2.5
8.5	Yes	37.5	100	3.75
8.5	No	37.5	100	3.75

Samples were divided into six groups ($n=2$) according to the laser fluence and with or without the presence of a photoabsorber, as follows: Group 1: irradiation at 2.8 J/cm^2 with application of photoabsorber; Group 2: irradiation at 2.8 J/cm^2 without application of photoabsorber; Group 3: irradiation at 5.6 J/cm^2 with application of photoabsorber; Group 4: irradiation at 5.6 J/cm^2 without application of photoabsorber; Group 5: irradiation at 8.5 J/cm^2 with application of photoabsorber; and Group 6: irradiation at 8.5 J/cm^2 without application of photoabsorber. This photoabsorber consisted of a triturated coal paste (± 10 μm diameter particles) diluted in 50% water and 50% alcohol, which was applied on the occlusal surface of samples with a No. 1 brush before laser irradiation, in order to increase the absorption of the laser beam at the enamel surface. The irradiation conditions and total energy are described in Table I.

The beginning of laser irradiation and temperature recording was synchronized but the thermal measuring finished 15 s after the end of the laser irradiation. For later analysis of temperature increments, two standardized points were chosen on the infrared images obtained: one located at the enamel surface immediately below the laser tip (spot 1) and the other located at dentin-pulp chamber limit (spot 2) at an approximate distance of 3.5 mm below spot 1.[12] Data were analyzed by ORIGIN PRO software.

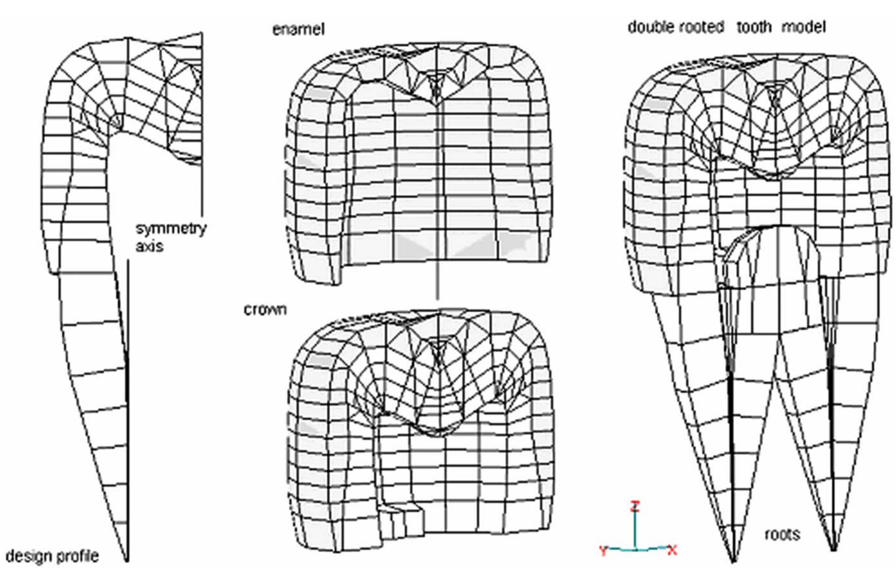

FIG. 1. (Color online) FEM model for a half-sectioned human molar tooth.

B. Computer calculation

A geometric FEM model of a half-sectioned double rooted molar tooth was constructed, as shown in Fig. 1. In order to obtain the geometric model, a typical profile of a tooth root was used, i.e., planar elements were designed to fit the profile and then a three-dimensional root structure was created revolving these planar elements around the vertical axis. Both roots are symmetrical with respect to the tooth axis and the geometric shape of the crown was also designed as axially symmetric. This is an acceptable approximation since the model was conceived only to be used in simulations of the thermal behavior of dental tissues. Stress and other static and dynamic characteristics that depend on the exact shape of the body under analysis are not objects of study in this work.

The dimensions of the model tooth are typical, corresponding to a total volume of $0.6\ \mathrm{cm}^3$ and total weight of 1.47 g. The enamel ($r=2.8\ \mathrm{g/cm}^3$) and the dentin ($r=1.96\ \mathrm{g/cm}^3$) are both represented in Fig. 1.

1. The thermal equations

Since the goal was to calculate the temperature distribution on the surface and inside the tooth, the FEM model was used to set up the equations of heat transfer through dental tissues.

In each element the total heat is given by the internal heat, determined by the material density (ρ) and specific heat (c), and the heat flux, determined by the element material thermal conductivity (k). The power density Q_i ($[\mathrm{J/m^3\ s}]$) corresponds to the heat H_i absorbed or lost by each element in each second is

TABLE II. Physical characteristics of dental hard tissues.

Physical characteristic	Enamel (typical)	Dentin (typical)
Specific heat (cal/g °C)	0.17	0.38
Thermal conductivity (cal/s cm °C)	2.33×10^{-3}	1.36×10^{-3}
Density ($\mathrm{g/cm^3}$)	2.80	1.96

$$Q_i = \frac{\partial H_i}{\partial t} = \rho c \frac{dT(\vec{r},t)}{\partial t}. \tag{1}$$

The heat flux ($[\mathrm{J/m^2\ s}]$) in direction $\vec{r}$ is

$$F_i = k\frac{\partial T(\vec{r},t)}{\partial r} = k\cdot\vec{\nabla}T(\vec{r},t). \tag{2}$$

Finally, the laser beam can be considered as an external energy source, represented by the function Q_{ext}, which, in each second (s), adds an amount of heat by volume (m^3) to each irradiated element ($Q_{\mathrm{ext}}\ [\mathrm{J/m^3\ s}]$).

Therefore, considering that the divergence of flux $\vec{\nabla}\cdot F = k\cdot\nabla^2 T(\vec{r},t)$ ($[\mathrm{J/m^3\ s}]$) corresponds to an amount of heat, lost or acquired, in each element, the energy balance in the tooth model can be represented by a matrix differential equation (the classical Poisson equation for the heat propagation also considering the laser energy as an external source), involving all the elements of the model.

$$[Q_i] = \nabla\cdot[F_i] + [Q_{\mathrm{ext}}], \tag{3}$$

$$\rho c\frac{\partial T(\vec{r},t)}{\partial t} = k\cdot\nabla^2 T(\vec{r},t) + Q_{\mathrm{ext}}. \tag{4}$$

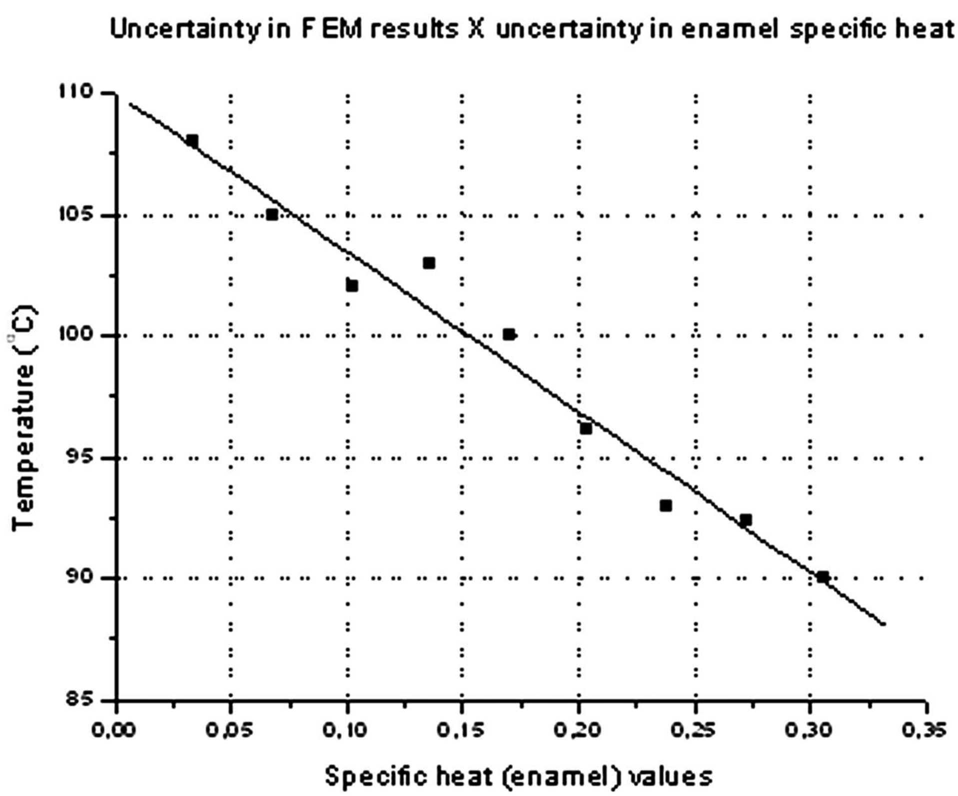

FIG. 2. The dependence between the uncertainty in specific heat and the uncertainty in maximum temperature reached.

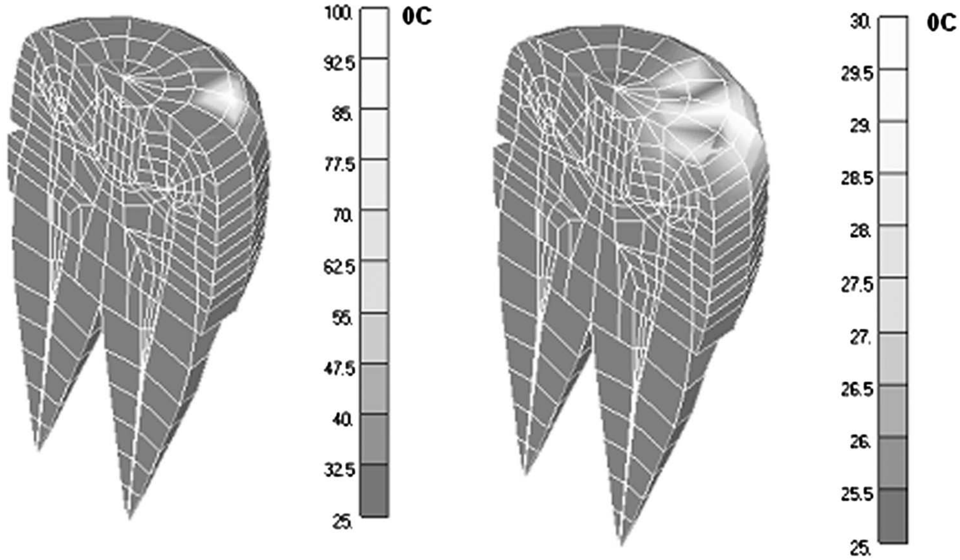

FIG. 3. Calculated temperature distribution: two gray scales are presented. The second one is limited to 30 °C in order to show details of temperature distribution inside the dentin; consequently the enamel surface, which reached a temperature of over 100 °C, appears to be saturated.

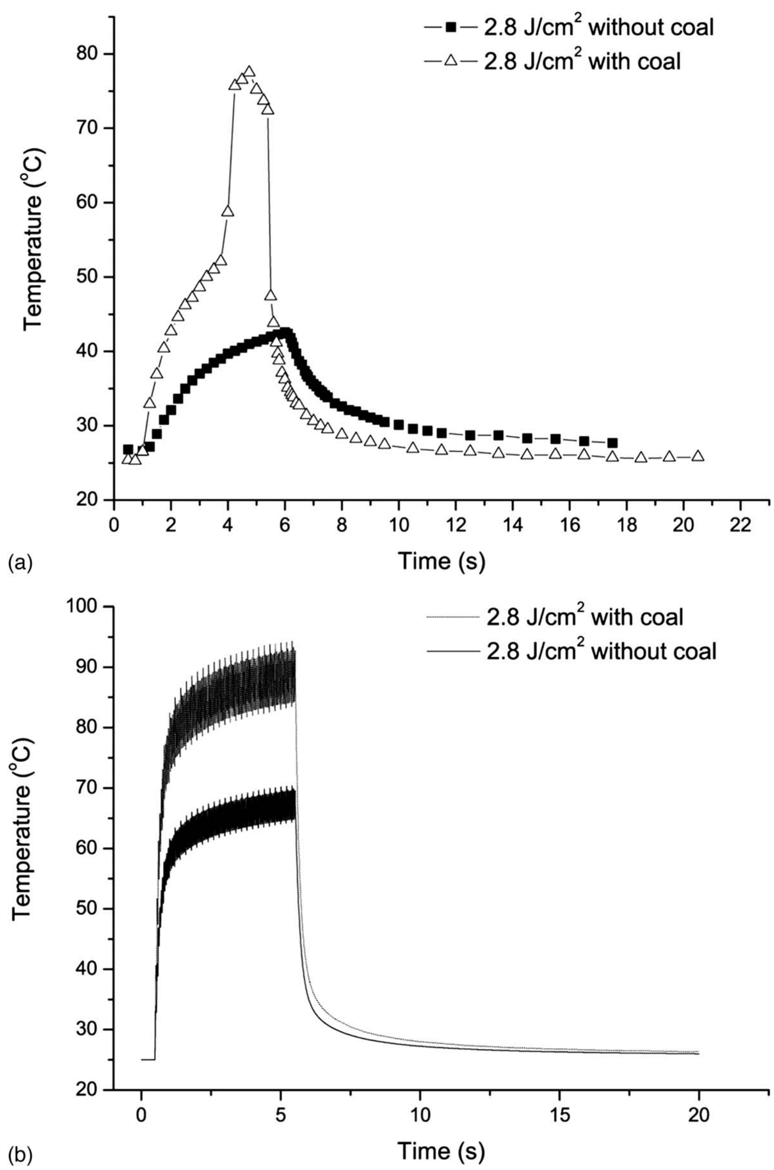

FIG. 4. Comparison between the temperature curves of tooth surface irradiated with Er,Cr:YSGG laser at 2.8 J/cm^2, obtained by thermographic camera (a) and FEM method (b).

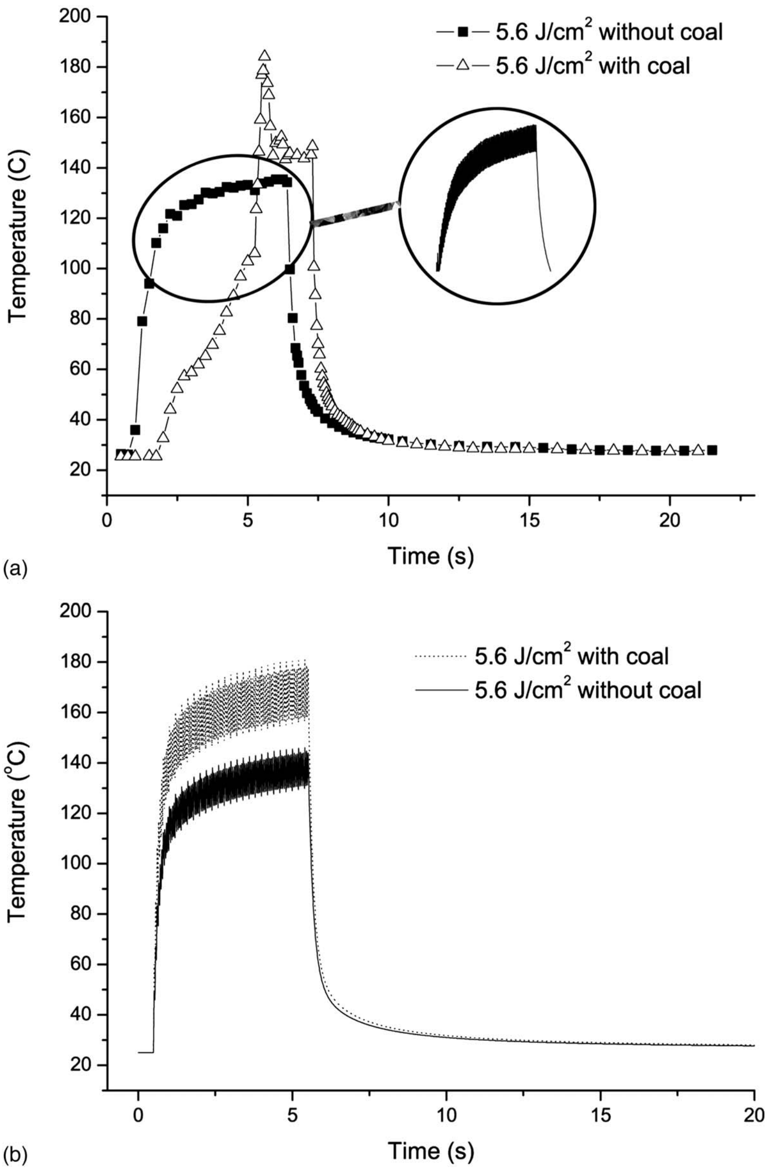

FIG. 5. Comparison between the temperature curves of tooth surface irradiated with Er,Cr:YSGG laser at 5.6 J/cm^2, obtained by thermographic camera (a) and FEM method (b). Inside the circle: detail of temperature curve showing the surface temperature change according to the laser pulses, which agrees with FEM data.

Initial and boundary conditions are necessary in order to solve these differential equations. These conditions are given by the supposition that at $t=0$, all the elements have $T=25$ °C and that the surrounding ambient has constant temperature $T=25$ °C. Therefore, as the laser beam begins to add energy to the dental material, the temperatures rise and the elements on external surface begin to irradiate, following the classical Stefan's law for the emission. These equations were solved using an educational version of the software NASTRAN FEM SOLVER (Santa Ana, CA, USA).

This model is used based on the fact that the optical heating source was considered purely superficial, as the temperature exhibits no dependence on thermal diffusivity. The relaxation time $\tau_B \approx 1/\beta^2\alpha^2$ (Mandelis and Royce)[13] was calculated as 7.9 μs, which is much smaller than the laser pulse (140 μs). The absorption coefficient was considered 7000 cm^{-1} (Stock *et al.*)[14] and α as 2.04×10^{-3} cm^2/s (Minesaky).[15]

2. The model analysis

In Table II some of the elastic and thermal characteristics of both enamel and dentin used in the numerical essay are listed as given in some previous studies.[16–19] There is considerable uncertainty involving these values since they refer to biological tissues. Thus, the values in the table must be considered as typical.[20]

In order to estimate the effect of this uncertainty on the results of FEM models, a large number of calculations were made, changing the physical characteristics of dental materials with regard to their typical values. In a band of 10% around the typical value, ten values were considered. Since there are three physical constants interfering in the thermal behavior (specific heat, conductivity, and density for two materials), 2000 combinations $(2\times 10\times 10\times 10)$ were obtained. Using a random numerical process, 50 of these combinations were drawn to run the FEM model. Considering, for example, the maximum temperature reached, the results formed a type of cluster around the mean value. The standard deviation of these values gives an idea about the uncertainty of FEM calculations. Figure 2 shows the results of this analysis with respect to specific heat. Similar results were obtained for all physical characteristics used. Based on these results it was considered that the

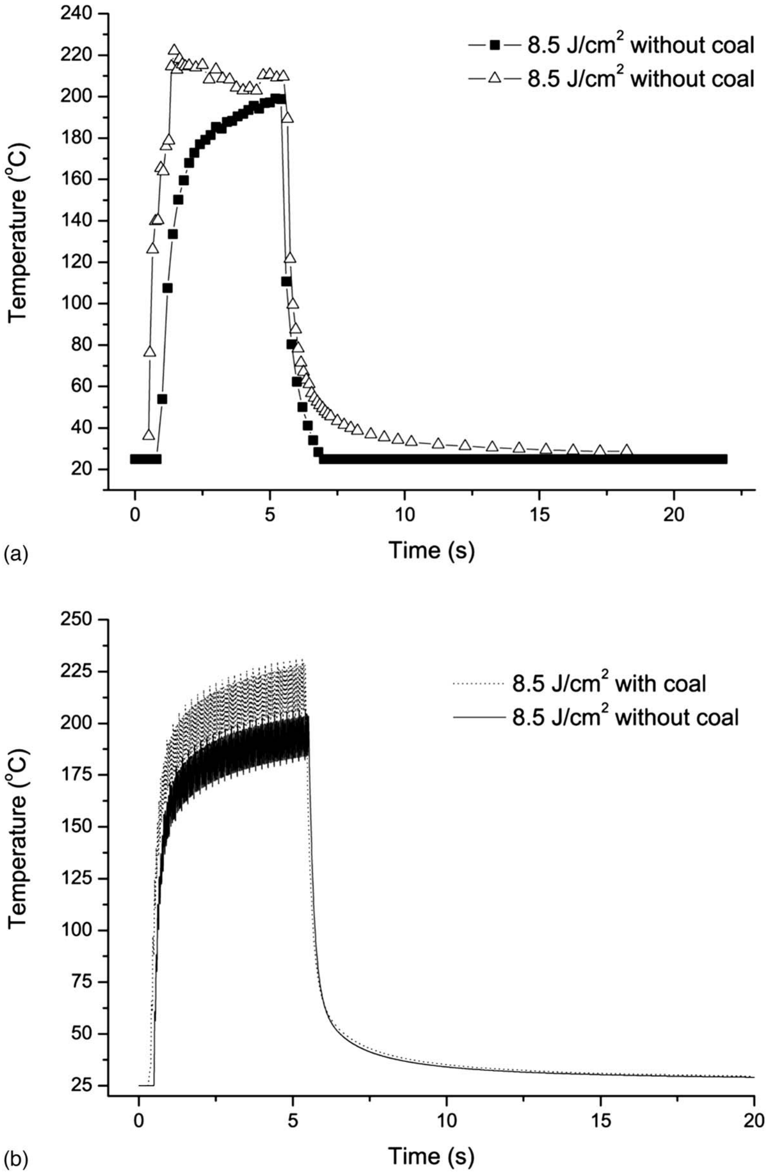

FIG. 6. Comparison between the temperature curves of tooth surface irradiated with Er,Cr:YSGG laser at $8.5\ J/cm^2$, obtained by thermographic camera (a) and FEM method (b).

calculations could be affected by an uncertainty of about $\pm 6\%$ and therefore, this error was attributed to all numerical data.

As a simplicity premise, the absorption of energy by the tissues has been supposed without any loss. In other words, the spectral response of the materials to the laser light has not been considered, mainly because of the high enamel absorption of the 2.79 μm from the Er:Cr:YSGG laser used in this study.

In practical situations, the laser beam is applied to the tooth in sharp pulses in order to avoid high temperatures that could represent damage to the dental tissues (pulpal necrosis) or uncomfortable conditions (pulpitis) to the patients. Thus, it is important to simulate the transient response of the dental tissues when exposed to these sharp laser pulses. All experimental conditions were reproduced in the model, such as three different values of total laser energy (1.25, 2.5, and 3.75 J), considering 100 pulses during 5 s with pulse length of 140 μs. For each of these energies two conditions were used: with or without application of a photoabsorber to the occlusal surface of the tooth. All these conditions were used in the simulation (see Table I). The transient analysis was performed for each of these configurations. Figure 3 shows the temperature distribution immediately after the 100th laser pulse was applied to the tooth.

III. RESULTS

A. *In vitro* experiment analysis

When analyzing the infrared images produced by thermographic camera, it was possible to observe the pattern of temperature change along the tooth and its gradual spread to dentin. The variations in the temperature of spot 1 point are shown in Figs. 4–6.

The maximum increases in spot 1 temperatures were 79.6 ± 0.8 and $42.7 \pm 1.9\ °C$ in samples irradiated at $2.8\ J/cm^2$ with and without photoabsorber, respectively; when lased with $5.6\ J/cm^2$, the maximum surface temperatures were 184.1 ± 29.3 and $136.1 \pm 13.0\ °C$ in samples with and without photoabsorber, and 247.6 ± 30.2 and $211.8 \pm 22.6\ °C$ in samples irradiated with $8.5\ J/cm^2$ with and without photoabsorber, respectively. After the end of ir-

TABLE III. Comparison of means of temperature rise on surface and in pulp obtained by FEM model and by thermographic camera.

Energy density (J/cm^2)	Presence of photoabsorber	Thermographic camera		Finite element method model	
		Surface (°C)	Pulp (°C)	Surface (°C)	Pulp (°C)
2.8	Yes	79.6	0.5	94.2	0.95
	No	42.7	1.0	66.0	0.9
5.6	Yes	184.1	1.5	178.0	1.9
	No	136.1	1.2	136.0	1.4
8.5	Yes	247.6	2.1	231.0	2.1
	No	211.8	1.9	188.0	2.3

radiation, the temperatures fitted into an exponential decay, almost reaching their initial temperature value ~10 s after laser was turned off.

The curves of spot 2 temperature rises showed a delay in temperature increase in comparison with the surface temperature, which corresponds to the time required for heat propagation. The maximum spot 2 temperature variations were 0.5 and 1.0 °C in samples irradiated with 2.8 J/cm^2 (with and without photoabsorber). In samples irradiated with 5.6 J/cm^2, the maximum variations were 1.5 and 1.2 °C with and without photoabsorber, respectively, and 2.1 and 1.9 °C in samples irradiated with 8.5 J/cm^2 with and without photoabsorber.

B. Computer simulation analysis

The numerical analysis was performed for all pulse configurations of Table III. Figure 4(b) shows the transient response results when pulses were applied directly on the enamel surface in order to transfer 1.25, 2.5, and 3.75 J to the tooth. The curves corresponded to a node near to the laser application point where the temperature reached its maximum value.

The model was able to reproduce the high frequency variation of tooth temperature imposed by the pulsed laser beam with good precision. Figures 7 and 8 show the results obtained when the laser spot was projected over a tooth region covered with a thin layer of photoabsorber. The data correspond to the maximum increase in temperature on the tooth surface and in the pulpal chamber wall, respectively.

The experimental and numerical data are almost coincident if the error bars are considered. The agreement occurs both in the surface temperature (enamel) and pulpal chamber wall temperature (dentin). Figures 9 and 10 show the same results for the case when the laser was projected directly onto the enamel surface without any photoabsorber.

IV. DISCUSSION

Irradiation of a laser wavelength on dental hard tissues is a critical procedure if the temperature increase in enamel, dentin, pulp, and periodontal tissues is not considered. An excessive increase in temperature can cause pulpitis, pulp necrosis, damage to enamel morphology and structure, and also injuries to the periodontal ligament and bone.[4,21] Therefore, investigating the temperature, particularly inside the pulp chamber, is the first step in choosing an irradiation parameter for a specific application in dentistry.[4,5,7] The *in vitro* evaluation of temperature changes is conventionally performed and widely accepted by researchers, considering that in some cases it is not possible to use vital teeth for ethical reasons. However, it must be pointed out that the experimental methods are sometimes unable to reproduce the *in vivo* conditions, such as the influence of the oral environment, presence of saliva, body temperature, blood flow, vital tooth conditions, and others.

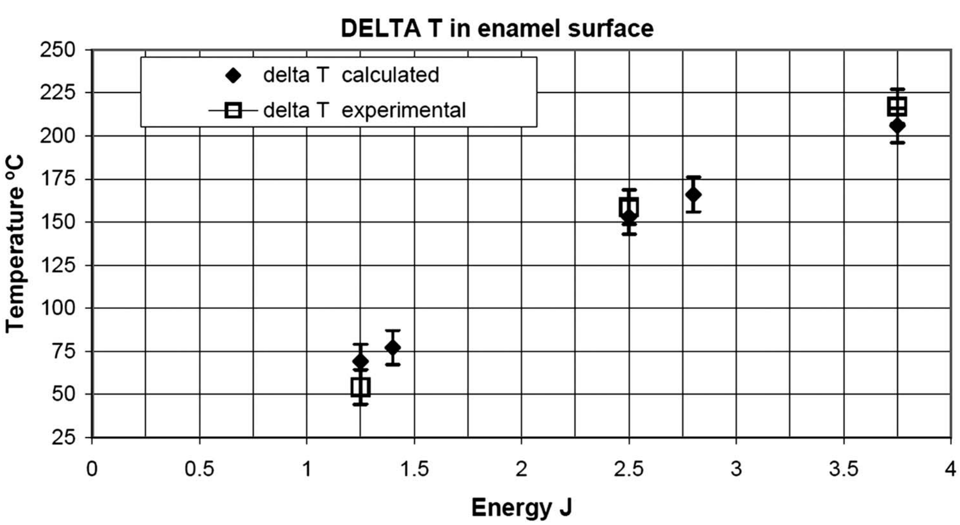

FIG. 7. ΔT reached at enamel surface in samples covered with photoabsorber. Experimental and calculated data.

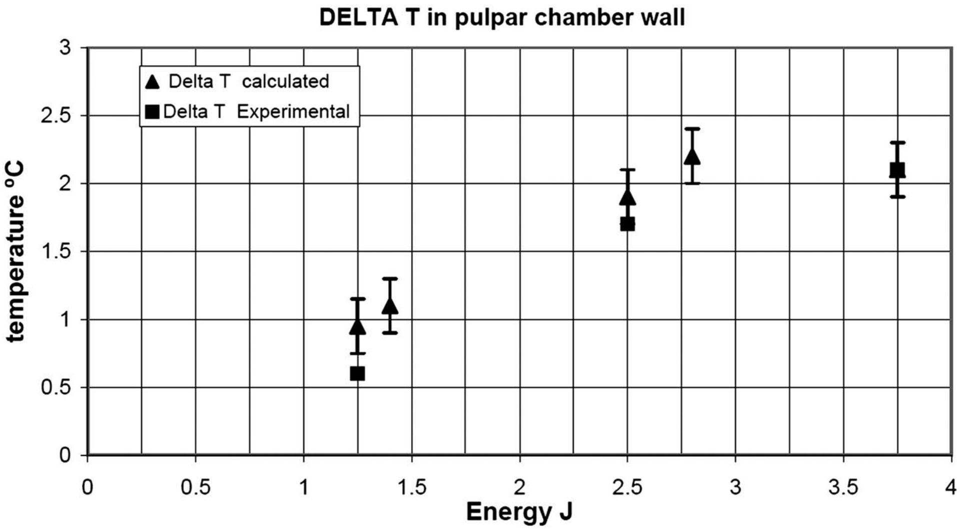

FIG. 8. Maximum ΔT reached at pulpal chamber wall in samples covered with photoabsorber. Experimental and calculated data compared.

In the experimental study, the use of longitudinally sectioned teeth immobilized in optical supports, and the laser handpiece, allowed the visual evaluation of temperature changes and heat diffusion from enamel into dentin and the pulp chamber by using thermographic imaging.[12] Taking into account that the variation in temperature is also dependent on the volume and weight of a tooth, the use of sectioned teeth does not correspond to an *in vivo* condition inside the mouth, but gives an idea of heat transfer inside the tooth and gives the exact value of surface temperature during laser irradiation. Moreover, in a clinical protocol, laser irradiation is performed by scanning all over the enamel surface, and it was not possible to reproduce this situation in the present study. To estimate pulpal temperature for therapeutical purposes, the use of thermocouples is the most accurate methodology, allowing the use of entire teeth, simulating the scanning mode of irradiation and immersion of the teeth in a thermal bath to simulate the body temperature of periodontal tissues.

Numerical mathematical methods do not present this type of problem. By using the FEM model, it was possible to analyze the temperature increase and distribution due to laser irradiation in a half tooth model. On the other hand, considering the higher heterogeneity of dental tissues, some of the physical characteristics were based on literature (conductivity, emissivity, density, and specific heat) and had to be assumed, and consequently, these assumptions sometimes cause a limitation in generalizing conclusions.

The FEM model has been progressively used in dentistry in studies of stress, load distribution, and temperature changes in restored teeth.[8–11,16–20] In the present study, the external heat source is due to instantaneous light absorption converted into heat [Poisson equation (4)]. Moreover, in spite of not considering wavelength dependence with absorption, reflection, transmission, and scattering, the FEM model predicts accurate values for temperatures inside the teeth, mainly because 2.79 μm is strongly absorbed by the dental hard tissue.[1,6] The optical penetration is very small (to the order of few micrometers) since the optical absorption coefficient of enamel is about 7000 cm^{-1}.[14]

As calculated in the present model and verified in the experimental procedure, the temperature increase in the pulp chamber would induce no severe pulpal trauma, considering the threshold of 5.5 °C for pulpitis.[21] The results of the present study are similar to those of a previous study performed with thermocouples, using the same wavelength, which found pulpal temperature increments of 0.8, 1.7, and 2.1 °C when laser was irradiated at 2.8, 5.6, and 8.5 J/cm^2, respectively, without the use of any photoabsorber.[12] The

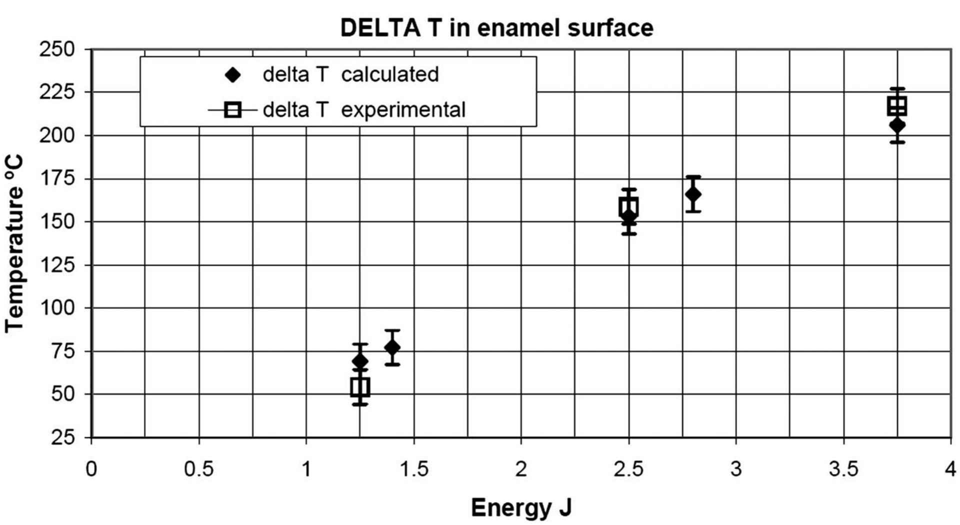

FIG. 9. ΔT reached at enamel surface in samples without photoabsorber covering. Experimental and calculated data.

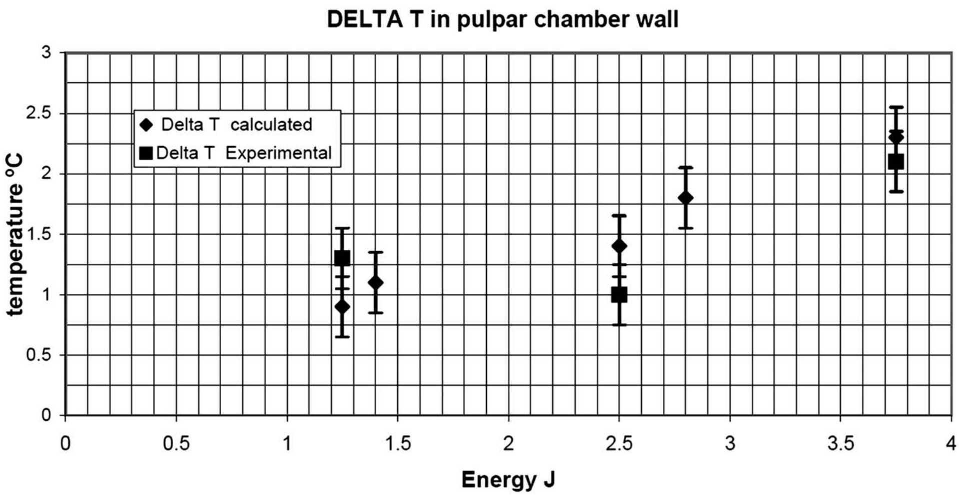

FIG. 10. Maximum ΔT reached at pulpal chamber wall in samples without photoabsorber covering. Experimental and calculated data compared.

above-mentioned study, in which thermocouples were placed inside the pulp chamber, also corroborated the strong decay of the thermal field in this location.

As regards the enamel surface temperatures, it was possible to observe that they changed according to the laser fluence, and the temperature rise of 247.6 °C found when teeth were irradiated with 8.5 J/cm^2 was lower than the temperature reported by Fried *et al.*,[6] who found approximately 400 °C measured by an elliptical mirror and a HgCdZnTe detector with a time resolution of 1 μs. Considering that the pulse width of Er,Cr:YSGG laser is 140 μs, even the 900 Hz recording rate of thermographic camera seemed to be unable to detect the highest temperature peaks during laser irradiation. Therefore, the thermographic camera gives an idea of temperature increments when teeth are irradiated with high intensity lasers; however, more accurate systems are required to precisely determine the maximum temperature peaks.

The results of the FEM analysis in this study revealed important agreement with the experimental data, estimating the temperature rises on the enamel surface as well as inside the pulp chamber according to the laser energies. It must be pointed out that this FEM model does not reproduce all the interferences of the oral environment in the photothermal response of enamel and dentin tissues, such as the influence of surrounding saliva, pulpal and periodontal tissues, presence of biofilm, body temperature, and other factors. However, under the given conditions, it can be concluded that the simulated model was shown to have a good approximation to the physical reality. The FEM model seems to give good results that can help to understand the thermal behavior of dental hard tissues under laser irradiation for preventive purposes.

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