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THE INFLUENCE OF PULSE DURATION ON THE STRESS LEVELS IN ABLATION OF CERAMICS: A FINITE ELEMENT STUDY

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Abstract

We present a finite element model to investigate the dynamic thermal and mechanical response of ceramic materials to pulsed infrared radiation. The model was applied to the specific problem of determining the influence of the pulse duration on the stress levels reached in human dental enamel irradiated by a CO_2 laser at 10.6 μm with pulse durations between 0.1 and 100 μs and sub-ablative fluence. Our results indicate that short pulses with durations much larger than the characteristic acoustic relaxation time of the material can still cause high stress transients at the irradiated site, and indicate that pulse durations of the order

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of 10 μs may be more adequate both for enamel surface modification and for ablation than pulse durations up to 1 μs. The model presented here can easily be modified to investigate the dynamic response of ceramic materials to mid-infrared radiation and help determine optimal pulse durations for specific procedures.

keywords: mesoscopic modelling; laser ablation; enamel; finite elements; CO_2 laser; pulse duration; stress transients.

1. Introduction

The effect of pulse duration on ablation by infrared (IR) lasers has been extensively studied. In general, it is accepted that to minimize thermal damage around the ablated site, the pulse duration, t_p, should be inferior to the characteristic thermal relaxation time, t_{th}, normally estimated as $t_{th} = d^2/(4\chi)$ where d is the smallest of the laser beam diameter or of the optical penetration depth and χ is the thermal diffusivity [1]. If $t_p << t_{th}$, the temperature at the irradiated site is maximized because only small amounts of energy diffuse out of it during the laser pulse. This condition is called thermal confinement, and is a requirement to maximize thermal stress in the material during the laser pulse, because thermal stress is proportional to the maximum temperature reached. It has been shown that pulses significantly shorter that t_{th} are much more efficient at ablating material and inflict much less thermal damage than pulses with duration comparable to or larger than t_{th} [2].

If t_p is significantly shorter than the acoustic relaxation time, t_{ac}, (the time it takes a stress wave to travel distance d, given by d/c_s where c_s is the speed of sound), then it is said that ablation occurs under conditions of stress or inertial confinement. Under stress confinement conditions, the stress transients generated are normally much higher than the thermal (static) stress generated in the material and, consequently, mechanical damage such as cracks is much more likely to occur [3, 4]. While these general guidelines are known and used

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to determine the order of magnitude of t_p to use for particular procedures, they do not easily allow the optimization of t_p beyond this. In particular, the behaviour of materials under laser pulses with $t_{ac} < t_p < t_{th}$ (for most materials, $t_{ac} << t_{th}$ [4]) is particularly difficult to predict based on these generic rules. There is consequently a need for models with sufficient predictive capability to allow the fine-tuning of laser operating parameters, in particular the pulse duration, easily adaptable to different materials and lasers.

In the work reported here we describe a finite element model of human dental enamel (a brittle, ceramic-like material) under radiation by a CO_2 laser at $\lambda = 10.6$ μm and use it to investigate the thermal and mechanical dynamical response of this material to pulses of varying duration, in the regime $t_{ac} < t_p \leq t_{th}$. The system chosen is of particular importance in the field of laser dentistry, where lasers are now being used to ablate dental hard tissue (enamel and dentine) and to modify the enamel surface (by heating) so that it becomes more resistant to acid attacks by cariogenic bacteria. While these procedures are already being used in dental laser treatments, there is still a need to optimize them in order to obtain higher ablation rates while minimizing thermal and mechanical damage inflicted to teeth. The model is generic in its nature so it can easily be applied to assess the dynamic mechanical behaviour of other ceramic materials under mid-IR radiation, making it an effective tool to optimize the pulse duration for particular applications.

2. Model description

In order to investigate the influence of the pulse duration on the stress levels reached during and after a single laser pulse in the material irradiated by the centre of the laser spot, we built a simple finite element model of human dental enamel using commercial finite element (FE) software ABAQUS 6.5-1. The model has dimensions $23 \times 23 \times 35$ μm^3 (containing 198144 nodes and 187765 elements) but does not account for enamel's microstructure or inhomogeneous chemical composition at this scale. The movement of the outer surfaces of the model, with the exception of the top surface directly irradiated by the laser, was completely constrained. All the outer surfaces were given adiabatic boundary conditions.

The model can be conceptually divided in two parts: the core and the restrain-layers. The core of the model corresponds to the part closer to the geometrical center of the structure and has the mechanical and thermal properties of hydroxyapatite (HA) - the substance representing 95% by weight of enamel - given in Table I. The restrain-layers (lateral restrain-layer and bottom restrain-layer), on the other hand, exist only to impose adequate boundary conditions on the core of the model, since the core of the model should not move entirely freely but should also not be completely constrained because it should represent a small piece of enamel, part of a tooth, where it is surrounded by more enamel. For this reason, the physical properties of the restrain-layers (Young's modulus, E, thermal expansion coefficient, and, for the bottom restrain-layer only, thermal conductivity, κ, and mass density) are not those of HA. Instead, they are estimated according to what is described in [5] so that the restrain-layers reproduce, in a computationally efficient manner, the constraints imposed by the large quantity of enamel and dentine that is surrounding the modelled structure. The alternative to this approximation would be to simulate an entire tooth, a computationally prohibitive task since it would necessarily have to be done with micrometer-scale resolution in order to capture the short wavelength/high frequency modes of vibration which we intend to capture with this work

The estimate of the physical properties of the restrain-layers is based on the properties of the enamel, the thickness of the restrain-layers themselves and the thickness of the material they are replacing. In the present case the lateral restrain-layer properties were obtained considering that a 6 mm thick layer of enamel surrounded the sides of the modelled structure, but only a 0.2 mm thick layer (the radius of the laser spot) underwent thermal expansion, and knowing that the width of the lateral restrain-layer is 2.8 μm. The bottom restrain-layer properties were calculated assuming that 6 mm of dentine ($E = 1.5 \times 10^{10}$ N/m^2) were beneath the modelled structure, and that thermal expansion was possible within the 6 mm of dentine. During the thermal simulations, the bottom restrain-layer was given a much higher density than that of enamel, so it acts as a heat sink. The scaling of the bottom restrain-layer thermal conductivity was not done in the work reported by us in previous articles, and therefore it is now described. According to the general diffusion equation [1], the heat flux per unit area (dQ/(Adt)) is proportional to the thermal conductivity of the material and the spatial gradient of the temperature. The spatial gradient of the temperature can be considered in this case to be dT/dz, because the laser spot (radius = 0.2 mm) is much larger than the optical penetration depth of λ = 10.6 μm in enamel (≈12 μm) and, consequently, the heat flux occurs primarily along the direction perpendicular to the irradiated surface, OZ.

$$\frac{dQ}{AdT} = -\kappa \frac{dT}{dz} \tag{1}$$

If the bottom restrain-layer is to be equivalent to 6 mm of dentine, then the heat flux per unit area through the bottom restrain layer must be equivalent to the heat flux per unit area through 6 mm of dentine considering that the inner part of the tooth (bellow the modelled structure) remains at 37 ºC. Therefore,

$$-\kappa_{RL} \frac{dT_{RL}}{dz_{RL}} = -\kappa_{dentine} \frac{dT_{dentine}}{dz_{dentine}} \tag{2}$$

Also, the temperature gradient throughout the thickness of the bottom restrain-layer must be the same as that throughout the 6 mm of dentine it is replacing. Therefore, the thermal conductivity of the bottom restrain-layer is given by

$$\kappa_{RL} = \kappa_{dentine} \frac{dz_{RL}}{dz_{dentine}} \tag{3}$$

where dz_{RL} and $dz_{dentine}$ are the thickness of the bottom restrain-layer (0.6 μm) and of dentine (6 mm), respectively.

Using the same model, several analyses were performed to investigate the thermal and mechanical response of the material to a single laser pulse of fluence 0.42 J/cm^2 emitted by a CO_2 laser at λ = 10.6 μm shining on the top 23 × 23 μm^2 surface. In the first set of analyses the pulse duration and the intensity of the radiation, given in Table II, were varied simultaneously so that the total deposited energy remained constant. The energy per unit volume, S(r,z), deposited in each finite element was calculated according to

$$S(r,z) = -\frac{\partial I(r,z)}{\partial z} = \mu I(r,z) \tag{4}$$

where

$$I(r,z) = I_0 \exp(-\mu z).\exp(-2r^2 / w^2), \tag{5}$$

z is the depth inside the tissue, I_0 is the intensity of radiation at the surface of the target and at the centre of the laser spot, μ is the absorption coefficient of the tissue (825 cm^{-1}), *w* is the beam radius (0.2 mm) and r is the radial distance from the centre of the laser spot. Note that under these irradiation conditions, d = 1/825 cm = 12 μm and, since χ_{enamel} = 0.5 mm^2/s [6] and the speed of sound in enamel is 6.5 × 10^3 m/s [7], t_{th} = 72 μs and t_{ac} = 24 ns. Note that scattering was not included in the model because the absorption coefficient of enamel at 10.6 μm is large, and therefore the effects of scattering are not expected to be dominant.

Because the temperature distribution influences the mechanical behaviour of the material but the deformation of the material does not influence its absorption of radiation, the thermal and mechanical parts of the simulations were performed independently to allow for shorter simulation times. First the thermal simulations were performed, using the implicit algorithm available in ABAQUS Standard and using eight-node finite elements with Lagrangian formulation, first-order interpolation and full-integration. Subsequently, the temperature as a function of time at each node was passed into the mechanical analyses, performed using the explicit algorithm available in ABAQUS because this algorithm is more suitable to study rapid events like laser pulses than ABAQUS's implicit algorithm: the nature of the explicit algorithm allows the easy use of very short time-steps and, consequently, the capture of dynamics of rapid events, something that can only be done at almost prohibitive computational cost when ABAQUS's implicit algorithm is used. In the mechanical analyses we used eight-node finite elements with Lagrangian formulation, first-order interpolation and reduced integration with hourglass control. Hourglass control is necessary because otherwise reduced integration elements are unable to resist bending loads, therefore leading to untrustworthy results. The total duration of the simulations varied between 100 and 250 μs; the duration of the laser pulses varied between 0.1 and 150 μs. The automatic incrementation schemes available in ABAQUS were used for both the thermal and the mechanical analyses.

In order to distinguish between effects caused by the lower temperatures reached in the material when longer pulses are used and effects caused by the actual pulse duration, a second set of simulations were performed. All the mechanical simulations in this second set share the same temperature distribution, the one obtained in the first set of simulations for a 0.35 μs laser pulse. This temperature distribution was divided into two sections, one containing the temperature as a function of time during the laser pulse for all nodes in the model, and the other containing the temperature as a function of time after the laser pulse. In this set of simulations the timescale of the first section was compressed or extended so that those temperature values were applied in different time intervals in the mechanical analyses, corresponding to different pulse durations: 0.1, 1, 10 and 100 μs. To continue the mechanical simulation for longer times than the laser pulse, the second section of the temperature distribution in question was applied to the model without any change. In this manner we could ascertain whether the observed behaviour of the model in terms of stress derived from the lower temperatures reached when longer pulses are used and the same incident fluence is kept, or if they are in fact a consequence of the duration of the laser pulse.

3. Results and discussion

The temperature distributions obtained for all simulations share the same qualitative features: the maximum temperature is reached at the surface of the model and at the end of the laser pulse, and the only appreciable temperature gradients are along OZ (the optical axis of the laser beam). The temperature maps are not shown here since they are similar to those published in ref. [5]. The maximum temperatures obtained for the first set of simulations, in which the same amount of energy is deposited by the laser in all simulations, are given in Table II. It is apparent that pulse durations between 0.1 and 2 μs cause little change in the maximum temperature reached (less than 10 ºC), but longer laser pulses are associated with significantly lower maximum temperatures (up to 45 ºC lower).

The stress results presented in Table II and Fig. 1 are given in terms of Von Mises stress (VMS), a scalar quantity that combines all the components of the stress tensor in a single value and that thus provides a convenient way of analysing them [3]. It is easily seen that both the mean and the maximum VMS reached at the centre of the irradiated face of the modelled structure are higher for shorter pulse durations if t_p is less than 10 μs. However, the increase of the maximum VMS with shorter pulses is very large while the increase of the mean VMS after the laser pulse is only moderate. In fact, the maximum VMS for t_p = 0.1 μs is 55% higher than the equivalent value for t_p = 0.2 μs, even though the maximum temperature reached by the model is the same in both cases. The magnitude of the difference between the stress values at longer and shorter pulse durations is more evident in Fig. 1, which shows the VMS values at the centre of the irradiated face of the model for 0.1 and 10 μs laser pulses, representative of results obtained for analyses with t_p up to 1 μs and t_p between 2 and 100 μs, respectively. In this figure it is readily apparent that, while the mean VMS for both analyses is relatively similar, the VMS for the short pulse simulation oscillates significantly around its mean value but the VMS for the longer pulse analysis does not. It is also shown that the stress at the free surface of the laser reaches a minimum value between 10 and 20 μs. This non-intuitive result is present for all pulse durations and explains the fact that the lowest VMS is reached when $t_p \approx 10$ μs and not at the longest t_p and also explains why the VMS values in Table II increase again when t_p is larger than 10 μs.

These results suggest that short laser pulses can generate large stress oscillations in the irradiated objects even when the pulse is far too long to be under stress confinement conditions (t_p should be shorter than ≈20 ns in this case). Furthermore, our results suggest that t_p influences the amplitude of the stress vibrations experienced by the irradiated object, independently of the maximum temperature reached. To further test these hypotheses, a second set of simulations was performed according to what was previously described in Section **2**.

The results obtained in the second set of simulations performed are given in Table III. It is apparent that, while the temperature distribution used as input to the mechanical simulations is the same, the maximum VMS reached at the centre of the irradiated face of the modelled structure is significantly higher for the shorter t_p's. At the same time, the mean VMS stress at the same location is only slightly higher for the shorter t_p's. An analysis of plots of VMS as a function of time (not presented, since they are similar to those given in Fig. 1) again indicates that a t_p shorter than 1-2 μs will generate a high frequency and high amplitude oscillation in the VMS stress values reached, the amplitude being higher for $t_p = 0.1$ μs.

Our results cannot yet be validated against experimental data since existing studies have not compared, under controlled conditions, the results of ablating dental enamel when $0.1 < t_p < 10$ μs pulse duration range. Furthermore, the results strictly only apply to the sub-ablative regime, where phase transitions and cracking in the material are not expected. Therefore the magnitude of the effect of the pulse duration described in this work in the ablation procedure cannot be fully assessed at the moment. Keeping these limits of validity in mind, our results may facilitate the search of the optimal laser parameters to ablate dental hard tissue and to modify the surface of enamel to make it less susceptible to caries. The higher stress transients experienced by the material when shorter (less than 2 μs) laser pulses are used suggest that these pulses may be more efficient than longer pulses at ablating tissue but, at the same time, they are more likely to inflict unwanted damage in the material. If our predictions are confirmed, then one should expect to have lower enamel ablation thresholds and ablation energy and, perhaps, higher ablation rates, for $t_p < 1$ μs than for $t_p \approx 10$ μs. For the same reasons, these results also suggest that $t_p < 2$ μs are less adequate to irradiate the surface of enamel to increase its resistance to acid attack. These results indicate that free-running lasers, which normally have a long macropulse (100-300 μs) composed of several micropulses, each with a duration of approximately 1 μs, may not be the most appropriate to use for enamel surface modification. However, further work investigating the response of the material to multiple pulses must be done to support this conclusion.

These results can be extrapolated to other wavelengths commonly used to ablate dental hard tissue, such as the Er:YAG laser at $\lambda = 2.9$ μm. This laser is very often used in free-running mode to ablate dental hard tissue, and some attempts have been made to use it to increase enamel resistance to acids [8]. Our previous work [9] indicated that Er:YAG lasers, which are primarily absorbed by water contained in water pores, would cause the pressure in pores to increase with increasing pore size, therefore making their effect on enamel more unpredictable than that of CO_2 lasers at $\lambda = 10.6$ μm for which the same effect was not observed. Our previous and present results thus provide an explanation as to why the free-running Er:YAG produce worse results in enamel surface modification [8] than longer pulsed CO_2 lasers [10].

4. Conclusions

This work suggests that pulse durations significantly higher than the characteristic time of acoustic relaxation of a material can still induce very high frequency and high amplitude stress variations in a material, capable of creating fractures. While the magnitude of the effects observed in our results must not be taken literally because the model has not been validated against experimental data, our results do provide guidelines for experimental procedures. For the specific case of dental enamel ablation by mid-IR lasers, our results seem to implicate that pulse durations on the order of 2-10 μs may be more appropriate to efficiently ablate dental enamel while significantly decreasing the probability of causing mechanical damage to this material and ensuring that thermal damage is still kept to a minimum. These results also indicate that pulse durations inferior to 2 μs may be less adequate to irradiate dental enamel with the aim of producing a more acid resistant surface. Finally, our results also suggest that free-running lasers, with their characteristic sequence of micropulses with duration approximately 1 μs, may still cause mechanical damage to materials despite the long duration of their macropulses. They also indicate that there may be a need to accurately characterize the pulse temporal profile in order to better interpret experimental results, something which very often lacks in the literature concerning dental laser ablation and treatment.

The model presented here can easily be modified to determine the optimal mid-IR laser pulse durations to treat or ablate any kind of ceramic material while minimizing thermal and mechanical damage at the irradiated sites.

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Table I: Material properties used in the model

	Enamel	Lateral Restrain-layer	Bottom Restrain-layer
Absorption coefficient (cm^{-1})	[11] 825	825	825
Density ($kg.m^{-3}$)	[12] 3.1×10^3	3.1×10^3	Therm. anal.: 3.1×10^6 Stress anal.: 3.1×10^3
Thermal conductivity ($J.s^{-1}.m^{-1}.^{o}C^{-1}$)	[13] 1.3	1.3	1.2×10^{-4}
Specific heat ($J.kg^{-1}.^{o}C^{-1}$)	[13] 880	880	880
Young's modulus ($N.m^{-2}$)	[14] 1.1×10^{11}	5×10^7	1.5×10^6
Poisson's ratio	[15] 0.28	0.28	0.28
Expansion coefficient ($^{o}C^{-1}$)	[16] 1.6×10^{-5}	$\alpha_{xx} = \alpha_{yy} = 1 \times 10^{-3}$ $\alpha_{zz} = 1.6 \times 10^{-5}$	0.17

Table II: Mean and maximum VMS stress and maximum temperature reached at the centre of the irradiated face of the modelled structure at the end of the laser pulse as a function of the maximum absorbed intensity and pulse duration. For each simulation, the mean VMS was averaged over 1 μs after the end of the laser pulse. Note that the incident fluence was maintained constant at 0.42 J/cm^2.

Maximum absorbed intensity, I_0 ($J.m^{-2}.s^{-1}$)	Pulse duration (μs)	Maximum temperature reached (ºC)	Maximum stress reached (N/m^2)	Mean stress at the end of the laser pulse (N/m^2)
4.20×10^{10}	0.10	162	4.5×10^{7}	1.6×10^{7}
2.10×10^{10}	0.20	162	2.9×10^{7}	1.3×10^{7}
1.20×10^{10}	0.35	160	2.7×10^{7}	1.2×10^{7}
7.00×10^{9}	0.60	159	1.9×10^{7}	1.2×10^{7}
4.20×10^{9}	1.0	158	1.7×10^{7}	1.2×10^{7}
2.10×10^{9}	2.0	155	1.3×10^{7}	1.1×10^{7}
4.20×10^{8}	10	147	5.5×10^{6}	4.8×10^{6}
8.40×10^{7}	50	132	8.0×10^{6}	7.7×10^{6}
4.20×10^{7}	100	123	1.2×10^{7}	1.2×10^{7}
2.80×10^{7}	150	117	1.3×10^{7}	1.2×10^{7}

Table III: Mean and maximum VMS stress and maximum temperature reached at the centre of the irradiated face of the modelled structure as a function of the pulse duration. For each simulation, the mean VMS was averaged over 1 μs after the end of the laser pulse. Note that the same temperature distribution was used as input for all the mechanical analyses reported here, and only t_p is different.

Pulse duration (μs)	Maximum temperature applied (ºC)	Maximum stress reached (N/m^2)	Mean stress at the end of the laser pulse (N/m^2)
0.10	160	4.5×10^7	1.6×10^7
0.35	160	2.6×10^7	1.6×10^7
1.0	160	1.8×10^7	1.2×10^7
10	160	1.3×10^7	1.2×10^7
100	160	1.3×10^7	1.2×10^7

Fig. 1: Von Mises stress as a function of time for the central top element for the same incident fluence and two different pulse durations: 0.1 and 10 μs.