

Review

# A review of heat transfer in human tooth—Experimental characterization and mathematical modeling

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#### ABSTRACT

With rapid advances in modern dentistry, high-energy output instruments (e.g., dental lasers and light polymerizing units) are increasingly employed in dental surgery for applications such as laser assisted tooth ablation, bleaching, hypersensitivity treatment and polymerization of dental restorative materials. Extreme high temperature occurs within the tooth during these treatments, which may induce tooth thermal pain (TTP) sensation. Despite the wide application of these dental treatments, the underlying mechanisms are far from clear. Therefore, there is an urgent need to better understand heat transfer (HT) process in tooth, thermally induced damage of tooth, and the corresponding TTP. This will enhance the design and optimization of clinical treatment strategies. This paper presents the stateof-the-art of the current understanding on HT in tooth, with both experimental study and mathematical modeling reviewed. Limitations of the current experimental and mathematical methodologies are discussed and potential solutions are suggested. Interpretation of TTP in terms of thermally stimulated dentinal fluid flow is also discussed.

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Abbreviations: DEJ, dentine–enamel junction; DFF, dentinal fluid flow; DRMs, dental restorative materials; DTs, dentinal tubules; FEM, finite element method; HSHPs, high-speed hand-pieces; HSPs, heat-shock proteins; HT, heat transfer; IPTR, intrapulpal temperature rise; LPUs, light polymerizing units; PBF, pulpal blood flow; TC, thermal conductivity; TD, thermal diffusivity; TPs, thermophysical properties; TTP, tooth thermal pain.

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#### 1. Background

Heat transfer (HT) in human tooth is a common process in both daily life [1,2] and clinical dentistry [3–6]. With advances in modern dentistry, instruments with high-energy output (*e.g.*, dental lasers [7,8], light polymerizing units (LPUs) [9–11] and high-speed hand-pieces (HSHPs) [12,13]) have been widely employed in dental treatments. Typical clinical examples of these treatments are laser assisted tooth ablation [7,14], caries detection and prevention [15,16], bleaching [17–19] and hypersensitivity treatment [20,21]. Table 1 lists the currently available therapies and the corresponding intrapulpal temperature rise (IPTR).

Heat generated within the tooth during the abovementioned treatments can cause thermally induced damage of tooth "hard" components (enamel and dentine) [2,29–31] and "soft" components (dental pulp) [32–34]. Temperature rise may also induce tooth thermal pain (TTP) [35–37]. The lack of detailed knowledge concerning these tooth thermal behaviors has hindered the further design and optimization of treatment strategies for clinical applications. Therefore, there is an urgent need to investigate the thermal behavior of human teeth.

#### 1.1. Structure of human tooth

Human tooth is a hard tissue with layered composite structure (e.g., enamel, dentine, cementum and dental pulp layers [38]) of complex geometry. Enamel is a highly mineralized layer consisting of 96% mineral, with water and organic material accounting for the remaining 4%. Dentine is a mineralized connective tissue layer with an organic matrix of collagenous proteins [39,40], composed of ~70% inorganic materials, ~20% organic materials, and ~10% water by weight. There are dentinal tubules (DTs) radiating from the pulp cavity to the exterior cementum or dentine–enamel junction (DEJ) [40]; see Fig. 1.

Human tooth is also a sensory tissue. The pulp is a soft connective tissue containing nerve fibers with diameter varying from 1 to 10  $\mu$ m [41]. There are also sensory nerve endings in DTs [42], which penetrate approximately 100–150  $\mu$ m into the tubules from the wall of pulp chamber [43]. These pulpal nerve terminals play an important role in sensing thermal stimulus [44].

#### 1.2. What induces HT in tooth?

HT in tooth occurs in both daily life and dental surgery. The thermal environment of teeth during daily life varies over a wide range of temperatures (-5 to 76.3 °C) [2,46], Table 2.

Since its first introduction as a tool for patient care in 1964 [48], laser has been found to be an exciting and rewarding technology in dental surgery (*e.g.*, dental ablation [7,49], cosmetic tasks [50,51], dental caries prevention [15] and hypersensitivity treatment [21–22]) due to advantages such as directivity, pulsed mode ability, and monochromaticity [52]. However, there is a major concern with the overheating of enamel and dentine during tooth-laser interaction, which causes carbonization, melting and cracking of the enamel and dentine, as well as inflammation and necrosis of the pulp [30,31].

Dental restorative processes are used to decrease the polymerization periods of resin composite and minimize its polymerization shrinkage. During these processes, teeth are exposed to the radiation of LUPs (*e.g.*, halogen polymerization lamps or semiconductor diode light) and experience substantial temperature increase of 10-18 °C within the resin and adjacent tooth [56–58], 7.5–29 °C at DEJ [53], and 2–9 °C at pulpal chamber wall [53].

Treatments with HSHPs are performed in dental clinics for applications such as cavity preparation and deceased tissue

Table 1 – Typical thermal therapies and relative intrapulpal temperature rise (IPTR).			
	Temperature rise (°C)	References	
Laser assisted tooth ablation	2.3–24.7	[22,23]	
Laser assisted caries prevention	1.2-4.0	[15]	
Bleaching (without light/laser assisted)	0.1–1.1	[24]	
Bleaching (with light/laser assisted)	1.1–16.0	[17,25]	
Polymerization of dental restorative materials (DRMs)	2.9–7.8	[10,26,27]	
HSHPs cavity preparation (without water, high load)	16.4–19.7	[12,28]	
HSHPs cavity preparation (without water, low load)	7.1–9.5	[12,28]	
HSHPs cavity preparation (with water, high load)	2.2–5.9	[12,28]	
	10.0–11.7		
HSHPs cavity preparation (with water, low load)	-1.8 (drop in temperature) to 5.0	[12,28]	

removal. Heat is generated by friction between the machinery (*e.g.*, driller) and tooth, resulting in IPTR [12,28,13]. This temperature rise depends on the pressure and speed of the hand-pieces [54] as well as the cooling methods used [12,55].

#### 1.3. Specialties of tooth thermal behavior

Unlike HT in engineering materials, the thermal behavior of tooth is mainly a heat conduction process coupled with tooth physiological processes (*e.g.*, dentinal fluid flow (DFF) [35], pulpal blood flow (PBF) [56,57]). The thermophysical properties (TPs) of teeth vary between different layers (*e.g.*, enamel and dentine) [58] and depend on their microstructures. For instance, the thermal conductivity (TC) of human dentine decreases with increasing volume fraction of dentine tubules [59]. The flow of dentinal fluid in the dentine tubules upon heating (or cooling) can also enhance HT within the pulp. In addition, PBF rate increases when the intrapupal temperature rises above 42 °C [56] and decreases during cooling [57]. The perfused blood plays an important role in the thermoregulation of pulpal soft tissue [56,60], working as a heat sink under heating and as a heating source when subjected to cooling.

#### 1.4. Thermally induced damage

Abrupt changes in tooth temperature can cause TTP and damage in tooth hard components (enamel and dentine), soft pulp tissue [33,34,32,61] and restorative interface (*e.g.*, interfacial debonding between the tooth and the DRMs) [62,63].

Enamel and dentine have different thermal and mechanical properties. For example, the thermal diffusivity (TD) and Young's modulus of enamel are  $\sim$ 2.5 and  $\sim$ 4 times larger than

Table 2 – Intraoral temperatures measured in vivo and calculated extreme temperature during consumption of hot beverage and food [47].			
Temperature (°C)	Hot beverage	Hot food	
Highest <sup>a</sup>	76.3	53.6	
Mean maximum <sup>b</sup>	46.4	41.6	
Calculated extreme <sup>c</sup>	61.4	50.2	

<sup>a</sup> Highest temperature measured in one volunteer between the lower incisors.

 $^{\rm b}$  Mean maximum temperature  $\pm$  standard deviation recorded by each electrode for all volunteers.

<sup>c</sup> Calculated extreme temperature obtained by adding two standard deviations to the mean maximum temperature measured *in vivo*.

that of dentine, respectively [64,65]. The difference in these properties may result in thermal stresses and cracking within tooth when subjected to thermal stimulus [2,29], Fig. 2. In addition, heat generated during laser treatment may result in carbonization, melting and cracking of the tooth structure [30,31]. Thermal denature of dentine collagen often occurs in endodontics treatments, where the tooth root canal dentine may be exposed to a temperature of ~300 °C [66]. The denaturation temperatures of demineralized dentine matrix have been reported to be  $65.6 \,^{\circ}$ C,  $148.5 \,^{\circ}$ C, and  $166.8-172.7 \,^{\circ}$ C for demineralized dentine saturated with water, saturated with methanol, ethanol or acetone, and bonded with resin, respectively [66].

Dental pulp, which is responsible for the maintenance of tooth vitality, is vulnerable to heat. When the IPTR exceeds  $\sim$ 5.5°C, irreversible pulpal damage (*e.g.*, cell death in pulp) will be induced [33,34]. However, pulp cells may survive such injuries [73,74]. This may be due to the increased synthesis of heat-shock proteins (HSPs) [67]. Amano et al. [68] found that a heat stimulation of 42 °C decreases dental pulp cell viability, whereas the HSPs would help recovering the pulp cell vitality.

Current restorative techniques are based on the adhesive properties of DRMs [69], which work normally in the temperature range of -5 to 55 °C [46]. Differences in TPs between tooth and DRMs facilitate the development of thermal stresses [63,70,71], with maximum stress developed on the bonding interfaces [72]. Together with stresses caused by mastication, these stresses can induce degeneration of the bonding interface and hence reduce the life-span of dental restorations [73–75].

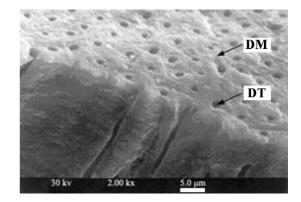


Fig. 1 – Scanning electron micrograph of dentine showing longitudinal and cross-sectional views of dentinal tubules (DTs) and dentinal matrix [45].

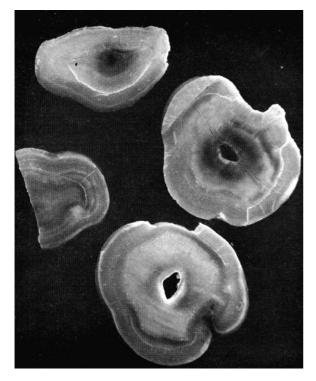


Fig. 2 – Sections of tooth after 7000 thermal cycles with crack depth and origin shown [29].

#### 1.5. Applications of tooth HT

The study of HT in tooth and thermally related effects (e.g., damage) is of great significance in modern dentistry, as summarized below.

- (i) Precise temperature measurement in tooth may indicate the pulp vasculature and hence help in endodontic diagnosis [76].
- (ii) In vitro investigation of HT in tooth under dental treatments can provide better approaches to evaluate the operation guidance, thereby reducing or preventing tooth damage so that a less empirical dental practice may be developed.
- (iii) It can help in choosing and designing suitable DRMs with thermomechanical properties similar to toot, so that postoperative complications such as pain, marginal staining and caries may be avoided [77,78].
- (iv) Tooth pain sensation is correlated with DFF [79].

A better understanding of HT phenomenon and thermally induced DFF in dental tubules will extend existing knowledge underlying TTP mechanisms and thus improve the relief methods for tooth pain sensation.

#### 1.6. Outline of this review

In view of the lack of a thorough review of the current development in tooth HT, we present the state-of-the-art of existing studies on experimental characterization and mathematical modeling methodologies. The challenges associated with these methodologies and potential modifications essential for addressing these challenges are discussed. Interpretation of TTP in terms of heat stimulated DFF is also presented.

# 2. Experimental characterization of HT in tooth

Investigation of HT in tooth requires both experimental measurements [2,10,35,58,80,81] and mathematical modeling [53,82–84]. Mathematical models can supply estimates of information (*e.g.*, temperature and thermal stress) over the entire continuum of interest, while experimental characterizations can validate the mathematical models and determine the various material properties (*e.g.*, thermal, optical and mechanical) needed for theoretical modeling.

#### 2.1. Measurement of tooth TPs

Knowledge of tooth TPs is crucial for accurate mathematical modeling and analysis of HT in tooth. The most important material properties for HT in tooth are tooth geometry, TC (*k*, W m<sup>-1</sup> K<sup>-1</sup>), specific heat ( $c_p$ , J kg<sup>-1</sup> K<sup>-1</sup>), and TD ( $\alpha$ , m<sup>2</sup> s<sup>-1</sup>). In view of physics, TC indicates the ability of a material to conduct heat and is given as  $k = (\Delta Q/\Delta t) \times (L/A \times \Delta T)$  where  $\Delta Q$  (*J*) is the heat transmitted during time  $\Delta t$  (s) through a thickness *L* (m), in the direction normal to a surface of area A (m<sup>2</sup>), due to a temperature difference  $\Delta T$  (°C). Specific heat is the energy required to increase a unit of temperature of a unit quantity of a substance. Thermal diffusivity  $\alpha \equiv k/\rho c_p$  is the ratio of TC to volumetric heat capacity,  $\rho$  (kg m<sup>-3</sup>) being the density of the material.

Traditional HT instruments and methods have been widely used to characterize the TPs of tooth components, such as the thermal couples [29,65,85–88], infrared camera (IR) technique [89], flash laser method [60,90,91], differential scanning calorimeter (DSC) [59], and traditional calorimeter cup [65,92]. The reported data on human teeth are summarized in Table 3, which shows significant differences between reported results. For example, TC of human dentine was reported to be ~0.11 W m<sup>-1</sup> K<sup>-1</sup> in one study [93], but to be 0.96–0.98 W m<sup>-1</sup> K<sup>-1</sup> in others [86,94]. Similarly, the reported TC of dentine covers a wide range of 0.36–0.88 W m<sup>-1</sup> K<sup>-1</sup> [59,64,85,95,96]. Whilst one study [91] reports the TD of enamel to be  $2.27 \times 10^{-7}$  m<sup>2</sup> s<sup>-1</sup>, its was measured to be ~4.20–4.69 × 10<sup>-7</sup> m<sup>2</sup> s<sup>-1</sup> by others [64,85].

The significant discrepancy between the reported results of tooth TPs may be attributed to several challenges associated with the measurement: (i) The microstructure of tooth is heterogeneous and varies significantly from one sample to another (*e.g.*, teeth donators are of different ages, races, healthy conditions and of different kinds such as incisors and molars). For example,  $c_p$  of dentine is found to depend on the orientation of dentine tubules [59,64,92], with  $873J \text{ kg}^{-1} \text{ K}^{-1}$ and  $1039-1181J \text{ kg}^{-1} \text{ K}^{-1}$  in directions perpendicular and parallel to tubules, respectively. (ii) When thermal couples are used, the imperfect contact between the probe and tooth structure (*e.g.*, existence of air gap) increases the measurement error. (iii) The thermal, spatial and temporal resolutions of the IR camera and the radiation/reflectivity of irradiated

Property	Tooth component	Values (method)	References
	Enamelª	4.69 <sup>f</sup>	Brown et al. [64]
	Enamel	4.20 <sup>f</sup>	Braden [85]
	Enamel <sup>d</sup>	2.27 <sup>g</sup>	Panas et al. [91]
	Dentine <sup>a</sup>	1.87 ( <sup>b</sup> ) <sup>f</sup>	Brown et al. [64]
		1.83 (°)	
X	Dentineª	1.99 ( <sup>b</sup> ) <sup>g</sup>	Magalhães et al. [59]
Fhermal diffusivity		2.04–2.65 ( <sup>c</sup> )	0
$\times 10^7 \mathrm{m^2  s^{-1}}$ ]	Dentine	2.58 <sup>f</sup>	Fukase et al. [97]
	Dentine	2.60 <sup>f</sup>	Braden [85]
	Dentine <sup>d</sup>	1.92 <sup>g</sup>	Panas et al. [91]
	Pulp <sup>e</sup>	1.520	
	-		de Vree et al. [98]
	Bulk value (enamel + detine)	3.49 (heating) <sup>h</sup> 2.78 (cooling)	Panas et al. [91]
	Enamel <sup>a</sup>	0.93 <sup>f</sup>	Craig and Peyton [99]
	Enamel	0.92 <sup>f</sup>	Braden [85]
	Dentine <sup>a</sup>	0.58 ( <sup>b</sup> ) <sup>f</sup>	Craig and Peyton [99]
		0.57 ( <sup>c</sup> )	0 , 1 ,
	Dentine	0.11 <sup>f</sup>	Johnson et al. [93]
	Dentine	0.96 <sup>f</sup>	Lisanti and Zander [86
	Dentine	0.98 <sup>f</sup>	Simeral [94]
2	Dentine	0.88 <sup>f</sup>	Little et al. [96]
Thermal conductivity	Dentine <sup>a</sup>	0.36 ( <sup>b</sup> ) <sup>g</sup>	Magalhães et al. [59]
$W m^{-1} K^{-1}$ ]	Dentine	0.48–0.66 (°)	Magaillaes et al. [59]
	Dentine	0.63 <sup>f</sup>	Prodon [95]
			Braden [85]
	Dentine	0.58 ( <sup>b</sup> ) <sup>f</sup> 0.57 ( <sup>c</sup> )	Craig and Peyton [99]
	Dentine	0.40 (Root <sup>c</sup> ) <sup>f</sup>	Soyenkoff and Okun [
	Dentine	0.45 (Crown <sup>c</sup> )	boyennon and onan [.
	Pulp <sup>e</sup>	0.63	de Vree et al. [98]
	Tulp	0.05	de viee et al. [56]
	Enamel <sup>a</sup>	0.71 <sup>i</sup>	Brown et al. [64]
	Enamel	0.75 <sup>i</sup>	Peyton and Simeral [9
	Dentine <sup>a</sup>	1.59 <sup>i</sup>	Brown et al. [64]
p	Dentine <sup>a</sup>	0.87 ( <sup>b</sup> ) <sup>j</sup>	Magalhães et al. [59]
Specific heat		1.04–1.18 ( <sup>c</sup> )	
$\times 10^{-3}  \mathrm{J  kg^{-1}  K^{-1}}$	Dentine	1.30 <sup>i</sup>	Fukase et al. [97]
	Dentine	1.17 <sup>i</sup>	Peyton and Simeral [9
	Whole tooth <sup>a</sup>	1.26 <sup>i</sup>	Brown et al. [64]
	Pulp <sup>e</sup>	4.2	de Vree et al. [98]
	Enamel(deciduous)	2.95	Berghash et al. [100]
	Enamel (permanent)	2.97	Manly et al. [101]
	Enamela	2.80	Brown et al. [64]
	Dentine (deciduous)	2.18	Berghash et al. [100]
)	Dentine (permanent)	2.14	Manly et al. [101]
Density [×10 <sup>-3</sup> kgm <sup>-3</sup> ]	Dentine <sup>a</sup>	1.96	Brown et al. [64]
	Dentineª	2.09–2.40	Magalhães et al. [59]
	Cementum	2.03	Berghash et al. [100]
			Brown et al. [64]
	Whole tooth <sup>a</sup>	2.20	

<sup>a</sup> From human third molar.

<sup>b</sup> Perpendicular to tubules.

<sup>c</sup> Parallel to tubules.
<sup>d</sup> From human premolar.

<sup>e</sup> Values taken from water according to de Vree et al. [99].
 <sup>f</sup> Data acquired using thermal couple method.

<sup>g</sup> Data acquired using flash laser method.

<sup>h</sup> Data acquired using monotonic heating regime method.

<sup>i</sup> Data acquired using traditional calorimeter cup method.

<sup>j</sup> Data acquired using DSC method..

sample surface for flash laser are the main restrictions in acquiring precise TPs with these measurement techniques.

#### 2.2. In vitro measurement of HT in tooth

Experimental characterization of tooth HT can be divided into two main types: in vivo and in vitro. In vivo characterization is desirable since it can reflect the active processes (e.g., blood circulation in pulp chamber and fluid motion in DTs [28,35,32]) not captured in vitro [89,102–104]. However, there are several challenges associated with in vivo experimental investigations [89,103]. (i) Some internal features are difficult to capture. For example, experimental measurement of in vivo temperature change within tooth pulp is impractical [81]. (ii) Experimental procedures are restricted by patient tolerance especially when extreme thermal loading conditions as used in clinical pulp vitality testing [35,105,106] are involved. (iii) In vivo HT investigations of tooth are usually performed in animals [107–109]. The extension of these results to human teeth is questionable.

In view of the challenges of *in vivo* tests, *in vitro* tests are also widely used, *e.g.*, for studying HT during pulp sensitivity testing [81] and for safety evaluation of light-activated bleaching, HSHPs cavity preparation and laser irradiation [3,17,28]. Existing *in vitro* characterization of tooth HT can be divided into three categories depending on how the contribution of pulpal tissue to the tooth thermal behavior is modeled (*e.g.*, with empty pulpal chamber [25,81], with simulated pupal tissue [10,23,80], with consideration of microcirculation [27]).

In vitro HT studies have been carried out in tooth with empty pulp chamber (pulp soft tissue was extracted [25,54,81]). However, in this case, the measured temperature change on pulpal wall does not necessarily indicate the temperature change in pulp soft tissue [112], as the TC and heat capacity of teeth with empty pulp chambers are significantly different from those with filled chambers.

To simulate the transfer of heat between dentine-pulp junction (DPJ) and soft pulp tissue, Preiskorn et al. [80] placed a copper wire within the pulpal chamber through tooth root canal, with its protruding part spirally shaped to intensify the HT between the wire and a water bath. IPTR were measured both with and without considering the influence of pulp HT, with significant difference in the measured temperature profiles observed. Similarly, to mimic the vital dental pulp, Attrill et al. placed a 'pulp phantom' into the pulp chamber [23], whilst Hannig et al. [10] filled the pulp chamber with warm water to mimic HT through soft tissue in the pulp chamber.

Although in vitro measurements with simulated pulp tissue are more reliable than those carried out with an empty pulp, both approaches ignore the influence of PBF and the dense capillary network adjacent to the odontoblast layer in the vital pulp. This deficiency limits the direct application of the measurement data to the *in vivo* situation [27,76]. Daronch et al. [27] proposed an alternative way to measure IPTR by connecting one of the tooth roots via a small diameter tube to an infusion pump, with the pump designed to deliver water at a speed of 0.0125 ml/min that mimics the PBF rate. The tooth was then immersed into a water bath up to the cement–enamel junction. As blood supply in the pulp chamber and HT through pulp soft tissue and periodontal ligament are both considered, the measurements, although still in vitro, are more applicable in clinical situations.

### 2.3. Response of tooth to heat stimulus in terms of blood circulation and DFF

The pulp is highly vascularized [43], with arterial vessels entering through the apex of tooth roots and passing into the tooth crown. The microcirculation of blood in the dental pulp plays an important role in tooth thermal behavior, besides providing nutrition to the peripheral tissue. Histophysiological studies reveal that the PBF rate is almost constant when the IPTR lies within the range of 33° to 42 °C [111], increases significantly when the temperature rises above 42 °C [56], and decreases with decreasing temperature under cooling [57]. This feature contributes significantly to the thermoregulation of pulpal soft tissue [56,60]: the PBF works as a heat sink under heating and as a heating source under cooling. However, the influence of PBF on HT is considered negligible in clinical settings due to the low blood volume in the pulpal vasculature [110].

Thermal stimulation (hot or cold) of tooth causes temperature change within tooth [10,35,112] and may agitate tooth pain response [36]. Three theories for pulp nerves activation have been proposed, i.e., the neural theory, the odontoblastic transduction theory and the hydrodynamic theory [113]. The neural theory assumes that direct thermal stimulus on the axons extending to the DEJ are responsible for TTP sensation. However, this assumption has been shown experimentally to be questionable, as the sensory response of teeth to thermal agitation occurred before a temperature change was detected in the pulpal wall (the locations of most sensory structures) [37]. Based on the observation that the human odontoblasts in vitro produce action potentials [114], the odontoblastic transduction theory proposes that odontoblasts may work as sensor cells that initiate tooth pain transmission. A strong argument against the transduction theory is the observation that dentin remains sensitive after local destruction of the odontoblasts [115,116]. At present, the most widely accepted theory is the hydrodynamic theory [115,117] which suggests that the free nerve endings located in the inner dentine and around the odontoblasts are activated by thermally induced DFF [36]. The DFF may be induced by the thermal expansion or contraction of fluid, pushing the fluid away from the pulp under cooling and toward the pulp under heating [118,119], or by the driving force of thermal expansion of enamel and dentine [35].

#### 2.4. Influence of different factors on tooth HT

HT in tooth is affected by a number of factors such as the temperature dependent TPs, geometry of teeth components, types of DRMs, pulp circulation and blood perfusion, as discussed below.

#### 2.4.1. Temperature dependent TPs

When the temperature change exceeds 10  $^{\circ}$ C, it is necessary to account for the temperature dependence of tooth TPs in modeling. The dependence of the tooth TC and TD on temperature may be approximated as:

$$\mathbf{k} = \mathbf{k}_0 + \mathbf{k}_1 \mathbf{T}, \quad \alpha = \alpha_0 + \alpha_1 \mathbf{T} \tag{1}$$

where  $k_0$ ,  $k_1$ ,  $\alpha_0$  and  $\alpha_1$  represent the linear fit values to test data. However,  $k_1$  and  $\alpha_1$  usually have values close to zero, implying that k and  $\alpha$  are only slightly influenced by temperature, especially when the temperature is relatively low. Consequently, existing studies of tooth HT [120–123] often assume that the TPs are independent of temperature to simplify the mathematical analysis.

#### 2.4.2. Geometry of tooth

Enamel has a unique microstructure consisting of aligned prisms/rods, which run approximately perpendicular from DEJ towards tooth surface [124]. This characteristic arrangement of prisms in enamel should have a significant influence on heat excursion in tooth. Besides, the presence of DTs is strongly correlated with the porosity of human dentine as well as its density and TC [59]. Furthermore, Pashley [125] and Komabayashi et al. [126] demonstrated that there is a marked increase in the number of DT, the tubular radius, and the total physical surface area available for diffusion in regions near the pulpal chamber wall, whereas a reverse situation was found in regions close to DEJ. This characteristic geometry of dentine facilitates a better transfer of heat into the pulp. Therefore, it is conceivable that the dentine material is adapting not only to enhance its endurance to thermal alterations but also to dissipate more heat toward the pulp [127].

# 2.4.3. Influence of the thickness of dentine and enamel layers

Enamel and dentine have relatively lower values in TC and diffusivity and thus protect the pulp from noxious thermal agitation. White et al. [128] and Paghdiwala et al. [129] proposed that dentine layer should be considered when analyzing tooth HT despite of its small thickness and that the prepared tooth with small amounts of remaining dentine thickness were more prone to temperature increases [59]. The effect of thermal stimulation on DFF has been investigated in tooth with exposed dentine [130], and it was shown that tooth with exposed dentine responded more quickly to thermal stimulation than intact tooth, due to direct transfer of heat to dentine in the absence of enamel.

#### 2.4.4. Dental restorative materials

The influence of DRMs on tooth HT has been studied extensively due to its significance in clinical applications [53,122,123]. It has been established that the thermal performance of restored tooth differs significantly from that of intact ones, due to the different TPs of DRMs and tooth.

#### 2.4.5. Heat transfer due to PBF and DFF

The PBF rate in the highly vascularized pulpal chamber [131,132] is correlated with peripheral temperature. For example, the PBF rate increases significantly when the temperature rises above 42 °C [56] and decreases under cooling [57]. Heat exchange between the perfused blood and peripheral tissue may significantly influence the thermal behavior of pulpal soft tissue [56,60]. In addition, heat can also stimulate DFF due to thermal deformation of DTs and the tissue fluid [35]. The outward (away from the pulp) or inward (toward the pulp) fluid movement under cold or hot stimulus [35] would inevitably cause the redistribution of pulp chamber temperature.

#### 3. Mathematical modeling of HT in tooth

HT in restored or unrestored human tooth has been studied extensively, with emphasis placed on assessing the risk of unexpected IPTR during dental treatments. Tooth temperature has been measured invasively, which however only provides information of tissue temperature at discrete points [10,35,80]. Mathematical modeling, in this aspect, can address this issue by predicting temperature distribution and its evolution within tooth.

#### 3.1. Theoretical analysis

Based on Pennes' bioheat transfer equation, various heat conduction problems solved by analytical means have been presented under different thermal boundary conditions [133–135]. The Pennes model is given as [136]:

$$\rho c \frac{\partial T}{\partial t} = \nabla (k \nabla T) + \rho_b c_b \omega_b (T_a - T) + q_{met} + q_{ext}$$
(2)

where  $\rho$  (kgm<sup>-3</sup>) is tissue density; c (J kg<sup>-1</sup> K<sup>-1</sup>) is tissue specific heat; k (Wm<sup>-1</sup>K<sup>-1</sup>) is tissue TC;  $\rho_b$  (kgm<sup>-3</sup>) is blood density; c<sub>b</sub> (J kg<sup>-1</sup>K<sup>-1</sup>) is blood specific heat; T<sub>a</sub> (K) is blood temperature;  $\omega_b$  (ml s<sup>-1</sup>) is blood perfusion rate; T (K) is temperature of surrounding tissue; q<sub>met</sub> (J) is metabolism heat generation; and q<sub>ext</sub> (J) is heat generation due to external heating sources.

In clinics, prediction of heat distribution in tooth is vital for optimizing parameters of dental treatments. Analytical solutions to the heat conduction equation for laser interaction with material and biological tissues have been well established [137,138]. However, the solutions are usually obtained by simplifying the problem (e.g., surface energy processes such as irradiation and convection are neglected), which put restrictions on modeling the spatial and temporal profiles of the incident pulse.

#### 3.2. Numerical simulation

HT in tooth dependents on its geometry, material properties and *in vivo* biological function. Due to the complicated topological structure of tooth, introducing more than one of its components into an analytical model leads to intractable solutions, while numerical methods such as the finite element method (FEM) and the finite difference method (FDM) offer an alternative approach [53,82,139,140]. In mathematical modeling, the tooth is generally simplified as a system of geometrical areas containing only enamel, dentine (in intact tooth) and DRMs (in restored tooth), with HT between pulpal wall and pulp tissue ignored [122]. However, these simplifications lead to approximate results [110], as HT in dental pulp is considered important [53,121,141].

Based on the Fourier law of heat conduction, various models with or without the consideration of soft tissue (dental pulp) have been proposed for HT in restored/unrestored tooth. The temperature and thermal stress fields have been quantitatively calculated using 2D or three-dimensional (3D) FEM.

#### 3.2.1. Modeling of normal heating

The thermal behavior of restored and unrestored tooth caused by food intake in daily life can be modeled as a cylindrical layered structure (*e.g.*, for human first molar during hot water drinking process [98]). With tooth taken as homogeneous and isotropic, one has [98]:

$$k_{i}\left[\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(r\frac{\partial T}{\partial z}\right)\right] = \rho_{i}c_{i}r\frac{\partial T}{\partial t}$$
(3)

where i is the index of sub-layers (i = 1, 2, 3, ..., n); r and z are the radial and axial coordinates; T is the temperature (which is a function of time t and location);  $k_i$ ,  $c_i$  and  $\rho_i$  are the TC, specific heat and mass density in sub-layer i, respectively. To mimic convective loading, warm water has been used, with its temperature decreasing linearly from 60 °C to 35.2 °C [98]. The temperature predicted by the above model matched well with the clinical experimental measurement of Trowbridge et al. [37].

## 3.2.2. Modeling of heat distribution in tooth under irradiation of LPUs

The need of tooth restorations leads to the use of light-activated resin composites [9,142]. However, rapid polymerization necessitates the usage of increased LPUs output energy which may damage the pulp tissue [10,11]. Tunc [53] and Preiskorn et al. [80] developed models to analyze the potentially overheating of pulp when tooth is irradiated with clinical relevant LPUs. However, a constant heat flux thermal boundary condition was assumed, which limits the universality of applying the mathematical model from one type of LPU to another. Jakubinek et al. [82] have recently developed a mathematical model that considers the light intensity of LPUs. It was assumed that heat generated within the nth layer of restored tooth due to curing light,  $Q_n$  (J), can be described by the difference between the light intensity entering and leaving a slice of material of thickness d divided by that thickness, as:

$$Q_n = \begin{cases} \frac{I_0}{d} (e^{-(n-1)d/x} - e^{-(nd/x)}), & \text{for } 0 \le t \le t_L \\ 0, & \text{otherwise} \end{cases}$$
(4)

where  $t_L$  (s) is the time duration of light exposure,  $I_0$  (W/m<sup>2</sup>) is the light intensity on tooth surface, and  $\delta$  (m) is the 1/e penetration depth. The numerical predictions of Jakubinek et al. [82] appear to agree well with experimental measurements.

3.2.3. Modeling of laser interaction with tooth hard tissue To analyze the heating of tooth hard tissue by laser, Zuerlein et al. proposed a one-dimensional (1D) heat conduction equation based on the Fourier conduction law and energy conservation equation [143,144], as:

$$\frac{\partial T(z,t)}{\partial t} = \frac{k}{\rho c_{\rm p}} \frac{\partial^2 T(z,t)}{\partial z^2} + \frac{Q(z,t)}{\rho c_{\rm p}}$$
(5)

where the source term Q(z, t) is the temporally and spatially varying laser power input:

$$Q(z, t) = (1 - R)F(t)\mu_a e^{-\mu_a z}$$
 (6)

Here, z (m) is the depth from tooth front surface; R is the reflectance of laser beam of a specific wavelength on a specific tissue surface; and  $\mu_a$  is the absorption coefficient; F(t) (J m<sup>-2</sup>) is the time dependent incident fluence of the laser pulse (assuming that absorption is consistent with the Beer–Lambert law). When a specific type of laser (e.g., CO<sub>2</sub>, Er:YSGG and Er:YAG lasers) is used, the important optical properties are the reflectance and the absorption coefficient, while scattering is negligible in highly absorbing materials (e.g., tooth) [144,145]. Combination of Eqs. (5) and (6) leads to:

$$\frac{\partial T(z, t)}{\partial t} = \frac{k}{\rho c_{\rm p}} \frac{\partial^2 T(z, t)}{\partial z^2} + \frac{(1 - R)F(t)\mu_{\rm a}e^{-\mu_{\rm a}z}}{\rho c_{\rm p}}$$
(7)

The distribution and evolution of tooth temperature can be determined from numerical solutions to Eq. (7). For thermal boundary conditions, the front and back surfaces of the tooth sample may be assumed thermally insulated so that the transient heat conduction equation can be solved in the axial direction only, since the absorption depth is much smaller than the laser beam diameter.

Clinically, the use of Nd:YAG laser ( $\lambda = 1064$  nm) offers a series of advantages compared with CO<sub>2</sub> laser, attributed mainly to the limited crack formation when the former is used [146]. However, when the wavelength of the Nd:YAG laser lies within about 300–1000 nm, the scattering of non-pigmented tissue dominates over absorption. To account for the scattering and its anisotropy, Moriyama et al. [140,147] modified Eq. (6) as:

$$Q(z, t) = \mu_a I_o(t) \exp(-\mu_{eff} z)$$
(8)

where z is the depth from tooth front surface;  $I_o$  is the power density; and  $\mu_{eff}$  is the effective attenuation coefficient defined as:

$$\mu_{\rm eff} = \sqrt{3\mu_{\rm a}[\mu_{\rm a} + (1-g)]\mu_{\rm s}} \tag{9}$$

In the above equation,  $\mu_s$  is the scattering coefficient and *g* is the anisotropy parameter.

The reflectivity of enamel and dentine accounts for about 8.8-49.4% of the energy loss on the irradiated surface [145]. However, Moriyama et al.'s model neglected the reflectance of laser beam on tissue surface and hence its clinical application is limited. Notice also that in both studies of Zuerlein et al. [143,144] and Moriyama et al. [140,147], heat radiation and convection from tissue surface were neglected which may be true in many cases. However, when the tissues are heated to high temperatures (e.q., dental ablation and caries treatment by laser), heat radiation and convection are particularly important as these are the processes allowing for cooling during and after the absorption and diffusion of laser energy. According to Sagi-Dolev et al. [148], neglecting the surface processes would lead to over-estimated temperature rises in tooth. Hence, they proposed a model that accounts for surface heat dissipation through convection and radiation by introducing two extra boundary conditions:

$$q_{\rm h} = H(T - T_{\infty}), \quad q_{\rm r} = \varepsilon \sigma (T^4 - T_{\infty}^4)$$
 (10)

where  $q_h$  is the convection heat flux on tissue surface; *H* is the surface convection coefficient; *T* is the temperature of tissue surface;  $T_{\infty}$  is the surrounding temperature;  $q_r$  is the heat radiation of tissue surface;  $\varepsilon$  is the emissivity; and  $\sigma$  is the Stephan-Boltzmann constant.

Nevertheless, the reflectivity of laser beam on tooth enamel surface was ignored by Sagi-Dolev et al. [148]. As previously mentioned, the reflectivity of enamel and dentine accounts for about 8.8–49.4% of energy loss on the laser irradiated surface [145]. This may explain why the model predictions of Sagi-Dolev et al. [148] deviate from the in vitro measurements.

Therefore, a mathematical model that accounts for all the important surface energy processes (reflection, radiation and convection) is needed for more accurate predictions.

#### 3.3. Limitations with existing models

In spite of the extensive research thus far, significant discrepancy still exists between experimental measurements and mathematical modeling. For example, Tunc [53] reported that the temperature predicted by existing numerical models could not be used directly as temperature changes in vivo because the models did not consider the cooling effect of blood perfusion in pulp chamber and DFF. The discrepancy indicates that some of the assumptions made when developing these models are not realistic. The factors that prohibit the development of a sound and conclusive mathematical model include: (1) the physical properties of tooth vary in different teeth (incisor, canine, molar) and different donors including ages, sex and races. Even for a single tooth, its physical properties differ from one layer to another and are anisotropic as well as inhomogeneous in each layer [45,149]. While, in the existing models, teeth are treated as layered materials and assumed to be homogenous, isotropic and linearly elastic in each layer. Such simplifications lead to an inaccurate presentation of tooth HT and hence prohibit the predictions to be directly used as guidance for clinical applications. (2) The current models assume that heat conduction occurs only between the pulpal wall and the pulp, with the influence of PBF and DFF neglected. (3) The thermal boundary conditions in tooth especially the part that under the gum is too complex to be determined. In the exiting models, these boundary conditions have been much simplified (e.g., using oral temperature as the constant temperature) [60,138].

#### 4. Future work

Characterizing how heat is transferred across tooth is of great importance which can contribute to a variety of dental medical applications as well as the fundamental understanding of tooth thermal pain. In this respect, the present review identifies the following topics for further research.

The lack of reliable and comprehensive data concerning tooth TPs causes great difficulties in the mathematical modeling of HT in tooth, which also impedes the development of DRMs possessing "tooth like" TPs to avoid post complications. It is therefore of great importance to systematically re-evaluate the TPs of teeth, where a number of factors should be properly considered, including the gender and age of the donors, the type of tooth (incisor, canine and molar), etc.

When studying the thermal behavior of biological tissue, thermomechanical coupling should be taken into account as mechanical loadings often accompany thermal stimuli [150,151]. For example, excessive heat deposition in tooth will cause significant tooth thermal deformation [129,152] and DFF [35]. The resulting thermal stresses may cause cracking in tooth [2,29,63] as well as marginal leakage of dental restorations interfaces [63]. More importantly, the thermally induced DFF and tooth deformation is critical for the study of TTP mechanisms [36,108].

Current mathematical models, although very helpful, still need further improvement. Previous models [55,59,106,137,138] have assumed that each layer of a tooth is made of isotropic material, and have neglected its biological features (both structure and function) such as: (1) biologically organized enamel prisms running from DEJ to enamel surface; (2) organized system of DTs filled with tissue fluid that run complexly through the tissue; and (3) cooling/heating effect of PBF in the capillarity. Improved modeling with consideration of the above-mentioned factors should provide a more accurate prediction of tooth HT which, eventually, may be practically used as guidance for clinical applications. Furthermore, experimental measurements are needed to check the validity of model predictions.

How do the external thermal stimuli (cold or hot) cause tooth pain sensation? Also, why outward fluid flow in DTs (away from the pulp that can be triggered by cold stimulus) is more efficient in evoking axonal activation than inward flow (toward the pulp that can be triggered by hot stimulus)? [108]. The answer may be obtained through a comprehensive study of thermal-relative DFF in DTs [36]. Due to the presence of mechanosensitive ion channels on pulpal neurons [153], the shearing force induced by DFF may be responsible for the activation of iron channels and consequently induce tooth pain sensation [40,153]. A holistic mathematical model capable of describing the complicated processes of heat stimulated pain sensation in biological tissue has been established [154–156], which may be applicable in the study of TTP.

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