



ORIGINAL ARTICLE

# Finite element modeling of the periodontal ligament under a realistic kinetic loading of the jaw system



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## KEYWORDS

PDL;  
Dynamic finite element;  
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Trajectory approach

**Abstract** *Purpose:* The stresses and deformations in the periodontal ligament (PDL) under the realistic kinetic loading of the jaw system, *i.e.*, chewing, are difficult to be determined numerically as the mechanical properties of the PDL is variably present in different finite element (FE) models. This study was aimed to conduct a dynamic finite element (FE) simulation to investigate the role of the PDL (PDL) material models in the induced stresses and deformations using a simplified patient-specific FE model of a human jaw system.

*Methods:* To do that, a realistic kinetic loading of chewing was applied to the incisor point, contralateral, and ipsilateral condyles, through the experimentally proven trajectory approach. Three different material models, including the elasto-plastic, hyperelastic, and viscoelastic, were assigned to the PDL, and the resulted stresses of the tooth FE model were computed and compared.

*Results:* The results revealed the highest von Mises stress of 620.14 kPa and the lowest deformation of 0.16 mm in the PDL when using the hyperelastic model. The concentration of the stress in the elastoplastic and viscoelastic models was in the mid-root and apex of the PDL, while for the hyperelastic model, it was concentrated in the cervical margin. The highest deformation in the PDL regardless of the employed material model was located in the caudal direction of the tooth.

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The viscoelastic PDL absorbed the transmitted energy from the dentine and led to lower stress in the cancellous bone compared to the elastoplastic and hyperelastic material models.

*Conclusion:* These results have implications not only for understanding the stresses and deformations in the PDL under chewing but also for providing comprehensive information for the medical and biomechanical experts in regard of the role of the material models being used to address the mechanical behavior of the PDL in other components of the tooth.

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## 1. Introduction

The periodontal ligament (PDL) is a soft connective tissue linking the tooth to the bone (Nishihira et al., 2003). PDL plays a crucial role in the orthodontic tooth movement and can actively bear both the tensile and compressive loadings (Cattaneo et al., 2005), and transfer them to the alveolar bone (Dorow et al., 2002). In the physiological process of orthodontic tooth movement, the PDL has a pivotal role in adapting orthodontic tooth movement as the microvasculature and blood flow contained within the PDL might be in part or fully occluded because of its exposure to a certain level of pressure (Jones et al., 2001). The pressure occlusion can trigger a dysfunction or necrosis of the PDL followed by a cascade of events directing orthodontic tooth movement via the recruitment of osteoclasts and osteoblasts (Meikle, 2006).

After the first contact between the tooth and food during chewing, a set of complex forces, whether translational, rotational or both are being applied to the tooth and transmit to the bone through the PDL (Bourauel et al., 1999). *In vivo*, analyzing the contours of stresses and deformations in the PDL under a kinetic loading of chewing is not achievable. Numerical approaches such as finite element method (FEM), can be applied to quantitatively calculate the stresses and deformations in the PDL under various types of static and dynamic loadings (Wakabayashi et al., 2008). However, the most crucial part of an accurate FE simulation is the mechanical properties of the components being implemented into the model. Since the PDL is a key asset in orthodontic tooth movement and deformation fields in the entire periodontium under an external force as well as remodeling process in bone (Dorow et al., 2003), its mechanical properties are of great attention (Komatsu et al., 2004). A wide range of material models have been proposed for the PDL, *i.e.*, linear elastic (Field et al., 2009; Poiate et al., 2009; Vecilli et al., 2008), nonlinear hyperelastic (Atkinson and Ralph, 1977; Maceri et al., 2007; Qian et al., 2009), and time-dependent viscoelastic (Komatsu et al., 2004; Toms et al., 2002; Wei et al., 2008). Some FE models have entirely ignored the role of the PDL (Kupczik et al., 2007; Strait et al., 2009; Wroe et al., 2007), or when it is considered is being modeled with a simplified geometry (Kupczik et al., 2009; Panagiotopoulou and Cobb, 2009). Orthodontic forces through FE study revealed the highest stresses in the root, alveolar bone, and the elastic PDL (Tanne et al., 1987). The role of the nonlinearity of PDL in the stresses and deformations of the entire periodontium was investigated using FEM (Aversa et al., 2009). A combined experimental and FE analyses have been carried out to investigate the full-field distributions of displacement, stress and strain, and their evolution with loading in the entire fresh periodontium under an

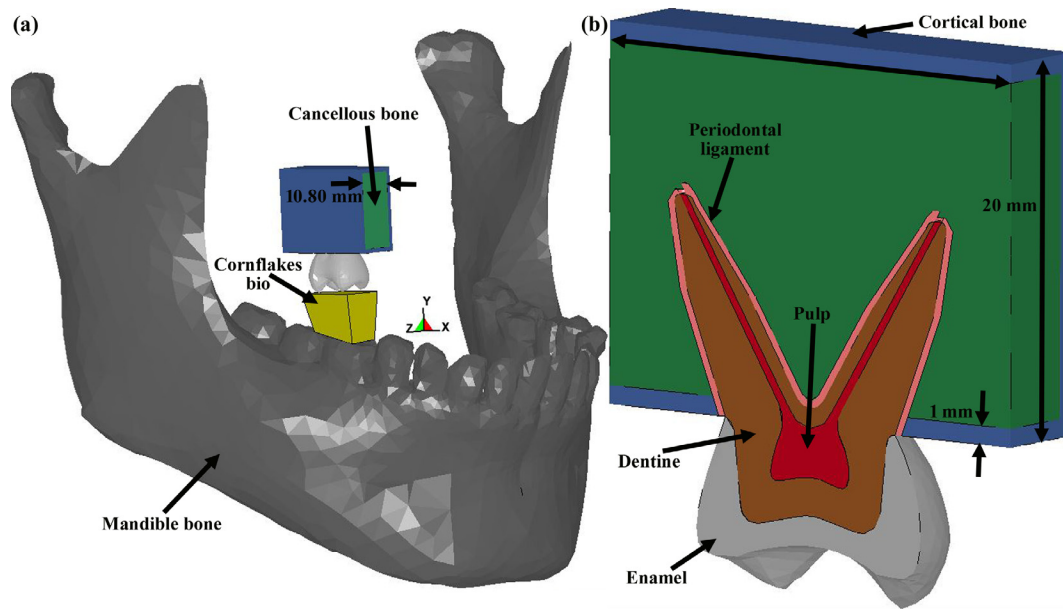
externally applied force (Qian et al., 2009). The major strain was found in the PDL with the highest value near to the tooth apices, at the tooth root, and the sides of the tooth roots. A two-dimensional (2D) FE model was employed to compare the importance of material models, *i.e.*, linear and nonlinear, of PDL in orthodontic tooth movement simulation results (Toms and Eberhardt, 2003). This study revealed that the non-linearity assumption for the PDL resulted in a considerable increase in the stresses at the apex and cervical margin compared to the linear model. When it comes to realizing the detailed orientation and amount of force which is being applied to the PDL, it is a challenging issue to have a precise numerical simulation. Having a realistic kinetic loading of the jaw system for movements such as chewing would help mimic the same pattern of motions that occurs during chewing in the mandibular system (Hannam et al., 2008). This approach to measuring kinetic loadings, such as muscle force and trajectory (Razaghi et al., 2017, 2016), has been used in the recent publications of our group to mimic the kinetic loading of a jaw system during chewing. FEM models have been developed to calculate the stresses and deformations in the PDL under a combination of chewing and orthodontic (Horina et al., 2018) or chewing only forces (Martinez Choy et al., 2017).

In studies that have been conducted so far, the role of the material models, which is being assigned to the PDL under the realistic kinetic loading of the jaw system, especially chewing, has not been thoroughly investigated. This study aimed to establish a simplified patient-specific FE model of the jaw system and tooth to compute and compare the stresses and deformations in the elasto-plastic, hyperelastic, and viscoelastic PDL under a realistic kinetic loading of chewing. The trajectory approach was used to mimic the chewing of food with a dynamic pattern of movements of the incisor point, contralateral, and ipsilateral condyles.

## 2. Materials and Methods

### 2.1. Finite element model

A 3D FE model of the human mandible was made according to our previous studies (Karimi et al., 2014; Razaghi et al., 2017, 2016). Briefly, the solid models which were meshed with hexahedral elements consisted of the mandible bone, cortical and cancellous bones, PDL, pulp, dentine, enamel, and food (cornflakes bio) as displayed in Fig. 1. Due to the complexity of the model, the structure of the model was a bit simplified, using average anatomical dimensions of the tooth components (Katrani et al., 2007; Ona and Wakabayashi, 2006). A con-



**Fig. 1** The (a) structure of the FE model. (b) The tooth including all its components.

stant thickness value of 0.20 mm was considered for the PDL (Natali et al., 2004).

The mechanical properties of the FE model components are listed in Table 1. Shell and brick elements were employed for the mandible and cornflakes bio, respectively. The number of elements and nodes of the system are summarized in Table 1. To achieve a dynamic separation and spatter effect, the elements in the interface of PDL and bone, as well as the contact between the enamel and cornflakes bio, were selected for node release. Using the orientation of the surface mesh for the maxillary nerve canal, the region was generated by removing some of the internal elements of the model. In the 3D FE model of the human mandible, the teeth were assumed to be part of the mandible and have the same mechanical properties as the cortical bone. Three different material models, the elasto-plastic, hyperelastic, and viscoelastic, were used to address the

mechanical response of the PDL under the applied load. The same experimental data (Toms et al., 2002) was used to calculate the elasto-plastic, hyperelastic, and viscoelastic mechanical properties of the PDL to minimize any errors in our stresses and deformations outcomes in the PDL and other components of the model.

## 2.2. Trajectory approach

The trajectory approach of the human mandible was adopted to mimic the realistic kinetic load of the jaw system during chewing (Hannam et al., 2008). The trajectory approach works based on the inverse kinematics of the system and takes advantage of an optimization algorithm to determine muscle functions through the natural trajectory of the human mandible

**Table 1** Materials properties and number of elements and nodes of the FE model.

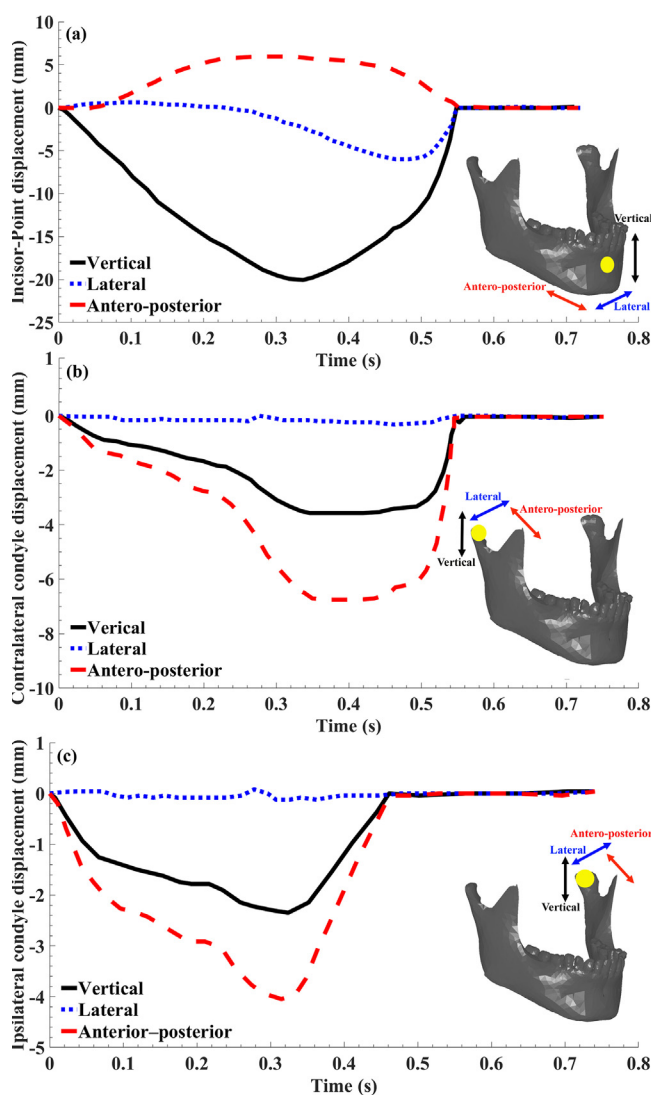
Material	Material model	Coefficients	Elements/Nodes
Enamel (Huang et al., 2005)	Elastic	$E = 77900 \text{ MPa}$ , $\nu = 0.33$ , $\rho = 3000 \text{ kg/m}^3$	12498/272
Dentin (Martinez Choy et al., 2017)	Elastic	$E = 18600 \text{ MPa}$ , $\nu = 0.31$ , $\rho = 2200 \text{ kg/m}^3$	17868/3962
Pulp (Huang et al., 2005)	Elastic	$E = 6.89 \text{ MPa}$ , $\nu = 0.45$ , $\rho = 1000 \text{ kg/m}^3$	2728/819
Cancellous bone (Chen et al., 2014)	Elastic	$E = 1970 \text{ MPa}$ , $\nu = 0.33$ , $\rho = 1400 \text{ kg/m}^3$	37345/7333
Cortical bone (Chen et al., 2014)	Elastic	$E = 15750 \text{ MPa}$ , $\nu = 0.33$ , $\rho = 1400 \text{ kg/m}^3$	16002/4230
Cornflakes bio (Razaghi et al., 2017)	Elastic	$E = 220 \text{ MPa}$ , $\nu = 0.45$ , $\rho = 1238 \text{ kg/m}^3$	1 brick element
PDL (Toms et al., 2002)	Elastic	$E = 0.40 \text{ MPa}$ , $S_y = 1.50 \text{ MPa}$ , $\epsilon_y = 0.80$ , $\nu = 0.49$ , $\rho = 1100 \text{ kg/m}^3$	6550/2033
	Hyperelastic	$\mu_1 = 0.99$ , $\mu_2 = -0.95$ , $\alpha_1 = 1.64$ , $\alpha_2 = -5.22$ , $\rho = 1100 \text{ kg/m}^3$	
	Viscoelastic	$G_1 = 0.0897$ , $G_2 = 0.1093$ , $G_3 = 0.7852 \text{ MPa}$ , $\tau_1 = 0.1548$ , $\tau_2 = 0.0038$ , $\tau_3 = 3.521 \times 10^{-5}$ , $\rho = 1100 \text{ kg/m}^3$	

$E$ : Elastic modulus;  $S_y$ : Yield stress,  $\epsilon_y$ : Yield strain,  $\nu$ : Poisson's ratio;  $\rho$ : density.

$W = \sum_{i=1}^n \frac{2\mu_i}{\alpha_i^2} (\lambda_1^{-\alpha_i} + \lambda_2^{-\alpha_i} + \lambda_3^{-\alpha_i} - 3)$ , ( $\mu_{i,j}$  and  $\alpha_{i,j}$ : Ogden material parameters).

$G(t) = G_1 e^{-\tau_1 t} + G_2 e^{-\tau_2 t} + G_3 e^{-\tau_3 t}$ , ( $G_i$ : Reduced relaxation function;  $\tau_i$ : Decay constant).

during chewing. During jaw opening, the superior and inferior lateral pterygoid muscles were co-activated. During early closing, the middle temporalis, superficial masseter, the left medial pterygoid, and superficial masseter muscles were all active. During late closing, the right superficial masseter and medial pterygoid, plus the temporalis and masseter muscle also participated (Murray et al., 2004, 2007). To address the function of all these muscles in our FE model, time-referenced displacement of the incisor-point and mandibular condyles, including the contralateral and ipsilateral, under the anterior, lateral, and antero-posterior movements were applied to the mentioned locations of the mandible as illustrated in Fig. 2. The initial stage, namely mouth opening, first contact with the cornflakes bio, and maximum contact that can be called clenching, was achieved in these diagrams.



**Fig. 2** Time-referenced displacement of the (a) incisor-point, and mandibular condyles, including the (b) contralateral and (c) ipsilateral, under the anterior, lateral, and antero-posterior movements (Hannam et al., 2008).

### 2.3. Finite element simulation

The numerical simulations were performed using the nonlinear explicit FE code of LS-DYNA. The contact algorithm of \*CONTACT\_SURFACE\_TO\_SURFACE' was employed to address the contact between the PDL and dentine on one side and the PDL and cancellous bone on the other side. The slave parts were the dentine and cancellous bone, while the master part was the PDL. The same contact was defined between the enamel, mandible bone, and cornflakes bio with the slave parts of cornflakes bio and enamel and the master part of the mandible. The merged contact was also defined between the other parts of the model.

Regarding the boundary condition of the model, the upper side of the tooth model (cortical bone) was constrained in all directions, and the lower jaw was allowed to move according to the pattern of the trajectory approach, mimicking the behavior of jaw in natural chewing (Figs. 1 and 2). The stress and deformation distributions in each region of the model were computed by the post-processing software (LS-PRE POST). To diminish the simulation time, only the clenching part of the curves in Fig. 2 was simulated as the highest amount of force during this action applies to the enamel of the tooth model.

## 3. Results

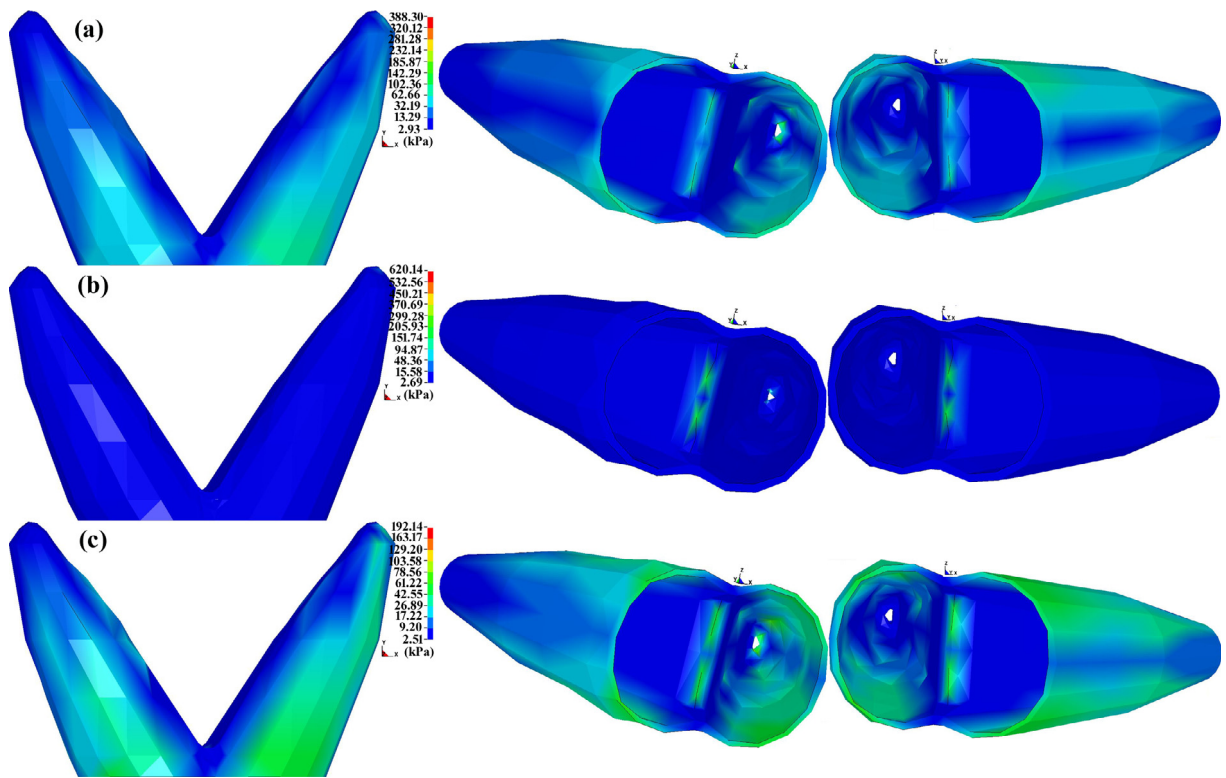
The contours of von Mises stress in the elasto-plastic, hyperelastic, and viscoelastic PDL tissues were calculated and shown in Fig. 3. The results revealed the highest stress of 620.14 kPa in the hyperelastic model, while the stresses of 388.30 and 192.14 kPa were observed in the elasto-plastic and viscoelastic models. The concentration of the stress in the hyperelastic model was in the cervical margin of the PDL, where it contacts with the dentine. However, when it comes to the elasto-plastic and viscoelastic models, the stresses were located in the mid-root and apex of the PDL.

The contours of deformation (resultant displacement) in the elasto-plastic, hyperelastic, and viscoelastic PDL tissues were also computed and indicated in Fig. 4. The results revealed the highest deformations of 0.21, 0.16, and 0.23 mm in the elasto-plastic, hyperelastic, and viscoelastic PDL. Chewing was shown to invoke a considerably higher deformation in the caudal compared to the rostral direction of the tooth.

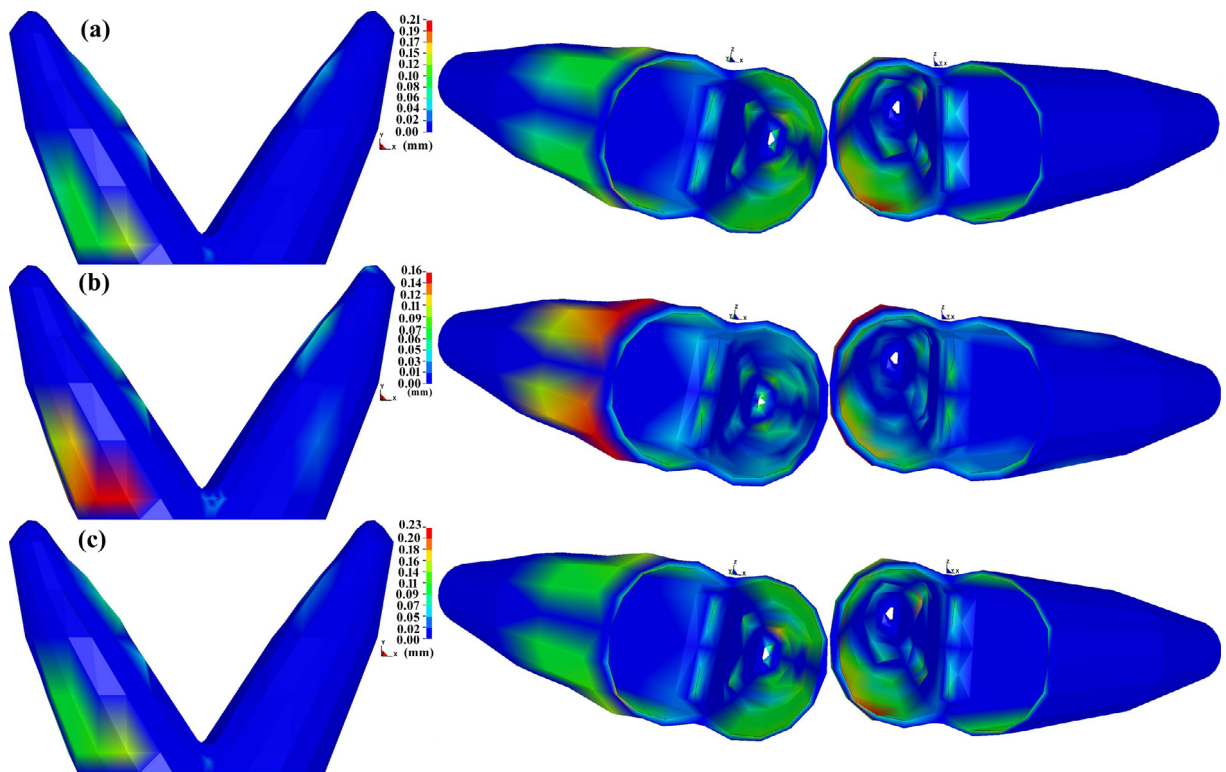
The von Mises stresses in other components of the model, such as the pulp, cancellous and cortical bones, enamel, and dentine, were calculated and plotted in Fig. 5. The results implied that the material model, which is being assigned to the PDL, has a vital role in the stresses of the cancellous and cortical bones as well as dentine. However, since the enamel and pulp were not in direct contact with the PDL, their stresses have not been affected.

## 4. Discussion

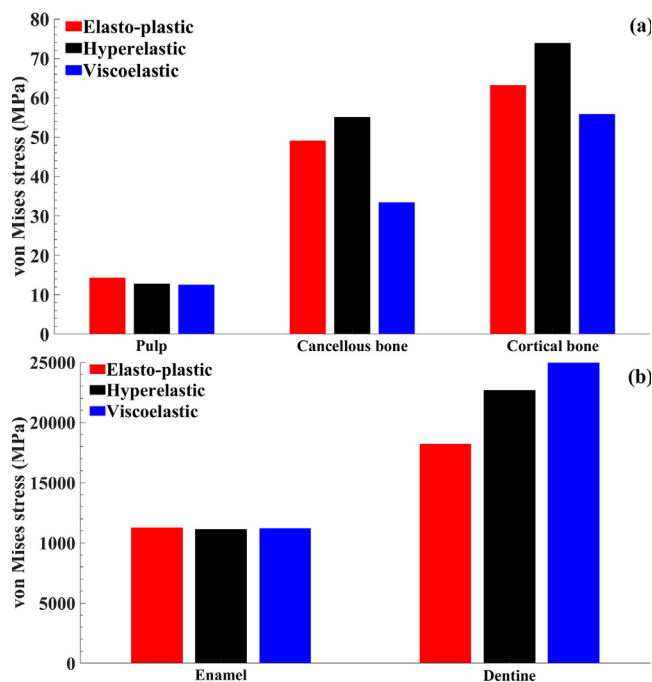
To the best of authors' knowledge so far, there has been a lack of research of the role of the PDL's material model in the induced stresses of other components of the tooth under the realistic kinetic loading of the jaw system. Establishing a precise FE model of tooth geometry is indispensable as the



**Fig. 3** The von Mises stress contours of the (a) elasto-plastic, (b) hyperelastic, and (c) viscoelastic PDL under chewing loading from different sides.



**Fig. 4** The deformation (resultant displacement) contours of the (a) elasto-plastic, (b) hyperelastic, and (c) viscoelastic PDL under chewing loading from different sides.



**Fig. 5** The bar plot representations of the stress in the (a) pulp, cancellous and cortical bones, the (b) enamel and dentine.

numerical results are highly sensitive to the assumptions made for the geometric modeling (Hohmann et al., 2011). Therefore, a simplified patient-specific FE model of the tooth, including the enamel, dentine, pulp, PDL, cancellous, and cortical bones, was established (Fig. 1). The realistic kinetic loading of the jaw system was mimicked using experimental trajectory data of the incisor point, contralateral and ipsilateral condyles under chewing and was implemented into our FE model (Fig. 2). The induced deformations in the PDL and the stresses in the other components of the tooth at the last step of clenching were calculated and reported. Since it has been shown that the angle of the forces applied on the tooth can considerably affect the resulted stresses in the components of the tooth (Huang et al., 2005), here in our simulations, we calculated the stresses and deformations under the realistic chewing loading.

The von Mises stress (Fig. 3) and deformation (Fig. 4) contours in the PDL showed the highest stress and the lowest deformation when the PDL was considered to be hyperelastic. The concentration of the stress in the hyperelastic model was in the cervical region of the PDL model, while the stresses in the elasto-plastic and viscoelastic models were concentrated in the mid-root and apex of the PDL. The same von Mises stress patterns were also observed in previous studies (Durkee et al., 1998; Toms and Eberhardt, 2003). The deformation in all the elasto-plastic, hyperelastic, and viscoelastic models was located in the caudal direction of the tooth, while in the rostral direction of the tooth, no considerable deformation was observed. In addition, the deformations, regardless of the material models being used for the PDL, were located in the cervical and mid-root regions. The location of the stress is related to the forces which are being transmitted from the food during chewing as the highest amount of deformation in the enamel was observed in the rostral direction. The point

where the deformation is the highest brings about a considerable momentum with translational force to the cervical and mid-root regions of the PDL following by higher stresses (Fig. 3) and deformations (Fig. 4). Understanding the mechanical response of the PDL under the complex chewing loading is crucially important for the simulation of orthodontic tooth movement (Jones et al., 2001; Kojima and Fukui, 2006). Simple linear elastic models may not be able to accurately measure the amount of deformation and stress at the interface of the dentine-PDL-bone (Dorow et al., 2003). Furthermore, it has been shown that the PDL may be subject to a large load of stresses and deformations from the dentine under biting forces during chewing (Maceri et al., 2007). Nonlinear material models for the PDL, such as hyperelastic, have shown to be more accurate when it comes to orthodontic tooth movement simulations under dynamic loadings (Pini et al., 2004). The stress magnitude of higher than 2.60 kPa has been shown to lead to the onset of bone remodeling (Penedo et al., 2010). Linear elastic and viscoelastic models showed the stresses of 23.93–60.35 kPa and 22.30–60.14 kPa under 1 N normal loading on the enamel, implying no considerable difference between these two material models (Yang and Tang, 2017). Here, the elasto-plastic, hyperelastic, and viscoelastic material models triggered the stresses 388.30, 620.14, and 192.14 kPa, respectively, implying that chewing a stiff food can be the initiation point of bone remodeling process following by necrosis and root resorption if this action continues over the time (Field et al., 2009).

The dentine and cancellous bone were in direct contact with the PDL. Consequently, the type of material model, which is being used, dramatically influences the stresses in these two components of the model (Fig. 5). The FE studies have been done before has also shown that stresses in the components of the tooth are affected by the presence of the PDL. A 40% difference in the strain of the dentine and cancellous bone were observed by the incorporation of the PDL into the tooth FE model (Panagiotopoulou et al., 2011). Our results also revealed that the viscoelastic PDL could considerably absorb the load from the dentine and trigger lower stress in the cancellous bone (Fig. 5a). It has also been shown that the viscoelastic PDL can absorb most of the applied energy from the dentine and minimize the transferred energy to the bone (Komatsu, 2010; Panagiotopoulou et al., 2011). The viscoelastic biomechanical behavior of the PDL also can better address the diverse tasks of the PDL, i.e., anchoring the tooth in the bone, damping during chewing, swallowing or clenching, force transmission to the bone, and converting long-term orthodontic force application into biomechanical signals for bone remodeling and orthodontic tooth movement (Keilig et al., 2016).

## 5. Conclusions

This study investigated the role of the PDL's material model in the stresses that occur in other components of the tooth under the trajectory realistic kinetic loading of the jaw system. Three different material modes, including the elasto-plastic, hyperelastic, and viscoelastic, were assigned to the PDL. The results suggested the importance of PDL material modeling as the viscoelastic PDL model led to lower stress in the cancellous bone compared to the elasto-plastic and hyperelastic models. The results have implications not only for understanding the stres-

ses and deformations in the PDL under chewing loading but also for shedding light on the role of the material models being employed for the PDL in the induced stresses of other components of the tooth.

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### Ethical issues

The use of humans for experimental purposes was approved by the committee of Basir hospital. This study was also entirely adhered to the declaration of the Helsinki 2008.

### Declaration of Competing Interest

The authors declare that they have no conflicts of interest.

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