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· 综述 ·

有限元分析联合拉曼光谱多模态技术在牙周组织创伤中的应用研究进展

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【摘要】 牙周组织创伤是指由多种因素导致的牙周组织病理性损伤或异常改变, 涉及复杂的物理学-化学-生物学耦合机制, 其精准诊断、评估与修复对口腔功能恢复和长期预后至关重要。传统单一技术常因力学表征不全或生物信息缺失等局限性而无法准确反映牙周组织状态。有限元分析通过有限元本构模型、多物理场耦合、有限元动态分析及多尺度建模的发展提升了物理模拟精度; 拉曼光谱基于非弹性光散射分子振动“指纹分析”获取的牙周组织分子化学组成及微环境信息, 可用于检测创伤后胶原构象变化、矿化梯度及炎症分子标志物, 具有较传统检测方法能更早发现微观损伤的技术优势。单独应用有限元分析或拉曼光谱只能对牙周组织创伤的应力-应变分析等物理模拟或分子化学检测, 功能较为局限; 但两者联合辅以人工智能(artificial intelligence, AI)形成的物理学-化学-智能分析多模态技术, 则可解析牙周组织创伤的生物力学机制、分子病理变化及动态修复过程, 并具有疾病早期精准诊断、个性化治疗方案优化等临床应用优势。有限元分析与拉曼光谱在牙周创伤研究中的联合应用尚处起步阶段, 现有研究存在多模态数据融合困难、实时反馈滞后、临床验证困难等不足, 未来需结合 AI 优化模型效率, 突破学科壁垒, 重点解决多尺度数据融合与临床转化问题并拓展跨学科技术整合。本文重点探讨有限元分析、拉曼光谱及两者联合的多模态技术在牙周组织创伤中的应用研究进展, 并提出了一类辅以 AI 的有限元分析-拉曼光谱多模态技术。

【关键词】 牙周组织; 创伤; 牙周炎; 有限元分析; 拉曼光谱; 人工智能; 多模态技术; 多尺度建模; 多物理场耦合模型; 牙槽骨; 骨代谢; 牙槽骨质量; 生物标志物

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Research progress on the application of finite element analysis combined with Raman spectroscopy multi-modal technology in periodontal tissue trauma LIU Yan^{1,2}, NI Qianwei², GAO Zan² 1. Xinjiang Medical University, Urumqi 830054, China; 2. Department of Oral and Maxillofacial Surgery, General Hospital of Xinjiang Military Command of PLA, Urumqi 830000, China

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【Abstract】 Periodontal trauma refers to the pathological damage or abnormal alterations of periodontal tissue caused by a variety of factors, involving a complex physical - chemical - biological coupling mechanism. Its accurate diagnosis, evaluation, and repair are essential for the recovery of oral function and long-term prognosis. The traditional single technique cannot accurately reflect the status of periodontal tissue due to limitations such as incomplete mechanical characterization or missing biological information. Finite element analysis improves the accuracy of physical simulation through the development of a finite element constitutive model, multi-physics coupling, finite element dynamic analysis, and multi-scale modeling. Based on the molecular chemical composition and microenvironment information of periodon-



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tal tissue obtained by inelastic light scattering molecular vibration “fingerprinting,” Raman spectroscopy can be used to detect the conformational changes of collagen, mineralization gradient, and inflammatory molecular markers after trauma. Raman spectroscopy can detect microscopic damage earlier than traditional detection methods. The application of finite element analysis or Raman spectroscopy alone can only be used in physical simulation, such as stress – strain analysis or molecular chemical detection of periodontal tissue trauma, and its function is relatively limited. However, the combination of the two modalities combined with AI (artificial intelligence) can analyze the biomechanical mechanism, molecular pathological changes, and dynamic repair process of periodontal tissue trauma, and it has clinical application advantages such as early accurate diagnosis of disease and personalized treatment optimization. The combined application of finite element analysis and Raman spectroscopy in the study of periodontal trauma is still in its infancy; studies have experienced issues with multimodal data fusion, clinical validation, and a lag in real-time feedback. In future work, it will be necessary to combine AI to optimize the efficiency of models, break through disciplinary barriers, and focus on multi-scale data fusion and clinical application, and expand interdisciplinary technology integration. This article focuses on the research progress of finite element analysis, Raman spectroscopy, and their combined multimodal techniques in the application of periodontal tissue trauma, and proposes a type of finite element analysis – Raman spectroscopy multimodal technology supplemented with AI.

【Key words】 periodontal tissue; trauma; periodontal inflammation; finite element analysis; Raman spectroscopy; artificial intelligence; multi-modal technology; multi-scale modeling; multi-physics coupling model; alveolar bone; bone metabolism; alveolar bone quality; biomarker

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牙周组织创伤是由机械性创伤、牙周炎等多种因素引起的牙周组织损伤,包括牙周膜、牙槽骨和牙龈等组织的破坏^[1-2],其力学机制复杂且具有显著个体差异。研究证实,机械性创伤(如击打伤、咬合过载、过度正畸矫治力等)可导致牙周膜纤维断裂、牙槽骨骨折及牙周血管神经损伤,进而可导致牙周组织炎症^[3-4]。牙周创伤导致的牙周组织炎症与糖尿病、心血管疾病等密切相关,牙周创伤引入的病原体可通过血液、唾液等途径引起全身疾病^[5-6]。

传统研究方式存在难以模拟牙周组织多向动态力学响应及组织交互模型简化的问题^[7-8]。有限元分析可通过分解复杂结构为有限单元进行物理分析,于牙周创伤而言,其核心优势在于既可进行应力-应变分析等物理学动态分析模拟,又可基于CT或Micro-CT数据构建涵盖牙周膜、牙槽骨及牙龈的个性化三维牙周组织模型,进而可揭示牙周创伤部分损伤机制^[9]。X线等传统诊断技术对早期牙周疾病的检测缺乏敏感性,无法在组织结构破坏前进行预警^[10-11]。拉曼光谱(Raman spectroscopy, RS)具有非破坏性检测、高化学特异性、多指

标同步分析、微米级空间分辨率等技术优势,能在分子层面对牙周组织化学物质进行分析,可实现牙周创伤早期诊治^[12]。这两种技术具有非破坏性检测、支持多物理场耦合分析、支持微观-宏观跨尺度关联的共性,可进行互补性技术整合。

1 有限元分析在牙周组织创伤中的研究与应用

1.1 有限元本构模型

有限元分析本构模型突破的关键在于材料属性研究的进步。牙周创伤中,牙龈、牙槽骨的有限元分析本构建模相对简单。牙龈在有限元分析中常被简化为低弹性模量的均质线性弹性体^[13]。该简化处理是可接受的,特别是当研究重点不在牙龈本身精细形变或非线性行为时。在简化模型中牙龈的主要作用是提供有限元分析边界条件和传导部分力。但实际上,牙龈表现出的是黏弹性、近似线性、横向各向同性特性^[14]。评估牙龈退缩、炎症响应及组织再生等研究,则需采用更精准复杂的模型。例如,应用有限元分析黏超弹性模型可更好反映在大变形及时间依赖性载荷下牙龈的组织响应^[15-16]。

牙槽骨的有限元分析材料定义通常有两种：一种是将牙槽骨定义为均质模型，模型相对粗糙，是研究需要或受限于研究条件的简化模型^[17]，虽是简化，但其背后蕴含着对生物力学分析复杂性的权衡与考量；另一种则是考虑到牙槽骨不同区域的骨密度差异，依据CT或Micro-CT图像灰度值对每个网格单元进行有差别材料赋值的非均质模型，模型相对精细，更符合真实生理情况^[18]。Zhang等^[19]研究发现非均质牙槽骨模型能更准确反映牙周膜应力集中区。牙槽骨模型的不同会显著影响牙周膜及周围骨的有限元分析模拟结果^[20]。牙槽骨高精度研究建议选用非均质模型。

牙周膜的本构建模及材料属性定义相对复杂。牙周膜作为“硬—软—硬”界面的核心力学缓冲器，具有超弹性、黏弹性、各向异性和非线性弹性特性，可被定义为非线性黏弹性体^[21-22]，常使用Ogden、Mooney-Rivlin超弹性模型（能较好拟合牙周膜的变形行为）、黏弹性模型（更适用于动态载荷分析）和应力松弛函数模型共同描述其非线性黏弹性生物力学特性^[22-23]，这种精准模型利于医学机制研究及临床转化。例如，Ortún-Terrazas等^[24]提出的“间质液过压会造成牙周膜损伤”理论，就是通过建立牙周膜多孔纤维超弹性损伤材料模型发现的。牙周膜线弹性模型常被用作简化模型，存在显著局限性。将牙周膜简化为线弹性会低估创伤载荷的能量耗散；虽建模方便、计算快速，但模拟结果准确度低，在有限元分析精细化建模中需谨慎使用^[23-25]。最近研究中，牙周膜被定义为具备超弹性模型、超弹性-黏弹性叠加本构模型，该有限元分析模型可通过整合结构非均匀性和时间依赖性提升牙周膜力学模拟的生理真实性^[26]。此外，基于牙周膜胶原纤维“在不同区域其纤维角度不同”的空间分布现象发展的多尺度横向各向同性、各向异性超弹性模型，显著提高了应力分布预测精度^[27-29]，为后续开发融合Micro-CT纤维追踪与深度学习（deep learning, DL）的多尺度各向异性模型奠定了基础。

1.2 多物理场耦合模型

物理学认为，现实世界不存在纯粹的单场问题，现实力学问题的本质都是多物理场耦合的结果，单场分析只是受限于技术条件的人为简化^[30]。现阶段，大量医学类有限元分析研究都是通过单一力场、流场等进行的实验；理论上讲，单场实验得到的数据较多场实验而言是相对粗糙的、不准

确的。

牙周创伤涉及力场等多物理场和多种生理因素的交互作用^[31]，有限元分析多物理场耦合模型可动态综合多个物理场因素，例如，在动态载荷下牙周组织的非线性力学行为（力场）^[32]、流体压力对牙周组织的影响（流场）^[33]等，可全面模拟牙周组织生理或病理情况。2019年，Ashrafi等^[33]首次通过流固耦合模型（fluid-structure interaction, FSI）量化了牙周膜内流体压力与组织形变的关系，发现忽略流体相会高估组织初始位移且无法捕捉组织能量耗散机制；Wang等^[34]通过FSI分析牙周膜孔隙压力、流速等流体力学响应时发现骨内缺损会导致局部应力增加、流体流速提高进而导致局部炎症反应增速。最近，Zhou等^[26]发现通过瞬时超弹性模型与时变非线性黏弹性模型进行多物理场超黏弹性耦合建模可深入研究牙周膜非线性蠕变力学行为。

1.3 有限元动态分析

有限元动态分析专注于研究结构或系统在随时间快速变化的载荷作用下的响应^[35]。牙周创伤有限元动态分析旨在理解牙周组织在受到快速力学冲击时或周期性载荷下的生物力学响应。早期牙周创伤有限元分析研究多用静态分析，现有研究也有采用准静态分析近似替代，然而，冲击性创伤涉及高速、短时的载荷，其瞬态效应显著，这些都是静态分析和准静态分析无法捕捉的^[36]。牙周组织受运动外伤、意外跌倒等撞击时，即使是短时冲击也可导致牙周膜不可逆性损伤^[4, 37]。动态分析可在瞬态事件中提供更准确的结果。Jayasudha等^[38]发现在创伤性冲击载荷下，有限元分析动态分析会更精确。

在机制研究方面，Zhou等^[39]通过有限元动态分析发现牙周膜在动态载荷下可表现出黏弹性阻尼效应并可调节牙槽骨的应力分布。临床转化方面，Oskui等^[40]发现动态载荷的静态简化分析可降低计算成本，在惯性对组织影响微弱时，可作为一种临床模拟替代方案。

1.4 多尺度建模

牙周创伤是涉及分子、细胞、组织及器官等复杂生物学过程，其宏观临床表现与微观病理变化息息相关^[41]。有限元多尺度建模通过整合分子动力学、细胞行为模型及器官仿真，为解析牙周创伤的物理机制、再生机制及制定临床干预策略提供了先进工具，推动完成模型计算与实验验证的闭

环,最终可实现从“模型预测”到“临床干预”的衔接,其最新进展体现在多模态数据整合^[42-45]。

尽管传统牙周创伤模型在牙周疾病机制研究和新疗法评估方面发挥了重要作用^[46],但其未考虑到细胞组分及血管、神经等结构多相性,无法反映出组织损伤后炎症级联反应和再生过程,而多尺度建模则可考虑到微观结构对宏观组织的影响,可模拟在生理或病理状态下的组织响应^[42]。

多尺度建模数据计算方面,人工智能(artificial intelligence, AI)发挥了重要作用。例如,多模态AI的多模态神经网络整合不同模态的数据与决策,融合成一个模型,表现为协同单一系统^[47]。Bhatia等^[44]通过机器学习(machine learning, ML)优化多尺度建模数据,实现了从量子尺度到宏观尺度的跨层次高效计算。未来研究可强化实验—模型闭环验证体系,推动临床转化应用。

1.5 AI与有限元分析

AI可提升有限元分析计算效率与精度。AI将有限元分析从“工具”升级为“智能决策系统”,核心优势是更快、更准、更自动化。Tundwal等^[48]研究发现传统有限元分析建模流程耗时且依赖专家经验,而AI可显著优化这一过程。AI可为评估个体牙槽骨丧失状况及预测牙周预后提供精准方案^[49],Jundaeng等^[50]发现AI能区分牙槽骨病变不同病理状态,可辅助鉴别组织适应性或病理性变化。此外,AI可根据患者CBCT数据构建临床个性化模型,使得个性化医疗成为可能^[51]。大量研究表明,有限元分析的未来发展方向是AI从CBCT等医学影像数据中进行快速个体化建模、牙周创伤预测,以及通过临床决策支持系统(clinical decision support system, CDSS)等智能诊疗系统辅助医生评估创伤风险、制定治疗方案^[52-54]。

1.6 有限元分析在牙周组织创伤中的临床应用及局限性

1.6.1 临床应用 有限元分析可帮助医生寻找病因、辅助临床决策、优化治疗方案。例如,Chen等^[55]通过有限元分析发现牙槽骨缺损可削弱根尖区骨组织对牙齿的支撑作用,进而可用于评估临床预后、制定修复方案。Akgün等^[56]通过有限元分析量化不同修复材料对牙周组织损伤的风险,模拟出了难以直接观测到的体内复杂解剖部位应力-应变关系,从而明确了病因、确定了治疗方案。

有限元分析可帮助界定临界骨吸收范围、优化手术方案,在预防术后并发症等方面提供量化依

据^[57]。此外,有限元分析还可评估不同防护措施的效果,为器械设计提供量化依据,例如,Doğan等^[58]通过有限元分析模拟牙-牙周膜-骨复合体在外部冲击下的力学响应,验证了定制护口器的物理保护作用,为围麻醉期牙外伤的预防提供了量化依据。

1.6.2 局限性 有限元分析于牙周创伤的主要局限性在于过度依赖牙周组织生物特性假设及将复杂材料属性假设简单化。例如,将牙槽骨视为各向同性材料(实为各向异性)^[59-60],或将牙周膜简化为线性弹性材料,而忽略其黏弹性或非线性特征^[23, 61]。这种简化可导致模拟结果与真实生物学行为存在差异。

有限元分析缺乏测量值的验证方法。临床中,很难从活体中取样进行传统测试,这使得模型验证变得困难。另外,高精度有限元分析依赖先进影像学成像系统,例如,用Micro-CT等进行有限元分析精细化程度会显著提高^[62],但Micro-CT等设备稀少昂贵,很多团队无法使用。此外,现阶段大量医学有限元分析实验只考虑单物理场因素、单条件因素,仅做有限元分析均质化粗糙模型,这会严重影响研究结果的临床适用性。

2 拉曼光谱在牙周组织创伤中的研究与应用

2.1 在牙周组织创伤研究中的优势

临床医学中,拉曼光谱(Raman spectroscopy, RS)已广泛用于疾病筛查、手术指导和疗效评估等方面^[63]。系统医学理念下,RS具备向牙周创伤医学迁移的理论共性。

牙周创伤可导致牙龈撕裂、水肿及炎症,严重者还可造成牙槽骨线性或粉碎性骨折^[4, 64]。相较于传统组织学检查或CBCT等影像学检查,RS更敏感、操作更便捷且避免了辐射风险^[65],利于口腔疾病早期防治。Haider等^[66]研究发现,相较于传统快速尿素酶试验,RS可在5 min内检测到幽门螺旋杆菌(*Helicobacter pylori*, *Hp*)的分子特征,还可同时获取*Hp*代谢活性、耐药性等分子信息。口腔是*Hp*储存库之一,这提示RS具有研究与全身疾病相关的*Hp*等口腔病原体的潜力。此外,在检测含水生物样本时,RS具有水分子干扰小的优势^[67],这使得RS在牙周创伤研究中比傅里叶变换红外光谱(fourier transform infrared spectroscopy, FTIR)、荧光光谱(fluorescence spectroscopy, FS)及太赫兹光谱(terahertz spectroscopy, TS)等更具优势。

综上,RS相较于传统检测方法能更早期发现牙周创伤病变:①RS可检测到牙周组织胶原合成紊乱、矿物质代谢异常等组织结构变化;②RS可识别唾液与龈沟液(gingival crevicular fluid, GCF)中的炎症标志物及病原体RS特征峰;③AI模型辅助诊断实现的。

2.1.1 在牙槽骨状态评估中的应用与优势 RS早已用于早期骨关节炎、骨质疏松症等骨骼疾病的诊断^[68-69]。牙周医学中,RS可监测牙槽骨损伤及修复过程中与骨代谢相关的关键分子变化;可提供牙槽骨羟基磷灰石(hydroxyapatite, HA)等矿物质组分和胶原蛋白等有机基质的分子信息,这使得研究人员能够量化矿物质与有机基质的比率、矿物质结晶度、碳酸盐含量、胶原交联度等与骨骼特性(如H、E和塑性)相关的指标^[70-72]。RS可通过检测异常矿化牙槽骨评估牙槽骨骨代谢状况。例如,Imamura等^[73]通过RS检测低磷酸酯酶症(hypophosphatasia, HPP)患儿乳牙样本时发现牙槽骨异常矿化及牙周膜胶原纤维交联缺陷会导致患儿牙周支持力下降。骨老化方面,Bracher等^[74]发现RS具有检测骨组织有机相(胶原)和无机相(矿物质)结构组成及变化的能力,并证明了这种变化与年龄和性别相关。

RS能无创、实时评估骨再生质量,可用于牙槽骨手术中、术后监测等方面。Gatin团队历经2019至2023年的研究,发现并强调了RS在评估牙槽骨骨质量方面的可行性。2019年,Gatin等^[75]识别了钙磷酸盐化合物的RS峰特征,并应用于牙槽骨样本;2022年,该团队通过追踪术中、术后不同阶段HA(960 cm^{-1})、PPi(725 cm^{-1})、胶原蛋白(酰胺I/Ⅲ峰)等RS特征峰,发现RS可区分不同骨质,确认了RS在口腔重建及再生手术中骨质量活体评估是可行的^[76];2023年,该团队继续研究发现:①RS可区分不同骨再生阶段,通过HA/胶原等指标可间接反映牙槽骨再生质量^[77];②牙周病患者牙槽骨中磷酸盐(inorganic phosphate, Pi)与焦磷酸盐(inorganic pyrophosphate, PPi)的比值显著低于健康者,PPi的RS特征峰与牙周炎进展呈负相关,PPi可作为牙周炎症性骨吸收的生物标志物,动态监测PPi峰值变化可量化牙周治疗后骨矿化程度,利于临床评估^[78]。

2.1.2 在牙周软组织及龈沟液检测中的应用与优势 Hines等^[79]证实,创伤会导致细胞外基质中活性氧等自由基增加。物理损伤会导致牙龈破坏,

伴随胶原纤维断裂^[4],导致自由基变化。RS可捕获此类氧化应激反应中RS特征峰的变化。例如,与牙周组织炎症严重程度显著相关的类胡萝卜素特征谱峰,主要包括位于 $1\,524\text{ cm}^{-1}$ (C=C伸缩振动)和 $1\,156\text{ cm}^{-1}$ (C-C伸缩振动)处的峰^[80-81]。牙周组织炎症会引起胶原合成紊乱及代谢异常。Timchenko等^[82]通过RS发现牙周炎患者与健康者牙周组织的光谱成分存在差异。Liu等^[83]进一步研究发现牙周组织炎症反应会造成胶原纤维定向排列破坏,导致胶原蛋白降解,这使胶原蛋白可作为检测早期牙周炎的生物标志物。

GCF是从牙龈结缔组织渗透到龈沟的液体,炎症早期GCF成分会发生变化,其成分变化可敏感反映牙周组织炎症程度^[84]。表面增强拉曼光谱(surface-enhanced Raman scattering, SERS)是RS的一个重要分支,灵敏度可达单分子水平^[85],可通过检测唾液、GCF中的病原标志物及病原体实现牙周组织炎症的早期发现。Fornasaro等^[86]发现SERS可快速识别GCF中代谢物变化,反映牙周生理或病理状态;Hernández-Cedillo等^[87]通过SERS发现牙周组织炎症患者唾液酸(sialic acid, SA)浓度高于健康者。此外,Nadeem等^[88]发现RS因具有水分子干扰小、适合检测含水生物样本的优势,使其能检测到牙菌斑生物膜等含水生物膜的生化组成。疾病防治方面,RS可整合至疾病早期预警系统。

2.1.3 在牙周病原体鉴定中的应用与优势 RS可实现活体样本细菌原位检测,减少对牙周组织的干扰。例如,SERS可利用等离子体微针阵列快速提取、检测并灭活细菌,并可快速分析分解的病毒成分^[89]。最近,Liu等^[90]研发了一种通过检测组织深层细菌光谱特征快速识别组织感染状态的磁性SERS技术,为指导牙周创伤清创范围、制订个体化抗菌方案提供了支持。此外,通过结合AI的ML算法,RS对牙龈卟啉单胞菌(*Porphyromonas gingivalis*, Pg)、伴放线聚集杆菌(*Aggregatibacter actinomycetemcomitans*, Aa)等病原体鉴别准确率大大提升^[91-92]。

2.1.4 作为连接牙周与全身健康研究工具的优势 大量证据证实,牙周疾病与心血管疾病、糖尿病、银屑病、癌症、妊娠结局及呼吸系统疾病存在关联^[93-94]。RS则可成为研究这个难题的有力工具。例如,Albahri等^[95]通过RS检测到唾液中的致病菌可驱动局部炎症反应并影响全身免疫应答;

Hu等^[96]通过RS对比分析多囊卵巢综合征(polycystic ovary syndrome, PCOS)合并牙周炎患者的血清与唾液样本,揭示了牙周炎与PCOS部分关联机制;这提示RS可用于牙周疾病关联全身疾病的研究。

2.2 拉曼光谱的发展应用于牙周组织创伤的前景

牙周创伤领域,新研发RS技术具有广阔应用前景。Bi等^[97]研发的数字化纳米胶体增强拉曼光谱(digital colloid-enhanced Raman spectroscopy, DCERS)实现了单分子水平、接近泊松噪声极限的检测灵敏度,可极大减弱口腔背景噪声干扰。Ideguchi等^[98]研发的双光频梳相干反斯托克斯拉曼光谱(dual-comb coherent anti-stokes Raman spectroscopy, CARS),通过双光频梳干涉效应实现了微秒级时间分辨的全谱测量,突破了传统RS覆盖范围限制,特别适用于牙周创伤的快速三维层析成像。Ilchenko等^[99]研发的一种面向临床的RS成像技术可实现厘米级组织区域实时可视化、术中分秒级成像,突破了传统RS微观局限,于牙周创伤而言,该技术可实现实时精准术中导航。

2.3 AI与拉曼光谱

RS可提供创伤牙周组织胶原纤维、炎症标志物等分子指纹信息^[83, 87],但面临信号微弱、数据复杂、噪声干扰、解释难度大等问题^[100-101],AI可通过自动化分析,快速处理海量光谱数据,减少人工解读偏差,使RS从数据采集工具升级为智能分析决策系统。生物医学中,通过ML、DL辅助分析至关重要^[102],它们显著提升了RS数据分析效率和疾病识别准确性,尤其在处理大规模数据集和复杂分类任务方面表现出色^[103-104],RS数据维度高、信息冗余,ML及DL能从中提取有效特征信息,构建分类或回归模型实现精确判别。Rathnayake等^[92]通过DL辅助SERS,以高准确度同时识别出了多种牙周病原体。Zhang等^[91]发现将RS与极端随机树(extra trees, ET)相结合,可快速区分Pg、Aa等主要牙周病原体。

此外,Bao等^[105]发现AI模块化连体神经网络可通过多投影层结构分离不同功能模块,使光谱编码器更灵活,可实现不同分辨率光谱联合应用,打破了传统模型对数据一致性的依赖。此外,AI还可通过自动标注和检测,减少因医生疲劳或经验差异等导致的知觉错误,减少主观判断带来的偏差^[106-107]。

2.4 拉曼光谱在牙周组织创伤研究中的局限性

RS存在组织穿透深度有限及信号干扰问题。牙周组织是强散射介质,入射光子在穿通过程中会经历多次散射,导致光能迅速衰减,这使得来自深层组织的RS信号非常微弱,难以有效收集^[108]。

因牙龈和血液等体液对光的散射、吸收干扰,导致RS对牙龈覆盖下的牙周膜及牙槽骨髓腔的信号捕获能力显著下降。在一项多模态技术验证研究中,Fitzgerald等^[109]尽管验证了RS+光学相干层析(optical coherence tomography, OCT)可弥补彼此不足(OCT提供形态学信息,RS提供生化信息),但发现唾液等会干扰RS信号。新兴的尖端增强拉曼光谱(tip-enhanced Raman spectroscopy, TERS)、共振拉曼效应(resonance Raman spectroscopy, RRS)和CARS、受激拉曼散射(stimulated Raman scattering, SRS)等非线性拉曼光谱,显著提高了RS信号强度^[63]。

RS检测结果缺乏验证方法。RS检测结果需结合组织学切片验证其与炎症程度、纤维破坏或骨吸收的对应关系后才能用于治疗决策。RS测得的胶原蛋白降解峰可能与牙龈纤维断裂、慢性溃疡或创伤修复共存,需组织学定位炎症细胞浸润区以确认病理来源^[110],避免光谱干扰导致的假阳性。

3 有限元分析联合拉曼光谱多模态技术在牙周组织创伤中的研究与应用

3.1 基本原理

传统研究方法在解析牙周创伤的物理机制及分子动态监测方面,仍存在显著局限性,而有限元分析、RS与AI组成的多模态技术,提供了全新的研究视角和方法:有限元分析可模拟牙周组织应力—应变力学响应^[9, 62],RS能提供组织成分变化的化学信息^[111-112],两者通过AI驱动,能够实现牙周创伤从宏观物理学行为到微观分子机制的全尺度解析,得到智能化“力学—化学”图谱,可揭示部分牙周创伤机制^[113],能更全面了解患者健康状况^[114],为个性化治疗提供准确临床策略^[9, 111]。

牙周创伤常伴随组织微结构损伤和炎症反应,细胞行为会随牙周微环境的改变而变化,而细胞行为的变化又会反作用于牙周微环境,使其发生改变^[115],RS可实时监测到牙周组织中的胶原降解、HA结晶变化、Pi/PPi异常等病变早期分子变化现象^[78, 83]。这些异常变化会影响有限元分析材料

属性设置。Topol等^[116]、Chen等^[117]发现微观上的胶原纤维重塑会影响宏观上的牙周组织刚度大小。有限元分析可分析、预测发生骨吸收或牙周膜断裂的位置^[118],RS提供的分子变化信息可提升有限元分析建模的生物真实性,AI可自动优化有限元分析模型参数、建模流程及RS数据处理质量^[119],实现结构-功能多维度智能化分析诊断。由此可揭示牙周创伤发生与发展的生物力学-分子化学关联机制,并进一步应用于临床治疗,充分发挥结合AI的医学多模态技术在人类无法感知的跨尺度、跨系统方面的核心优势^[120-121]。

3.2 临床应用场景

临床转化方面,有限元分析联合RS多模态技术可实现牙周创伤个性化治疗方案动态优化、早期诊断与风险预测、术中导航与术后监测。通过RS检测患者牙周组织生化异常,同时用有限元分析模拟其力学后遗症,利用多模态数据融合架构整合多模态数据,通过ML实时优化疾病分期、治疗策略^[122]。

有限元分析个性化建模可根据患者个性化牙周解剖结构及骨密度数据进行构建,可实现对个体患者牙周生物力学行为精准预测^[123],大幅提升治疗精准度并降低并发症发生几率,结合RS、AI实时监测优化个性化治疗^[124-125],可模拟不同治疗对牙周组织的影响。医生可在治疗过程中动态监测组织对治疗的响应,例如炎症消退、组织愈合或骨代谢改善,从而实现治疗方案的实时优化与参数动态调整,实现真正个性化治疗,确保治疗效果最大化、创伤最小化^[126]。

RS能够检测到早期牙周病变在宏观结构损伤显现之前就已存在的微观分子变化^[127]。例如,微观上的胶原结构改变或炎症标志物,RS可在疾病早期进行识别。有限元分析可识别患者易发生损伤的牙周组织薄弱部位与高应力区。将这两种信息结合,可为患者提供更精准的风险预测模型,从而可实施早期干预,在疾病未进展到不可逆阶段之前进行有效干预^[128]。

未来研究可研发AI驱动的有限元分析预测模型联合RS实时反馈的术中导航系统;术后监测方面,该多模态技术可监测治疗后组织生化恢复情况,对于改善患者预后至关重要。

3.3 临床价值及科学意义

有限元分析联合RS多模态技术具有提升诊断精度与效率、加速预后评估、推动个性化医疗发

展、优化医疗资源分配的临床价值,以及推动跨学科方法融合,促进精准医学发展,加速基础研究与临床转化的科学意义(表1)。

3.4 现有研究不足及未来挑战

3.4.1 研究不足 现有研究存在多模态数据融合困难、实时反馈滞后等不足^[129]。Acosta等^[130]研究发现结合AI的医学多模态技术存在不同模态数据格式差异、跨模态特征提取算法兼容性差及计算资源需求不足等问题,严重影响了多模态数据融合。由于受光学时频共轭理论限制,RS需处理分子振动信号的时频转换;而有限元分析依赖物理模型的动态迭代计算^[131],两者数据采集频率和格式差异会导致实时数据融合延迟。针对该问题,Fan等^[132]利用纠缠光子研发的超快受激拉曼光谱,发现了经典光无法比拟的时间-频率尺度。Zhang等^[133]研发的时间-频谱解耦量子飞秒拉曼技术(quantum femtosecond Raman spectroscopy, QFRS),突破了传统时频共轭限制,实现了飞秒级时间分辨率与高光谱精度的同步测量。此外,若要充分发挥AI在牙周疾病中的预测能力,还需要大样本量和复杂的预测因子^[49]。

3.4.2 未来挑战 未来研究需开发更高灵敏度和分辨率的RS技术,开发更完善的有限元分析模型;需推动AI与临床深度融合、优化算法泛化性并拓展跨学科技术整合以实现大规模推广^[134]。研究发现,DL能从结构生物学精细模型中提取信息,在多尺度建模方面有巨大发展空间^[44]。在AI多模态融合方面,需解决注意力机制等算法解释性问题,避免“黑箱”决策^[114]。特别注意的是,在医疗场景下,降低受试者工作特征曲线下面积(area under the curve, AUC)换取100%可解释性,往往是合规的唯一路径。多尺度计算模拟一直是个难题,Bhatia等^[135]研发的一种自适应多尺度模拟新范式能以微观尺度的有效精度实现宏观的长度和时间尺度模拟,可显著提升在宏观尺度上以微观精度进行复杂系统模拟的能力。

此外,多模态技术涉及整合多种数据源,在促进创新的同时也带来了严重的伦理与隐私问题^[136],多模态数据由于模态间相关性,比单模态更易泄露患者隐私。因此,未来研究需系统分析伦理、隐私和安全的权衡机制,关注伦理与数据隐私问题。

表 1 有限元分析联合拉曼光谱多模态技术在牙周组织创伤中的优势、局限性、功能、应用场景

Table 1 Advantages, limitations, functions, and application scenarios of finite element analysis combined with Raman spectroscopy multimodal technology in periodontal trauma

Technical name	Function	Application scenarios	Advantages	Limitations
Finite element analysis	① Physical field simulation	① Trauma mechanism simulation	① Non-invasive detection	① Reduced model error
	② Virtual experiments		② Dynamic simulation capability	② Resource-intensive computation
	③ Mechanism analysis	② Surgical and treatment scenario simulation ③ Physics optimization of treatment devices	③ Multi-physics field integration capability	③ Reliance on experimental verification
Raman spectroscopy	① Molecular recognition	① Mechanism research	① Non-destructive testing	① Signal interference
	② <i>In vivo</i> detection	② Early diagnosis	② High chemical specificity	② Shallow penetration
	③ Pathological quantification	③ Health and prognosis assessment	③ Simultaneous multi-index analysis	③ High equipment cost
	④ Chemical imaging		④ Micrometer-level spatial resolution	
Finite element analysis-Raman spectroscopy multimodal technology	① Trauma mechanism analysis	① Cross-scale pathological analysis	① Cross-scale analytical capability	① Model simplification error
	② Treatment optimization and monitoring	② Precise diagnosis	② Non-invasive dynamic monitoring	② Spatial-Temporal scale differences
	③ Tissue regeneration evaluation	③ Early disease and prognosis monitoring	③ Precise diagnosis support	③ Operational complexity
		④ Personalized treatment plan optimization	④ In-depth mechanism exploration	④ Data fusion barriers

4 小结与展望

在牙周创伤研究中,有限元分析通过物理分析,回答了“力如何导致损伤”;RS通过无创检测早期微观损伤的分子RS特征峰变化,揭示了“损伤的分子表现”。有限元分析引入AI可加速建模、优化参数、智能预测并得到相应的物理场数据;RS引入AI可使数据采集优化、光谱解析智能化并进一步得到分子化学数据;再通过AI驱动的多模态融合系统进行跨尺度数据关联建模。由此,该多模态技术可研究部分牙周创伤机制,并可应用于临床治疗;有望引入系统医学及其他科学的研究应用。

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