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Research Progress on Artificial Intelligence-Driven Development of Oral Biomaterials

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Abstract: Artificial intelligence has penetrated into many aspects of oral biomaterials research. In this paper, the application progress of AI in the research and development of oral biomaterials was reviewed from five aspects : precise oral microbiome analysis, design and optimization of targeted materials, performance prediction and simulation, targeted delivery and intervention, effect evaluation and dynamic regulation. The role of AI in the clinical treatment of oral diseases such as caries, periodontitis, peri-implantitis and root canal infection was also introduced. Through literature analysis, it can be seen that there are problems of technology first and verification lag in this field, and the lack of data standardization, insufficient clinical verification and lagging regulatory framework are three prominent bottlenecks. On this basis, this paper makes a preliminary discussion on the possible direction of the follow-up.

Keywords: Artificial Intelligence; Oral Biomaterials; Machine Learning; Clinical Translation.

1. Introduction

Oral infectious diseases (caries, periodontitis, peri-implantitis, root canal infection) are one of the most common chronic diseases in the world. The main feature is the formation of three-dimensional biofilms on the surface of teeth. The extracellular polymer barrier can make bacteria evade host immunity and reduce the effect of antibiotics [1]. At present, conventional treatment methods such as local or systemic antibiotics and various biological materials cannot effectively break through the biofilm barrier, and are prone to drug resistance, which cannot adapt to the frequently changing pH value and saliva erosion environment in the oral cavity. Researchers are looking for a new generation of biomaterials with selective antibacterial activity, microenvironment responsive release or microbiome regulation function [4,10] to achieve the purpose of precise intervention in microecological imbalance.

After the combination of material science, microbiology and stomatology data, the research and development of biomaterials has changed from repeated trials to data-driven [2]. The above functions of artificial intelligence mainly rely on three types of algorithms : supervised learning for material performance prediction and component optimization, unsupervised learning for microbiome data clustering and anomaly detection, and generative models to complete material microstructure generation and crown restoration shape design [1]. In practical research, these three algorithms are used together to do their own work in different links of the R & D chain [1]. Cheng et al. summarized the application of AI in the development of dental materials into five aspects : from microbiome analysis to effect evaluation, Lam et al. systematically sorted out the application distribution of 407 clinical studies in this field from the perspective of digital dentistry as a whole, so that we can see which aspects of digital dentistry are currently used most, and provide clear information on the direction in which AI can enter next. [23].

The existing research algorithms have made great progress, but there are still some problems : there is no systematic evaluation of the quality of the existing research methodology, the data obtained under laboratory conditions are inconsistent with the situation in the clinical real environment, the model has not been verified, and the lack of supervision has not been discussed substantively [1,2].Material informatics has achieved good results in other fields, but the data base in the direction of oral materials is poor and the cross-modal integration ability is weak [2].

Previous reviews mainly focused on mechanism induction and technical classification. This paper mainly discusses two issues that have not been systematically studied : what is the comparability of existing research methodologies and evidence, and what are the sticking points in the laboratory to clinical transformation. According to these conditions, according to the research progress of AI in oral material design, performance prediction, clinical application and other aspects, it provides a theoretical and practical reference framework for the design and transformation of such materials.

2. Application Progress of AI in Oral Biomaterial R&D

2.1. Application of AI in the Oral Material R&D Process

On the basis of relevant reviews [1,10], Cheng et al. summarized the application of AI in the development of dental materials into five aspects.

2.1.1. Precision Oral Microbiome Analysis

There are two effects of AI on oral microbiome analysis : one is to select microbial targets before design, and the other is to evaluate the effect of materials after use. The composition of oral flora in healthy people and patients is different. AI can use metagenomics, transcriptome, metabolomics and other data to analyze structural differences. Machine learning can quickly find important information from a large number of microbial data, that is, which bacteria are related to caries or periodontitis, and how they are related to each other. These information directly determine the targeted design of biomaterials [1].Taking 16S rRNA sequencing as an example, ML algorithm can distinguish the β diversity of healthy samples and diseased samples after dimensionality reduction and clustering, and find the characteristic strains related to diseases. The same analysis method can also detect whether the flora returns to a healthy state again [1].

2.1.2. Targeted Material Design and Optimization

Traditional material research mainly uses experiments to obtain results, which is time-consuming and costly. This situation has been changed after the emergence of material informatics. Using computational methods and artificial intelligence techniques, researchers can quickly find promising combinations [2]. On this basis, the application of AI can be divided into three levels.

The first layer is the basic performance prediction and monitoring. At present, the ML model is more accurate in predicting the mechanical properties of composite materials, and deep learning can also automatically determine whether the material is degraded [1].

The second layer of micro-functional design is that artificial intelligence can not only predict performance, but also make nanozymes play a more accurate role in oral antibacterial, anti-inflammatory and other aspects through surface modification, doping elements or bionic structure [20]. Zhao et al. [15] obtained that the prediction accuracy of ML model for nucleoside derivative hydrogel was 71 %, and the prediction R2 of bending strength of CAD / CAM composite resin was 0.93 ~ 0.99.

The third direction is from single-objective optimization to multi-objective collaboration. The supervised learning algorithm trained with high-throughput experimental data can establish a mapping relationship between material composition and performance, and quickly screen out millions of candidate formulations in virtual space. In the past, only one indicator was focused on for optimization. Now AI can comprehensively balance the parameters of strength, degradation rate and biocompatibility. This is particularly critical in the design of oral materials, because most clinical scenarios require multiple performance standards at the same time. Reverse design is another way : first set the target performance, and then let the generative model reverse the optimal composition, eliminating a lot of repetitive labor of ' synthesis-test-resynthesis ' [2].

2.1.3. Performance Prediction and Simulation

The influence of material composition change on mechanical properties is often encountered in the research and development process. At present, AI has given some answers. One is to use actual measurement data to train prediction models, such as deep learning models such as LSTM to predict the wear of 3D printed dental resin materials during use [1]. The other is to add artificial intelligence to the simulation analysis, so that the mechanical calculation is closer to the actual situation. After the combination of finite element analysis and artificial intelligence, the personalized dental mechanics simulation has a more reliable basis [11]. Different from the traditional empirical formula, the AI-driven performance prediction does not assume the constitutive equation, but directly finds the relationship between the microstructure of the material and the macroscopic performance from the data : how to arrange the microstructure, and what performance will be shown on the macro level. Such a complex relationship is completely dependent on data-driven, and different neural networks perform different tasks. For example, the convolutional neural network (CNN) can infer the fracture toughness based on the fracture morphology image of the material, and the graph neural network (GNN) can simulate the mechanical signal transmission path between the particles inside the material [1,9].

2.1.4. Targeted Delivery and Intervention

When and where the drug is released is a very important part of the design of the drug delivery system. Artificial intelligence can obtain release kinetic parameters, and can also design a delivery system that responds to external environmental signals. It begins to release in the presence of acid or a specific enzyme [1].Taking intelligent hydrogels as an example, hydrogels designed with artificial intelligence can not only evaluate the severity of periodontitis, but also adjust the amount of drug release according to the evaluation results [1]. Metal-organic framework materials (MOF) have also attracted people 's attention. They can release antibacterial components under pH changes, enzyme effects, redox reactions, or light conditions to achieve the effect of on-demand treatment. [5] Multi-physics simulation combined with artificial intelligence can simulate the behavior of drug release in the oral environment before formal synthesis. Saliva erosion, pH fluctuations, temperature changes, etc., can be taken into account, so that the drug release curve can be optimized to reduce the waste of time and raw materials caused by repeated trial and error. [1] Combine organ chip technology with artificial intelligence. It can provide an in vitro model closer to physiological conditions for drug screening and material evaluation in the oral microenvironment [17].

2.1.5. Efficacy Evaluation and Dynamic Regulation

Artificial intelligence has two effects on effect evaluation and dynamic regulation. The first is to extract useful information from images and clinical data, and the second is to adjust the treatment plan according to useful information [1]. For example, after obtaining the image of the tissue under the prosthesis by optical coherence tomography (OCT), artificial intelligence can be used to quantify the depth of dentin remineralization, and the range of inflammatory cell infiltration can be marked, giving an objective data support to the repair effect. This method can reduce the difference in evaluation results between different doctors and facilitate long-term follow-up observation of material properties [1].

2.2. Clinical Application of AI in Treating Oral Diseases

The five functions of AI R & D stage will finally be implemented in specific disease treatment scenarios. Here are several aspects to introduce its application.

2.2.1. Application in Oral Infectious Diseases

The methods of AI-driven biomaterials used in different pathological conditions are different [1]. For caries, artificial intelligence is used to assist in the design of enamel biomimetic membranes. Antibacterial materials are mainly designed to play a role in Streptococcus mutans biofilms. The antibacterial effect in vitro is much better than traditional materials. In the treatment of periodontitis, the use of AI-assisted local delivery systems and microbiome-regulated hydrogels can inhibit Porphyromonas gingivalis and promote symbiotic bacterial colonization [4]. Choi et al. [4] divided this kind of material into four categories : probiotic delivery platform, metal ion release hydrogel, antibacterial / antioxidant material, and enamel bionic membrane. From animal experiments, it can be seen that artificial intelligence is used to assist design is a new direction to be studied in this field. Due to the different treatment methods of peri-implantitis, artificial intelligence is more used in surface engineering, and micro-nano structures are used to regulate the host immune response. The AI-optimized root canal irrigation and disinfection scheme for root canal infection is still under exploration [1].

2.2.2. Progress in Prosthodontics

In 2015, Cheng et al. used BP neural network to predict the changes of soft tissue after complete denture restoration [19]. Sun et al. developed MeshSegNet software in 2022, using the method of preset template and adaptive deformation to realize the intelligent matching of complete denture [13].After that, the research team sorted out the overall workflow of data intelligent complete denture [18]. In 2023, Revilla-León et al. summarized 36 articles from 1985 to 2021, and concluded that artificial intelligence is feasible for tooth color selection, automatic restoration design, edge line detection and RPD design. [7] In the same year, Urkande et al. conducted exploratory research on the application of image analysis, treatment simulation and prognosis prediction in cast post-core repair, but there is no empirical support [22]. In 2026, the research focus of AI in prosthodontics is further focused on the automatic design of crowns. According to the Meta-analysis of Holiel et al. (17 studies, 13 quantitative synthesis), it is concluded that the shape accuracy and internal fit of crowns designed by artificial intelligence are not significantly different from those of traditional CAD, but the design time is reduced by 25 % -50 %, and the edge accuracy is greatly improved (SMD = -1.00) [3]. The deep learning single crown design has morphological and temporal advantages, but Lemos et al. think that most of the evidence comes from in vitro experiments. [21]At the same time, Ma et al. summarized the current status of generative AI in the fields of prosthodontics, orthodontics, radiology, and oral education. They believed that GAN and diffusion models can be used for crown design, tooth arrangement, and three-dimensional reconstruction, and have the potential to become an important direction for clinical applications. However, there are still problems such as lack of verification and lack of standardized data sets [6].Lam et al. sorted 407 articles on clinical research according to prevention and treatment, including 127 articles on prosthodontics and 112 articles on maxillofacial surgery. It provides a macro reference for understanding the impact of artificial intelligence technology on the field of prosthetics [23].

2.2.3. Applications in Oral and Maxillofacial Surgery and Bone Regeneration

The reconstruction of tissue defects in oral and maxillofacial surgery is more complicated than that in prosthodontics. Du et al. constructed a set of preoperative three-dimensional visualization technology system with multimodal data fusion. Under this framework, they have done a lot of intelligent tools, including automatic tumor segmentation and classification, automatic generation of jaw reconstruction scheme, postoperative appearance prediction, prognosis prediction of salivary gland cancer, etc., basically stringing up the preoperative, intraoperative and postoperative stages [14]. In the direction of bone regeneration, Zhou Yongsheng and others put 4D printing technology and AI-driven design and manufacturing platform together to make a bone repair scaffold, whose shape and function can be dynamically adjusted as needed. [16]. Regarding injectable hydrogels, Sakhrani et al. have tried to design patient-specific scaffolds using AI combined with computational modeling, but it is mainly methodological exploration, and there is still a distance from clinical application [12].

2.3. Key Issues in Current Research

An obvious feature of artificial intelligence in the field of oral biomaterials is that technology advances faster than clinical verification. The following aspects are discussed from the aspects of literature type, research focus, methodological basis and clinical transformation evidence.

Literature type and evidence level. At present, the most extensive coverage is the review of Cheng et al. They screened 99 articles from three databases and systematically reviewed the application of AI in oral material development and clinical treatment [1]. Although the scope review of Lam et al. includes 407 articles, it mainly focuses on the overall situation of digital dentistry, and the analysis in the cross direction of AI and material research and development is relatively limited. [23] Most of the other related reviews [2,6,8] are narrative reviews, which do not clearly explain the retrieval strategy, nor do they conduct bias risk assessment, and the overall level of evidence is low.

The differentiation of research focus. There are obvious differences in the focus of different literatures. Cheng et al. mainly focused on the technical application of AI in the entire material development chain [1]. Yamaguchi et al. take material informatics itself as the analysis object, and believe that insufficient data volume is the main obstacle to AI landing. [2]. Ma et al. focused on the application of generative AI in various branches of the oral cavity [6]. A direct consequence of this differentiation is that the evaluation indicators used in each study are not uniform, some look at the physical and chemical properties, some measure the antibacterial activity in vitro, and some use animal models to observe the degree of inflammation improvement. It is difficult to compare directly between studies [1, 2].

Methodological basis. Most AI models lack interpretability. In other words, it is often unclear why the model recommends a formula and what to make decisions based on. If this problem is not solved, it is difficult for clinicians and regulators to trust the results given by AI [2]. In addition, the algorithms used in different studies are also very different (machine learning, deep learning, genetic algorithm). The sample size varies from dozens to thousands, and most of them are based on single-center, retrospective data. Once the model is placed in a multi-center, multi-device, multi-crowd scenario, whether it can maintain stability has not been systematically tested [1].

Clinical transformation evidence. There are not many studies that really promote AI-optimized materials to the patient level for effect evaluation. Most of the work remains in the stage of computer simulation or in vitro experiments. The phrase " many papers, not many clinical " can roughly summarize the current situation [1,2,23].

In addition to the above limitations, the research of AI-driven oral biomaterials also faces three key bottlenecks.

Data bottleneck. A prominent problem is the lack of standard database. Although there are many research data on dental materials, the format, test methods, and evaluation indicators are not uniform, and it is difficult to directly use them for model training or cross-laboratory integration [2]. Multimodal fusion is not sufficient, and the information of microbial composition, immune status, and mechanical environment in the oral microenvironment is still relatively dispersed, and has not been effectively integrated into the AI-driven material design process [1].

Verify the bottleneck. The reliability of AI model in real clinical environment has not been fully verified. Most of the studies are based on single-center, retrospective data. Whether the model can maintain stable performance after replacing the equipment or the study population is still a lack of systematic testing. Taking AI crown design as an example, Holiel et al. pointed out that most of the evidence comes from in vitro experiments or computer simulations, and prospective clinical verification and long-term follow-up are insufficient [3]. The long-term performance of smart closed-loop materials in complex oral environments - such as degradation product toxicity, chronic inflammatory response, and long-term failure modes - also lacks systematic data [5,12]. In addition, most of the studies did not disclose the code and training data, resulting in the results could not be reproduced, which directly reflected the existence of the " reproducibility crisis " in the field of AI in the direction of oral materials.

Regulatory bottleneck. There are no registration guidelines or approval procedures for AI-driven biomaterials worldwide. The decision-making basis of AI recommendation scheme is often difficult to trace, and there is a certain mismatch between it and the current medical device evaluation system based on deterministic knowledge, so the evaluation promotion faces great resistance [2]. At the same time, there is also a lack of effective interdisciplinary collaboration framework and standardized data sharing platform among material scientists, AI engineers and clinicians [1].

3. Conclusion and Outlook

Based on the systematic review of Cheng et al., this paper mainly supplements from two aspects : one is to sort out the shortcomings of the existing literature in methodology and clinical evidence, and the other is to summarize the three key bottlenecks of data, verification and supervision. On the whole, the technology advancement in this field is faster than clinical verification. The inconsistent data standards, insufficient verification evidence, and imperfect regulatory framework are the current prominent problems.

In order to solve the above problems, we may need to work together in the following directions. At the data level, the construction of standardized databases and the unification of data formats are the basic conditions for improving cross-study comparability. At the verification level, the transition from in vitro research to multi-center prospective clinical trials is a necessary path to obtain higher-level clinical evidence. For regulation, AI-driven biomaterials review systems also need to keep pace with technological developments.

In terms of the overall development stage, AI-driven oral biomaterials are still in the transition period from concept verification to clinical application. It is still difficult to achieve large-scale clinical application and promotion in the short term, but this is only phased. With the gradual establishment of the data base, the continuous accumulation of clinical evidence and the continuous improvement of the regulatory system, it is expected that the field will gradually enter routine clinical use in the next five to ten years.

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