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The Role of Inorganic Trace Elements on Hard Dental Structures in the Context of Mineralization

PhD Thesis Abstract

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CONTENTS

Contents 1

List of Published Works 4

Abbreviations 5

List of Figures 6

List of Tables 8

Acknowledgments 9

Introduction 10

Motivation for Choosing the Topic 10

Importance and Relevance of the Topic 11

Framing the Topic within International, National, and Regional Concerns 12

Scientific Objectives for Resolution within the Research 13

Specific Objectives of this Research: 14

Summary Comments on the Research Methodology and Approach 14

Highlighting the Interdisciplinary Nature of the PhD Thesis 15

1. Macroscopic and Microscopic Structure of Hard Dental Tissues in the Context of Mineralization 17

1.1. Macroscopic Structure of Hard Dental Tissues 17

1.1.1. Enamel 17

- 1.1.3. Pulp Chamber and Root Canal 20
- 1.2. Microscopic Structure of Hard Dental Tissues 21

1.2.1. Enamel 21

1.2.2. Dentin 23

1.3. Specifics of the Chemical Composition of Hard Dental Structures 25

1.3.1. Enamel 25

1.3.2. Dentin 26

1.3.3. Mineralization versus Demineralization of Teeth 28

1.3.4. Remineralization of Root Canals Using Filling Materials 29

2. Natural and Synthetic Compounds Involved in the Mineralization of Hard Dental Tissues 32

2.1. Dietary Supplements Involved in the Mineralization of Hard Dental Tissues 32

2.2. Prescription and Over-the-Counter Drugs Rich in Calcium, Magnesium, and Phosphorus 33

2.3. Oral Hygiene Products with Plant Extracts or Synthetic Components Involved in the Mineralization of Hard Dental Tissues 34

2.4. Topical and Internal Fluoridation Products Involved in the Mineralization of Hard Dental Tissues 36

2.5. Filling Materials Rich in Bioelements Involved in the Mineralization of Hard Dental Tissues37

- 3. Techniques for Characterizing Hard Dental Structures 39
- 3.1. Scanning Electron Microscopy (SEM) and X-ray Diffraction (XRD) 39
- 3.2. Finite Element Model (FEM) of Teeth 40
- 4. Hypotheses, Aims, and Objectives of the Research 42
- 5. General Research Methodology 44
- 5.1. Scanning Electron Microscopy and Finite Element Model 44
- 5.2. Preparation of Metallographic Samples 45
- 5.2.1. Surface Preparation 45
- 5.2.2. Chemical Etching 51

6. Study 1. Research on the Variability of Chemical Composition by SEM Analysis of a Set of Teeth from a Population in the Bucharest Area 58

- 6.1. Introduction 58
- 6.2. Material and Method 60
- 6.2.1. Chemical Determination in Teeth Using SEM Microscopy 60
- 6.3. Results 60

6.4. Discussions 65

6.5. Conclusions 67

7. Study 2. FEM Modeling of Tooth Behavior Based on the State of Mineralization 68

7.1. Introduction 68

7.2. Material and Method 69

7.2.1. Finite Element Modeling of the Behavior of a Normal Tooth Compared to a Mineralized One 69

7.3. Results 71

7.4. Discussions 76

7.5. Conclusions 78

8. Study 3. Analysis of Bioactive Element Concentrations at the Dentin-Sealer Interface of Bioceramic 79

- 8.1. Introduction 79
- 8.2. Material and Method 80
- 8.3. Results 83
- 8.4. Discussions 95
- 8.5. Conclusions 97
- 9. Final Discussions 98

10. General Conclusions, Original Aspects, and Future Research Directions 107

Bibliography 110

The issue of mineralization of hard structures in the human body in the context of variations in their chemical elements depending on age is a topic of intense concern in contemporary medicine and pharmacy. Currently, the pharmaceutical market offers a wide range of dietary supplements containing various chemical elements predominantly found in bone structures. Since teeth also represent such structures and are more accessible for study, the mineralization of dental hard structures has been an important subject of research and discussion over time due to its influence on the functioning of the entire human system. In practice, various dietary supplements are available today to improve the mineral concentration in bones. However, less research has been conducted on the chemical composition of teeth and how these mineral concentrations influence their behavior.

The choice of this research topic was also motivated by the imperative need to better understand the relationship between filling materials and their impact on dental structures, especially in the context of mineralization. It has been observed that while many filling materials are effective in sealing the root space, their long-term effects on dental health can vary significantly, and some materials may even inhibit natural regeneration processes.

Hypotheses, Goals and Research Objectives

The primary goal of this doctoral thesis is to analyze and characterize dental structures in the context of mineralization processes and pharmacodynamic interactions. The research focuses on elucidating how filling materials can influence the natural processes of remineralization and regeneration of dental tissues, both at the coronal and root levels.

Specific Objectives:

1. Evaluate the chemical composition of hard dental structures: dentin and enamel.

2. Describe the structural and mineralogical changes in enamel and dentin when they come into contact with saliva.

3. Analyse the concentrations of bioactive elements (Ca, Na, Mg, P, etc.) in dentin at the interface with root sealing material as a bioceramic sealant in the context of remineralisation.

General Research Methodology

The research methodology involved the structural analysis of teeth using Scanning Electron Microscopy (SEM), Finite Element Modeling (FEM), and chemical etching through electrolytic polishing. SEM is an advanced imaging technique that uses a beam of electrons to produce highresolution images of specimen surfaces.

FEM is a numerical method used to analyze the mechanical and structural behavior of teeth under various loading conditions. FEM involves creating detailed three-dimensional models of teeth, based on medical imaging such as CT scans. These models allow for simulation and evaluation of stress and deformation distribution in dental structures, providing a deeper understanding of how teeth react to masticatory forces and other stresses.

Study 1: Research on the Variability of Chemical Composition Through SEM Analysis in a Set of Teeth from a Population in the Bucharest Area

The purpose of this study was to evaluate the chemical composition of hard dental structures: dentin and enamel.

Material and Method

The chemical determination in teeth was performed using SEM microscopy in the enamel and dentin areas for 32 teeth randomly selected from patients in the Bucharest area. The selection criterion was age.

Results

A sample from a 50-year-old patient is presented in Figure 1. In Zone 1, a significant crack can be observed on the left side, while on the right side, in Zone 2, a well-defined inclusion can be seen. Additionally, the interface between dentin and enamel is very well defined. The zones where the chemical compositions are determined are clean and specific to them.

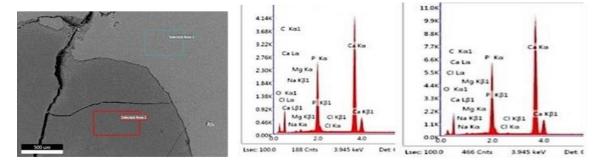


Figure 1. Chemical Analysis of a Tooth from a 50-Year-Old Patient

Discussions

For interpreting the results provided by SEM analysis, the chemical compositions of the 32 analyzed samples were determined, and the volumetric percentages of carbon, oxygen, phosphorus, magnesium, calcium, and silicon were recorded. Figure 2 shows the variation of these components in dentin based on the age of the patients from whom the teeth were collected. A closer evaluation shows a correlation between them depending on age, all having a certain characteristic with one exception. Around the age of 40, with the exception of the carbon content, all other chemical elements reach a minimum value. The variation graph of the carbon percentage (dark blue) reaches a maximum value at this age. The oxygen percentage has the highest values compared to the other chemical elements and shows a minimum around the age of 40. The variation of the calcium percentage shows a minimum content around the age of 40 (green line), with a maximum around the age of 23. The third chemical element studied is phosphorus, which shows a maximum value around the age of 23, followed by a minimum value at approximately 40 years of age. This element also shows the same variation as the other two. The fourth chemical element, carbon, shows a completely different variation compared to the other elements. Over time, different variations have been recorded, but the maximum value is also around the age of 40. An interesting fact is the cycle of maximum and minimum values of carbon. The maximum values are approximately at 24, 34, 43, 54 years, and the minimum within these periods. Sodium content (gray color) shows a relatively uniform variation, without excessive maxima and minima, but as observed with the previous elements, the minimum value is also around the age of 40, while the maximum is around the age of 35-38. The last chemical element recorded is magnesium (yellow line). As with sodium, its variation is relatively constant, with the lowest value starting from the age of 40 towards 50 years. The maximum is also found around the age of 25.

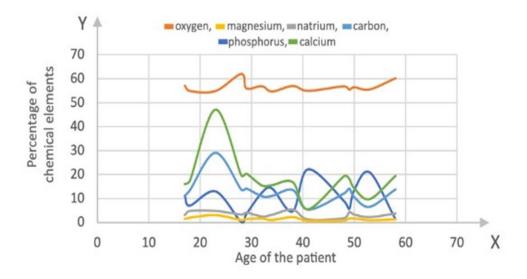


Figure 2. Variation of Chemical Composition in Dentin.

In the case of enamel, the variation of chemical elements according to age is much better defined and distinct (Figure 3). As in the case of dentin, the oxygen content is the highest compared to the other chemical elements. Its minimum is clearly at the age of 40. The second chemical element is calcium, which shows a cyclic variation with clear maximum and minimum values, but not cyclic. Around the age of 40 (green line), a very pronounced value is recorded, as in the previous variation. The phosphorus content in enamel (light blue) is relatively constant, but with a clear minimum value around the age of 40. For the same reason, the variation of sodium in dentin, in enamel, has a relatively uniform variation (gray color). A very similar and uniform variation is also observed for magnesium, represented by the yellow color. The minimum value is also observable for this age. As in the case of the chemical analysis in the dentin structure and in the enamel case, the carbon content reaches a maximum value around the age of 40. Moreover, this chemical element has a behavior exactly opposite to the others (dark blue).

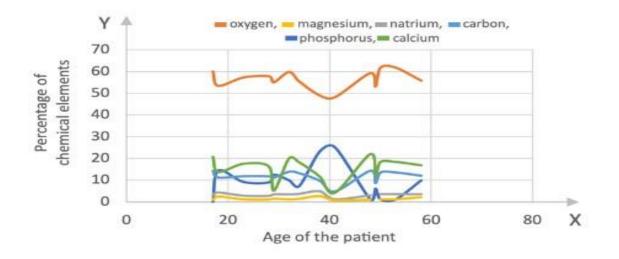


Figure 3. Variation of Chemical Composition in Enamel.

Conclusions:

This research initially aimed to find interdependencies of the chemical elements that are part of dentin and enamel of randomly selected teeth based on their age. The existence of this condition among the selected population living around Bucharest is not yet established at this time. Using SEM microscopy, the chemical compositions of oxygen, carbon, magnesium, silicon, phosphorus, and calcium were determined in well-defined and representative areas of dentin and enamel. Corresponding graphs were drawn for the two areas of the tooth, and it was observed that, except for carbon, the other elements have minimum values around the age of 40. On the other hand, carbon shows a maximum value at this age. In this regard, we consider that the research can continue by introducing and interpreting other variables, but which would involve a much larger number of tooth samples.

Study 2: FEM Modeling of Tooth Behavior Based on Mineralization State

The purpose of this study is to characterize the structural and mineralogical changes in enamel and dentin in contact with saliva.

The research method was finite element analysis of the behavior of a normal tooth compared to a mineralized one. The meshing was done using the ANSYS program with the SOLID187 discretization element, which provides output data on the displacements of the structure under the application of a force and the stress state that develops in the body as a result of the application of a force system.

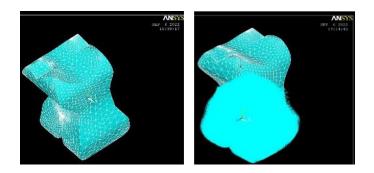


Figure 4. Meshed Tooth Volume; b - Input Data of the Model: Force F and Presentation of Displacement

Results

This study was conducted considering several variables, the first variable being the degree of mineralization of the tooth, the second variable being the value of the forces applied to the tooth surface during the chewing process. In all four situations, the tooth undergoes movements of the order of hundredths of a millimeter, observing that:

- In the case of applying the force F2, the displacements are larger for both types of teeth.

- In the case of mineralization, the calculated displacements are smaller than in the case of a normal tooth.

The second category of results refers to the stress map that appears in the tooth structure. In the theory of material resistance, the stress state cannot be defined using a single criterion, so to obtain a complete picture of the integrity of a structure, several types of stress must be analyzed, such as those corresponding to the OX, OY, OZ axes, shear stresses in the XOY, XOZ, and YOX planes, as well as stresses of the S1, S2, and S3 types, which describe the predominant tensile stress state, the balanced stress state between extension and compression, and the compression stresses.

Stress States that Appear in a Mineralized Tooth When a Concentrated Force F2= 190 N is Applied.

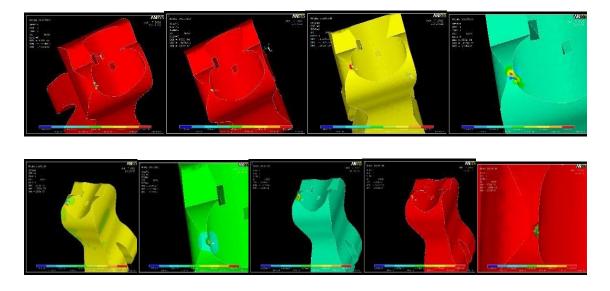


Figure 5. Type of Stress: a - Sx, b - Sy, c - Sz, d - Sxy, e - Syx, f - S1, g - S2, h - S3 at F=190 N for a Normal Tooth

Discussions

The mineralization process contributes to changing the properties of bones or teeth in the human body. In addition to other benefits that are exclusively part of the medical field, engineering can study what happens to bone structures that undergo such beneficial changes. Teeth have a relatively similar structure.

Conclusions

In general, the stresses corresponding to the mineralized tooth (TM) are lower than those in a normal tooth. The smallest stresses are the shear stresses in the XOZ plane, meaning that tooth rotation in this plane cannot produce significant effects. In conclusion, it can be said that the mineralization process is beneficial for the tooth structure, with its resistance being particularly evident under larger, potentially critical forces that may occur during mastication.

Study 3: Analysis of Bioactive Element Concentrations at the Dentin Interface with Bioceramic Sealer

The aim of this study was to evaluate the bioactivity of AH Plus Bioceramic Sealer (Dentsply, Konstanz, Germany) by analyzing the concentrations of bioactive elements in dentin at the interface with the bioceramic sealer.

Material and Method: A total of 110 incisors (upper and lower) with mature apices and a single canal, extracted for periodontal reasons, were selected. The teeth were ultrasonically

cleaned of all debris and stored in a 0.1% thymol solution for 3 hours. The incisors were decoronated by sectioning 1 mm above the enamel-cement junction, access cavities were created, working length was determined with a manual K ISO number 10 instrument (Dentsply/Sirona, Switzerland), and then prepared with the Trunatomy system (Dentsply/Sirona, Switzerland) to a foraminal diameter of 0.25 or 0.35, depending on the case.

Results

SEM images allow detailed observation of how the endodontic sealer interacts with dentin (Figure 7).

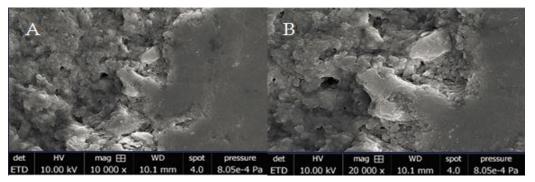


Figure 7. SEM Images of the Sealer/Dentin Interface, Indicating a Mineral Infiltration Zone at the Interface Between Dentin and the Bioceramic Sealer, Highlighting the Sealer Tags, at Magnifications of A. 10,000X and B. 20,000X.

To interpret the results provided by SEM analysis, the chemical compositions of the analyzed samples were determined in the dentin immediately adjacent to the interface with the endodontic sealer, as well as in the peripheral dentin. For this purpose, mass and volumetric percentages of carbon, oxygen, phosphorus, magnesium, calcium, and silicon were recorded:

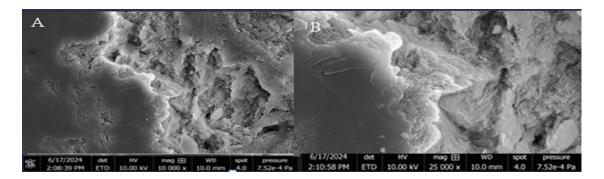
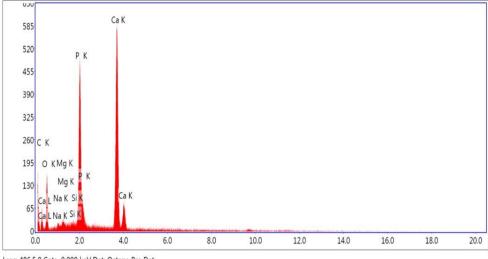


Figure 8. SEM/EDS Analysis of the Interface Between AH Plus Bioceramic Sealer and Root Dentin Showing Precipitation with Chemical Elements: Ca, Si, P, C at Magnifications of A. 10,000X and B. 25,000X.

Table 1 and Figure 9 describe the elemental composition of a sectioned sample from an upper incisor, linked to the SEM images of the interface between dentin and the bioceramic sealer (Zone 1). The dataset shows a composition rich in oxygen, phosphorus, and calcium, indicating a strong presence of phosphate compounds such as hydroxyapatite.

Element	Weight %	Atomic %	Net Int.	Error %	Kratio
СК	5.46	9.59	0.34	36.45	0.01
ОК	43.96	57.93	4.55	12.14	0.06
NaK	4.89	4.49	1.35	15.33	0.01
MgK	3.37	2.92	1.82	13.72	0.01
SiK	1.02	0.77	1.12	19.95	0.01
РK	16.62	11.32	19.69	5.93	0.10
CaK	24.68	12.98	28.09	3.27	0.21

Table 1: Chemical Analysis of an Upper Incisor for Selected Zone 1



Lsec: 486.5 0 Cnts 0.000 keV Det: Octane Pro Det

Figure 9. Chemical Analysis of an Upper Incisor for Selected Zone 1

Discussions

In this study, the concentration of calcium ions was higher at the interface with the bioceramic sealer than in the peripheral dentin. This can be explained by the fact that the calcium silicate in bioceramic sealers reacts with dentinal fluids to form calcium hydroxide. This transforms into hydroxyapatite, a naturally occurring calcium apatite mineral in dental tissues. Hydroxyapatite binds the sealer to the dentin walls, strengthening the seal and remineralizing the dentin. Additionally, calcium ions help periapical tissues heal by differentiating and proliferating odontoblast-like cells, which can contribute to the regeneration of periapical tissues.

Conclusions

Using Energy Dispersive X-ray Spectroscopy (EDX) analyses, we can understand the elemental compositions of the dentin interface and endodontic bioceramic sealers, evaluate their biological characteristics, and analyze the impact of their elements. Bioceramic sealers have revolutionized endodontic therapy due to their intrinsic bioactive properties, which facilitate effective interactions at the sealer-dentin interface. Additionally, they demonstrate significant bioactivity through their dynamic interaction with dentin at the root canal level. The bioactive capacity of bioceramic sealers enhances the durability and efficacy of endodontic treatments, promoting long-term success.

Final Discussions

In our research, SEM analysis allowed for the detailed identification of microstructural and chemical variability in enamel and dentin. It was observed that elements such as calcium and phosphorus, essential for the hardness and strength of teeth, show significant fluctuations in concentration. This variability can be correlated with metabolic and hormonal changes that occur with aging, thus affecting the mineralization and demineralization processes of teeth. Furthermore, the study highlighted that external factors such as diet, oral hygiene, and fluoride exposure can significantly influence the chemical composition of teeth. For example, a diet rich in sugars and acids can accelerate the demineralization process, while regular use of fluoride-containing oral hygiene products can support remineralization. These findings emphasize the importance of constant monitoring and appropriate dental care to maintain optimal dental health in the long term.

It is important to note that in the case of a mineralized tooth, its displacements are smaller, while the mechanical stress state, if the applied force is the greatest, is lower than in the case of a normal tooth. From the perspective of mechanical stress, it can be said that the mineralization

process of a tooth has a noticeable effect when the tooth is subjected to more difficult functional situations, which is an important benefit.

The differences in displacement and resistance capacity of mineralized versus nonmineralized teeth underline the importance of maintaining an adequate level of mineralization to prevent fractures and other dental injuries. These findings are consistent with the results of other studies that have used FEM to evaluate the impact of mineralization on teeth.

Regarding the use of bioactive materials for root canal obturation, our study aligns with research highlighting the potential of bioceramics and bioactive composites in stimulating remineralization and tissue regeneration processes. These materials not only provide an effective seal of root canals but also support natural healing processes, thereby reducing the risk of post-treatment complications.

GENERAL CONCLUSIONS OF THE RESEARCH

The studies conducted in this research highlight the following general conclusions:

- The percentage of CARBON reaches a maximum value at the age of 40.

- The percentage of OXYGEN has the highest values compared to the other chemical elements, with a minimum around the age of 40.

- The variation in the percentage of CALCIUM shows a minimum content around the age of 40 and a maximum content around the age of 23.

- PHOSPHORUS shows a maximum value around the age of 23, followed by a minimum value around the age of 40.

- SODIUM presents a relatively uniform variation, without excessive maxima and minima, but the minimum value is also around the age of 40, while the maximum is around the age of 35-38.

- MAGNESIUM shows a relatively constant variation, with the lowest value starting from the age of 40 towards 50 years. The maximum is also found around the age of 25.

- Around the age of 40, except for the carbon content, all other chemical elements reach a minimum value.

- The stress values that appear in the tooth structure are close to the values of the Young's modulus of dentin and are slightly lower than the elastic modulus of enamel.

- Stress arises as a result of the application of a masticatory force, but if this force is exceeded during mastication, the stresses will increase and may even exceed the elastic moduli of dentin and enamel, leading to cracks or even fractures in the tooth structure.

- The mineralization process is beneficial for the tooth structure, with its resistance being particularly observed under larger, potentially critical forces that may occur during mastication.

- The average concentrations of elements in dentin located immediately adjacent to the interface with the bioceramic sealer were: C (6%), O (43%), Na (5%), Mg (4%), Si (2%), P (19%) and Ca (25%).

- The average concentrations of elements in peripheral dentin were: C (25%), O (30%), Na (2%), Mg (1%), Si (1%), P (13%) and Ca (20%).

- Bioceramic sealers facilitate effective interactions at the interface between sealer and dentin,

Original Aspects:

- Analysis of the Variability in the Chemical Composition of Teeth Using SEM. The use of Scanning Electron Microscopy (SEM) to study the variability in the chemical composition of teeth based on age and exposure to various environmental factors is an original aspect of this thesis. The study highlighted significant fluctuations in the concentration of essential elements such as calcium and phosphorus, providing a new perspective on the impact of aging and external factors on dental health.

- FEM Modeling of Tooth Behavior Based on Mineralization. Applying Finite Element Modeling (FEM) to evaluate the mechanical behavior of teeth based on their degree of mineralization represents an original contribution. This study demonstrated significant differences in the displacement and resistance of mineralized teeth compared to non-mineralized ones, underscoring the importance of adequate mineralization for the prevention of dental injuries.

- Analysis of Bioactive Element Concentrations at the Dentin Interface for Investigating the Potential of Bioactive Filling Materials. The analysis of bioactive element concentrations at the dentin interface to explore the potential of bioactive materials, such as bioceramics (bioceramic sealer), in promoting remineralization and regeneration of root canals is another original aspect of the thesis. The study showed that these materials not only efficiently seal root canals but also stimulate natural processes of mineralization and healing, offering innovative solutions for endodontic treatments.

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