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APPLICATION OF OPEN SOURCE SOFTWARE FOR CREATING THREE-DIMENSIONAL DENTAL MODELS, MATHEMATICAL CALCULATING THE MASS PROPERTIES OF GOLD, ZIRCONIUM AND TITANIUM AND FINANCIAL IMPACT ON THE HEALTH CARE SYSTEM

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Abstract Dentistry, associated with the construction of crowns, bridges and other structures, accompanies many people. It is often necessary to use quality materials that are compatible with living tissue and have the necessary biocompatibility. These are gold (Au), zirconium (Zr) and titanium (Ti), as well as the titanium alloy Ti6Al4V. They are the basis for acquiring a healthy dental restoration when a tooth or teeth are already missing, or the existing ones are compromised and non-functional. Restoration of the dentition is associated with certain financial burdens, which have specific costs of dentistry, materials, labor and more. This report covers the stage of creating the basic digital three-dimensional geometry of dental models through open source software. Methods for generating 3D geometry by scripting and specialized add-ons in the Blender software environment are presented. The mass properties of the applicable dental materials have been calculated mathematically, as well as the financial impact on budgeting has been calculated. The results of the study are directly applicable and cover a large segment of modern healthcare, such as dentistry.

Keywords: Open source software; 3D; mass properties; financial impact; health care.

1. INTRODUCTION

Dental healthcare is a significant subdivision of the Health Care system [1-3]. It takes a long time to build specialists, dentists, dental technicians and assistants [4-6]. It is no longer enough to study only conventional methods of dentistry in specialized institutes, universities and dental centers. It is necessary to build specialists working well with modern design technologies, including conventional and specialized software for designing 3D geometry, working with additive technologies, 3D printers and scanners, CNC machines and others [7-9]. Combined with the knowledge of human physics and methods of treatment, it can be said that the current generation of dental professionals have interdisciplinary knowledge and skills [10-12]. Of course, the most important thing for the dentist is to be able to accurately and with high quality carry out his usual dental activities with the materials provided to him by the dental technician and/or the assistant.

This report focuses on the following main areas:

• Overview of the leading 3D modeling software products and applications with simulation and mathematical calculation capabilities.

• Creating three-dimensional geometry of dental models / structures using open source software, through conventional 3D design and direct scripting.

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• Obtaining accurate mathematical values by computer calculation of the volume of the threedimensional dental models.

• Calculation of the mass of the materials: gold (Au), zirconium (Zr), titanium and titanium alloy Ti6Al4V.

The main goal of the study is to build a strategy for predicting the cost of expensive materials such as gold and others that are applicable in dental dentistry at the level of the digital design. This in turn optimizes the whole vision of calculating dentistry, where competent clarity can be justified for all parties involved (dentist, dental technicians, patients, etc.). The in-depth analysis of each detail in the design process guarantees a good strategy along the entire production line. At first glance, models of relatively small size are being studied, but globally it is a colossal industry, where the production of dental components is in millions of pieces. The research experience will enable all stakeholders to get acquainted in detail with the process of precise design of dental models in a computer environment.

2. MATERIALS AND METHODS

2.1. Materials

In order to create a real dental model (crowns, dental structures, etc.), it is necessary to anticipate what material base is needed. Modern dentistry is unthinkable without the integration of modern technologies [13-15]. It is important that these are available:

• Computer systems with correspondingly good hardware and software characteristics;

• Additive technologies and machines, including 3D printers and scanners, CNC machines, kilns for firing materials (eg zirconium) and others;

Deep knowledge of biocompatible materials is also required [16]. To date, materials such as gold, zirconium and titanium (as well as their alloys) have been shown to be the best choice for making dental models that possess the required biocompatible properties [17-19]. This is of great importance for maintaining oral hygiene and hence to maintain good health. It is known that some of the metals used in dental dentistry not only do not help, but cause serious and irreparable damage to health through the release of metal micro particles in patients' bodies [20]. This problem needs to be thoroughly researched and presented to the public. It is inadmissible to neglect the mass process of placing metals with poor biocompatible characteristics in the biological organism [21].

The research in this report focuses on the following important materials:

• Gold and zirconium (mainly for making dental crowns) [22-26];

• Titanium and titanium alloy Ti6Al4V (mainly for the production of dental implants, with Ti6Al4V being a priority) [27].

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2.2. Methods

The research is focused on the leading initial stage of creating three-dimensional digital geometry. Optimizing the design process of dental models is absolutely necessary [28]. This requires the creation of an entirely new methodology, covering in detail each important stage of design in a computer environment. It contains the stages of obtaining data from the study of the problem of the clinical case / and the appointment of treatment using developed dental models. It is associated with the manufacture of various structures such as dental crowns, implants, dental bridges, specialized braces for bruxism and others [29]. Emphasis is placed on the calculation of the volume of the three-dimensional digital models, and the obtained data is transferred to specialized platforms for calculating the mass of the material. With this calculation of the financial impact, the subsequently obtained mass data is used to calculate the final price of the used material. This is especially applicable for gold. The visually optimized methodology is presented in Figure 1.

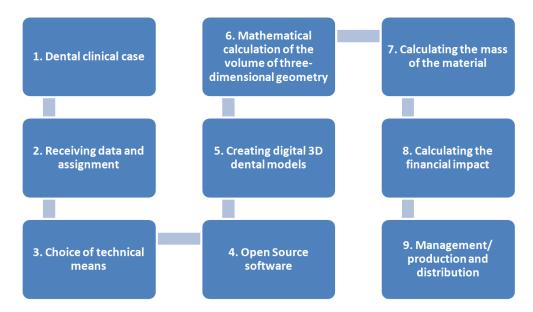


Figure 1. Optimized methodology for creating three-dimensional digital geometry of dental models and financial impact.

The components of the optimized methodology include the following main stages and required components to them:

1. Dental clinical case. The complaints of the patients in the dental clinics are documented.

2. Receiving data and assignment. Patients' pain and needs are examined. Some dental clinics require informed consent for the status of intolerance to allergies, metals and others [30]. If treatment is scheduled with placement of external dental models (crowns, implants, etc.) an order is made for ordering or production of ready-made ones according to the standard (often these are implants), as well as making dental crowns.

3. Choice of technical means. X-rays are taken (local or of the entire jaw). 3D scanners are also used to digitize the problem area in the mouth [31].

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4. Open Source software. Leading Open Source Software (OSS) such as Blender [32] for polygonal mesh [33] 3D models and FreeCAD [34] for solid 3D models [35] are available to create quality 3D geometry. They are in constant technological progress, with numerous users around the world, leading to a sharp rise in software innovations and the relatively frequent launch of new and/or updated versions. Also highly developed and freely available is OSS Bforartists (Blender based) [36].

5. Creating digital 3D dental models. Depending on the software, there are different modeling techniques in 3D designing. Generally speaking, the basic principles of operation include conventional modeling [37, 38], generating ready-made 3D models using specialized add-ons [39, 40], generating models by writing scripts directly in a software environment (OSS specific) [41] as well as hybrid modeling using combined techniques [42, 43].

6. Mathematical calculation of the volume of three-dimensional geometry. Looking for opportunities for mathematical calculation of the volume of 3D geometry directly in the OSS environment, there are tools – add-on type, respectively for the leading Blender and Bforartists (Nikitron tools Addon [44]), and respectively for FreeCAD there is an additional script "Macro FCInfo" [45].

7. Calculating the mass of the material. Calculating the mass of the material of three-dimensional geometry requires accurate mathematical calculations. These are possible directly in the environment of solid 3D CAD software such as SolidWorks [46], where the calculation process is automated in the presence of already built three-dimensional geometry, defining the exact standard material and calculating through the operation "mass properties" [47]. SolidWorks software has this feature in the basic package, which is a convenience for users. What is specific about this software is that it is paid, as well as that it is not open source. The Macro FCInfo script for FreeCAD already mentioned in item 6 provides an opportunity to calculate the mass of the material in a CAD environment. This is definitely a good opportunity, as the challenge remains for designers to find the right approach to accurate 3D modeling of dental models and components, which usually have complex three-dimensional geometry characteristics. Often 3D dental models such as crowns have a difficult geometry to make with many irregular shapes and curves, which requires the use of sculpting tools or specialized add-ons. Of course, there is always the possibility of transferring digital data between software, which in turn with good associativity one can achieve the desired results. As a rule, the difference in the structure itself between the polygonal mesh and solid 3D models is compensated by an additional correction of the three-dimensional geometry (with functional admissibility). Due to all these features, the Blender and Bforartists software provide the maximum conditions for calculating the mass of the material of the dental models. They are flexible, have quality sculpting tools. Conventional construction of three-dimensional geometry is always correct. That is, we have no violation of the polygonal mesh. It also has the "remove doubles" cleaning correction function, which ensures maximum quality. They work perfectly with specialized dental add-ons: "ODC - Open Dental CAD" [48] and "Dents 3D - Human Teeth Addon" [49], as well as the add-on for calculating 3D volume "Nikitron tools Addon". With the help of these add-ons, mathematical values of the volume of three-dimensional geometry are obtained, which are transferred to online specialized calculators such as: "SensorsOne" [50]. In order to be

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able to calculate the mass of the material used, it must be defined using standardized data for the respective material [51-53].

8. Calculating the financial impact. Accurate calculation of the financial impact be-comes possible after the mass of the material has been calculated. As a result of all ma-thematical calculations and the availability of data, they are defined in specialized cal-culators for calculating the financial value. For example, the online calculators "ARCH EnterPrices: SILVER AND GOLD VALUE CALCULATOR" [54] and GoldPriceZ [55] are fully available. It is used to perform operations to calculate the financial value of gold, which is one of the most important dental materials in the manufacture of dental crowns and bridges.

9. Management/production and distribution. The huge volume of activities related to dental dentistry is related to the global production of dental accessories, tools, components, services and others [56]. This is due to the large scale of financial activities. Calculating the financial value is of great importance for the management of dental model manufacturers (dental companies, clinics and laboratories). The availability of data on the cost of the material allows for accurate calculation of financial investments. This leads to the optimization of the overall production, where to the estimated cost of expensive materials (such as gold and others), the manufacturer calculates the costs of production, labor, distribution, etc. Having all the calculations leads to proper management, which is a prerequisite for a successful business. Globally, applying such an approach will shed light on an entire segment of the health system, such as dental health care in terms of material costs and accurate prices to end users.

3. MATERIALS AND METHODS

The technical implementation includes exemplary dental models such as gold and zirconium crowns, as well as implants made of titanium and titanium alloy Ti6Al4V. They are considered in 2 groups, respectively, the first relating to implants and the second to crowns. The second group, including the gold, will contain an extended study of financial value.

The main possibilities for creating three-dimensional geometry in the environment of Blender software are presented in sequence. Python scripts are included directly in the Blender environment, as well as specialized add-ons "ODC - Open Dental CAD" (GPL LICENSE: The program is free software; can redistribute it and/or modify it under the terms of the GNU General Public License and published by the Free Software Foundation) and "Dents 3D - Human Teeth Addon" (CC BY-NC-SA 2.5 - free to: share & adapt) to generate 3D models of whole teeth, crowns and implants. Some of the modifiers were used to create a solid volume of the initially studied surfaces, and the final results of the volume are calculated using the specialized add-on "Nikitron tools Addon" (GPL LICENSE – free software). The data of the obtained volumes of the models are transferred to the online specialized environment and are calculated respectively for mass as well as for financial value (gold).

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3.1. Interface and Creation of Three-dimensional Geometry in Blender Software

Blender software is fully available for Windows, Linux and macOS [57]. The software license is the GNU General Public License [58], which in practice gives complete freedom to work and present developments. A stable version of Blender is 2.79, which can be provided in the "release" section of the main site [59].

Creating 3D geometry in Blender is done by conventional construction from 0, generating 3D primitives (which are further refined), writing scripts directly in the work environment and generating fully finished 3D dental models. Figure 2 shows the Blender software interface and basic possibilities for creating 3D dental models.



Figure 2. Interface (Theme Science Lab) of Blender software (version 2.79b) and basic possibilities for creating 3D dental models. In the green boxes are marked: the specialized dental add-ons: "ODC - Open Dental CAD" and "Dents 3D - Human Teeth Addon", the operating mode "Scripting" and the main options for conventional creation of 3D geometry. (In the middle are presented rows of upper and lower jaw obtained through Dents 3D addon).

Activation of specialized add-ons in Blender is performed in: File> User Preferences> Add-ons> Install Add-on from file.

Before starting the construction of the three-dimensional dental models, it is recommended to adjust the system in millimeters so that the dimensions correspond to the real ones. This is done in the Scene> Units> Millimeters work panel.

Using the specialized ODC add-on, two sample models of dental implants (figures 3 a and b) with numbers 0848 and 1248 were created, and the Python scripts for them are:

^{• 4.8} mm/4.8 mm / 8 mm (figure 3 a)

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bpy.ops.opendental.place_implant(objs=[{"name":"0848"}])

• 4.8 mm/4.8 mm / 12 mm (figure 3 b)

bpy.ops.opendental.place_implant(objs=[{"name":"1248"}])

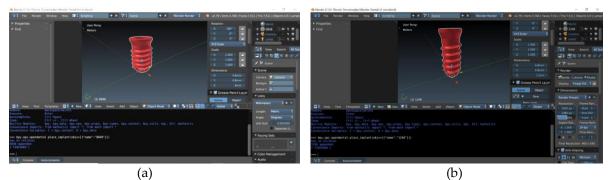


Figure 3. Standardized dental implants built using Python scripts, via ODC add-on in Blender software environment (a) dental implant 0848; (b) dental implant 1248.

3.2. Automated Computer Calculation of the Volume of 3d Geometry of Dental Models

Once the three-dimensional geometry of the dental implants is ready, their volume is automatically calculated using the NTA add-on in a Blender environment. The obtained values are:

• For dental impant model 0848: 64.1782 mm3

• For dental implant model 1248: 96.2677 mm3

3.3. Mathematical Calculation of the Mass of Materials of Dental Models (Implants and Crowns)

The resulting implant volume values are added to the required formula for calculating the mass of the material in the SensorsOne online calculator. The value of the density of the metal is also required, which must be accurate and comply with world accepted standards. [51-53].

The mathematical calculations of the mass of the material, which are realized in the online environment of SensorsOne, are calculated according to the following formula [50]:

$$\mathbf{m} = \mathbf{V} \times \boldsymbol{\rho} \tag{1}$$

Symbols:

• m = Mass

• V = Volume

• ρ = Density

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After performing the calculation, the following results were obtained for the mass of materials shown in Table 1.

Table 1. Obtained values of the mass of materials, of the 3D dental implants in the environment of Blender
software, by means of automated calculation using the online calculator SensorsOne [50].

3D Dental Implant / N:	Material	Density	Volume	Mass
0848	Titanium (Ti) Ti6Al4V			$0.2894 \\ 0.2842$
	Zirconium (Zr)	6.51		0.4178
1248	Titanium (Ti)	4.51		0.4341
	Ti6Al4V	4.429	96.2677	0.4263
	Zirconium (Zr)	6.51		0.6267

Dental crowns can be created conventionally from the initial stage of manual work, and it is necessary to comply with the standard ISO 3950: 2016 [60]. ODC or Dents 3D add-ons are optionally used for optimized development of dental crowns, and in both cases additional conventional modeling in Blender software is required. An exemplary ODC standardized dental crown No. 46 has been developed in Figure 4 (a), having an anatomical shape but at the same time having only external surfaces. The Python script is as follows:

• ODC Dental Crown:

bpy.ops.opendental. get_crown_form (objs=[{"name":"46"}])

Figure 4 (b) shows a completed solid 3D model of the dental crown using the "solidify" modifier [61], with a defined thickness value of 0.5 mm. This is an absolute prerequisite to be able to calculate exactly the Volume of 3D geometry.



Figure 4. ODC standardized dental crown with N: 46, 3D created using Python scripts in the environment of Blender software (a) 3D basic model of the crown (b) 3D ready model of the crown with a thickness of 0.5 mm.

Using the same methodology, the mass of all dental crown models is calculated, and Table 2 shows the obtained values of ODC models of dental crowns with numbers 46 and 45. They are placed in two groups with differences in the material used, respectively: Gold and Zirconium, as well as with differences in thickness.

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Table 2. Obtained values of the mass of materials, of the 3D dental crowns in the environment of Blender software, by means of automated calculation using the online calculator SensorsOne [50].

3D Crown/ N:	Material	Thickness	Density	Volume	Mass
	Gold (Au)	0.5	19.3	132.0311	2.5482
46	Gold (Au)	0.7	19.3	178.3377	3.4419
	Gold (Au)	0.9	19.3	221.1173	4.2675
	Zirconium (Zr)	0.5	6.51	132.0311	0.8595
	Zirconium (Zr)	0.7	6.51	178.3377	1.1609
	Zirconium (Zr)	0.9	6.51	221.1173	1.4394
	Gold (Au)	0.5	19.3	68.4567	1.3212
	Gold (Au)	0.7	19.3	91.4234	1.7644
45	Gold (Au)	0.9	19.3	112.0344	2.1622
	Zirconium (Zr)	0.5	6.51	68.4567	0.4456
	Zirconium (Zr)	0.7	6.51		
	Zirconium (Zr)	0.9	6.51	91.4234	0.5951
			0.01	112.0344	0.7293

3.4. Mathematical Calculation of the Price of Gold (Au) Used for Dental Crowns in Real Time

In order to use the online "ARCH EnterPrices SILVER AND GOLD VALUE CALCULATOR" [54] it is necessary to enter the data for weight (in our case the obtained mass of gold), grade or purity, current market price in troy ounces of pure gold. Two important features should be noted, that the only available data on the mass of the material is used, and that the calculator calculates the current price of gold in real time according to "CNN Commodities Prices" [62]. Also a very good option is the online calculator "GoldPricesZ" [55], where it is necessary to define a value of Quantity. "GoldPricesZ" provides visual information about Gram gold, and USD rate 1 Gram Weight: 0.03215 Oz, as well as for the period about the Gold Price and US Dollar Information Last Updated: Gold price updated on 13-Dec-2021 (time of financial calculation 14K Gold / Gram in USD = 33.5294 USD) at 04:30:03 pm (GMT-04: 00) according to America New-York time. This is a very important point to note, because changes in gold prices are very dynamic and the calculation of values must be done according to the specified period.

The financial results obtained for 10K (42% Pure Gold), 16K (67% Pure Gold) and 22K (92% Pure Gold) are shown in Table 3. It is possible to include calculations for 1K (4% Pure Gold), 2K (8% Pure Gold), 3K (13% Pure Gold), 4K (17% Pure Gold), 5K (21% Pure Gold), 6K (25% Pure Gold), 7K (29% Pure Gold), 8K (33% Pure Gold), 9K (38% Pure Gold), 11K (46% Pure Gold), 12K (50% Pure Gold), 13K (54% Pure Gold), 14K (58% Pure Gold), 15K (63% Pure Gold), 17K (71% Pure Gold), 18K (75% Pure Gold), 19K (79% Pure Gold), 20K (83% Pure Gold), 21K (88% Pure Gold), 23K (58% Pure Gold), 24K (99.99 % Pure Gold) as well as the Pure Gold option.

According to The Gold Center, the selected 10, 16 and 22 K are among the possible options for making gold dental crowns, with 16K being the most preferred compared to the specified interval of 10K (minimum) - 22K (maximum). This type (16K) of gold alloy may also contain amounts of palladium, platinum and silver [63].

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Table 3. Obtained values of the price of gold (10, 16 and 22 K) used for dental crowns by automated calculation	
using the online calculator GoldPricesZ [55]. The values are calculated on 13-Dec-2021.	

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3D Crown/ N:	Material	Mass	10K / \$	16K / \$	22K / \$
46	Gold (Au)	2.5482	61.00	97.61	134.28
		3.4419	82.40	131.84	181.37
		4.2675	102.16	163.47	224.87
		1.3212	31.63	50.61	69.61
45	Gold (Au)	1.7644	42.24	67.59	92.96
		2.1622	51.76	82.82	113.91

4. RESULTS

The results of the study give data on the exact values of:

- Volume of the three-dimensional geometry of dental models implants and crowns;
- Mass of gold, zirconium, titanium and titanium alloys Ti6Al4V used;

• Pricing of the Gold cost (gold price data in \$ are updated in real time and refer to the specific time: date and time).

The work methodology allows for the application of other metals and alloys of choice.

The add-ons and scripts used successfully generate the required 3D models. With regard to 3D digital models, no inaccuracies have been identified in polygonal mesh. Creating Thickness of 3D geometry is correct, without the presence of legs on the polygonal grid. Blender's "Solidify" modifier successfully builds additional geometry. There are no inaccuracies. The developed models of 3D digital dental models are fully completed and functionally prepared for production.

5. CONCLUSION

Many different technical means have been used in the present study. They have found an approach to creating, improving and generating three-dimensional digital geometry through precise mathematical parameters, the use of scripts and specialized add-ons. An approach has been found to calculate the volume of developed 3D dental models in OSS. Available free resources for calculating the mass of the material are presented. Calculating the cost of expensive materials used for dental models of implants and crowns are mathematically calculated in real time. This report has a strong financial dimension.

The methodology and data from the research are directly applicable and financially substantiated.

The author of the study is of the opinion that at the time of writing the report is not known as extensive work to calculate the cost of precious metals such as gold, widely used in world dental practice at the level of 3D digital design. The author of the study offers all StakeHolders accumulated research experience and many fully available free and Open Source resources providing:

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• Optimized creation of complex 3D dental models;

• Technological approach and methodology for calculating the volume of three-dimensional geometry in Open Source environment, data transfer for calculating the mass of the material and calculating the financial impact.

This paper has been prepared after many years of practice with various technical tools, software, program code, interdisciplinary research and studies in the fields of Industrial Design, 3D computer modeling and Dentistry. The advantage of the research is that in one paper it is possible for a comprehensive view of the topic, and the desired result is the optimization of the strategic vision in an entire segment such as dental health, as a key unit in the Health care system.

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