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COMPUTER HYBRID DESIGN USING PYTHON SCRIPTING AND CONVENTIONAL 3D MODELING TO BUILD (FCC) CRYSTAL STRUCTURES OF PRECIOUS METALS AND THEIR PREPARING FOR 3D PRINTING

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Abstract: Developing a properly constructed 3D geometry is essential for obtaining high quality digital and real 3D models. Gold (Au 79) and Platinum Crystal (Pt 78) Face Centered Cubic (FCC) Crystal Structures are designed to illustrate the training content of models invisible to the human eye. The present study optimizes the design approach by applying Python programming language directly in Blender 3D environments, and further developing it into software compatible with 3D printers to produce the final model.

Key words: 3D, Blender, digitalization, open source, printing, Python, visualization

1. INTRODUCTION

Computer 3D visualization is a complex process that goes through various stages of design. At the core of 3D CAD and 3D polygonal-mesh programs there are complex mathematical models, through which the technical part of the realization of three-dimensional geometry is performed. In addition, it must be considered that the modern process of digitalization requires complex knowledge and solutions for building digital real models by assignment, which is often accompanied by the application of many technical means, standards and formats, integrated systems and others involved individually or in symbiosis with other technical means ensuring the overall functioning of a system building the design of three-dimensional geometry - digital and real materialized [1-5].

The development of design models through the application of mathematical models and accuracy calculations are a modern way to improve the quality of the elaboration [6, 7].

The educational process is based on the transfer of information. This increases the importance of the visual presentation of information in education, which is a modern requirement of the digital age and is recommended by several leading scientists [8].

The principle of visualization of modern education is oriented towards the use of various visual aids in the learning process and the correct presentation of information through graphic images and videos, explaining the text and specific objects [9].

Establishing the right approach for making the three-dimensional geometry of mathematically correct models from reality is of great importance. The creation of a polyhedron unit is a prerequisite for the generation of different configurations of lattice, which has a direct application in modern practice [10-15].

Many polyhedral can be designed to be space-filling as well and are often used in the design of AM porous biomaterials, Figure 1 [10].

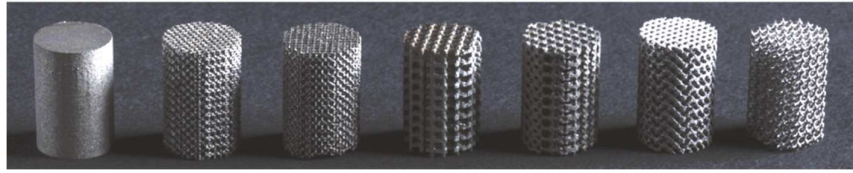


Fig. 1. A number of different polyhedron cylindrical specimens designed by using different types of beam-based unit cells as well as a solid specimen [10].

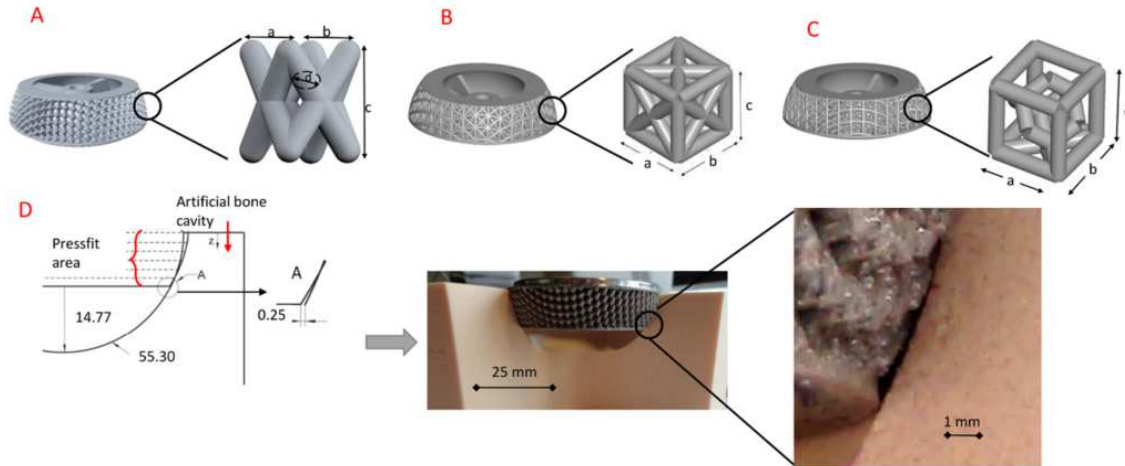


Fig. 2. Designs of artificial acetabular cups with an open-porous load-bearing unit cell in abbreviated version; (A) Illustration - twisted unit cell, (B) Illustration - combined unit cell, (C) Illustration - combined open unit cell substitute, (D) Press-fit area and gap in case of reduced cup model (negative press-fit) - schematic figure and photograph, all units are in mm [11].

For the needs of biomedicine and in particular implantology, fully developed models of Acetabular Press-Fit Cups with Open-Porous are shown in Figure 2 [11].

Biocompatible precious metals such as gold and platinum are essential in the biomedical industry [12; 13; 14]. They have unique antibacterial properties. They are popular with dental and orthopedic implants. The present study shows the necessary technological process of making FCC (Face centered cubic) models, which allows the production of precise three-dimensional geometry.

The present study aims to digitize and recreate 3D models invisible to the human eye, designed for public presentation to students at different levels, as well as to illustrate the learning content. Part of this strategy is the digitization and subsequent prototyping of important for science and practice models of metal crystal structures, in this case gold and platinum are selected. In parallel, the present work offers an innovative approach to the development of three-dimensional geometry,

which makes it possible to improve the quality of the final models

2. METHODOLOGY

Modern technical tools allow the use of hybrid 3D modeling techniques, by scripts and conventional design. Face Centered Cubic (FCC) Crystal Structures of Gold (Au 79) and Platinum (Pt 78) [16] are developed in the present work. A methodology covering various design stages containing the main activities for model development is successfully implemented.

To maximize the location accuracy of 3D spherical details (atoms) along the edges and center positions, Python scripts are used to directly produce geometry in Blender 3D three-dimensional environment according to location and scale [17-23]. The three-dimensional models have the correct construction, based on the parameters specified by science concerning FCC of precious metals, to which gold, platinum and others belong [24-28].

The digital modeling of Au and Pt in Blender 3D ends with the construction of the thickness of the connecting elements of the cubic structure. Suitable additional software compatible with the available 3D Printer is implemented to deliver the finished 3D printed model of Gold FCC Crystal Structure. The developed FCC digital Au and Pt models and the real-printed Gold Crystal Structure model serve to illustrate the learning content of precious metal models invisible to the human eye. Mathematical values and equations are used to achieve maximum accuracy during the work process, and the work methodology is optimized through synchronization between the technical means. For convenience, hybrid design techniques are applied, which shows the advantage of this type of technical implementation of digitalization, which confirms the principle of operation as relatively new and innovative. The illustrative example explains why different types of technical software and software tools manage to combine into one working system to achieve effective results. The technical part of implementing three-dimensional geometry goes through various successive stages. This includes using Blender 3D, Autodesk MeshMixer, XYZ software compatible with 3D Printer XYZ. For the development of 3D digital models, Python codes are applied in the Blender 3D Scripting section. Figure 3 presents an optimized methodology for obtaining final digital and real three-dimensional FCC Crystal Structures models of Gold and Platinum.



Fig. 3. An optimized methodology through the development of FCC of Gold and Platinum with maximum accuracy is possible.

As seen in Figure 3, the principle of operation is consistent, using conventional and hybrid design techniques in Blender 3D environments.

All technical systems use import-export *.OBJ, *.STL and other compatible file standards.

3. THREE-DIMENSION (3D) DIGITIZATION AND PRINTING

The three-dimensional design process begins with the launch of Blender 3D (using the stable version of Blender 2.79b), which automatically obtains an initial primitive-Cube, which can be used in principle for the present work, and is required in Transform / Scale to enter suitable values for X, Y and Z. Or building a brand-new Cube using Python (Interactive Console 3.5.3) scripting. The following script is written to create the 3D Cube (Figure 4):

1. Cube:

```
bpy.ops.mesh.primitive_cube_add(radius=2,
view_align=False, enter_editmode=False,
location=(0, 0, 0), layers=(True, False, False,
False, False, False, False, False, False,
False, False, False, False, False, False,
False, False, False))
```

The second step goes directly to the generating of three-dimensional spheres (atoms), specifying the location and size (Figure 5):

2. FC Atom (up)

```
bpy.ops.mesh.primitive_uv_sphere_add(view
_align=False, enter_editmode=False,
location=(0, 0, 2), layers=(True, False, False,
False, False, False, False, False, False,
False, False, False, False, False, False,
False, False, False))
```

```
bpy.ops.transform.resize(value=(0.55, 0.55,
0.55), constraint_axis=(False, False, False),
constraint_orientation='GLOBAL',
mirror=False, proportional='DISABLED',
proportional_edit_falloff='SMOOTH',
proportional_size=1)
```

The third and subsequent steps only specify the locations of the other spheres (atoms), the dimensions being identical (Figure 6):

3. All atoms (1 already done + more 13)

```
location=(2, 2, 2), location=(-2, -2, 2),
location=(2, -2, 2), location=(-2, 2, 2),
location=(0, 0, -2), location=(2, 2, -2),
location=(-2, -2, -2), location=(2, -2, -2),
location=(-2, 2, -2), location=(0, 2, 0),
```

$location=(0, -2, 0)$, $location=(-2, 0, 0)$,
 $location=(2, 0, 0)$.

the FCC. 3D Cube is edited to the save state only
Edges (Faces are removed).

Figure 5 shows the construction and
arrangement of the resulting primary version of

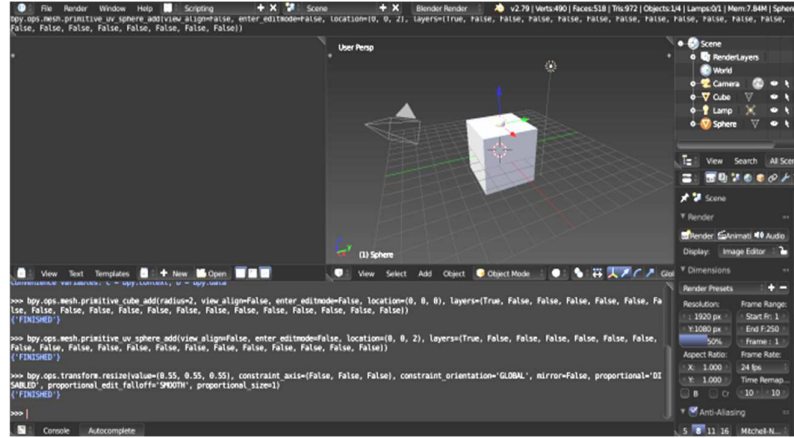


Fig. 4. Creating 3D Cube model with Python Scripting in Blender software field.

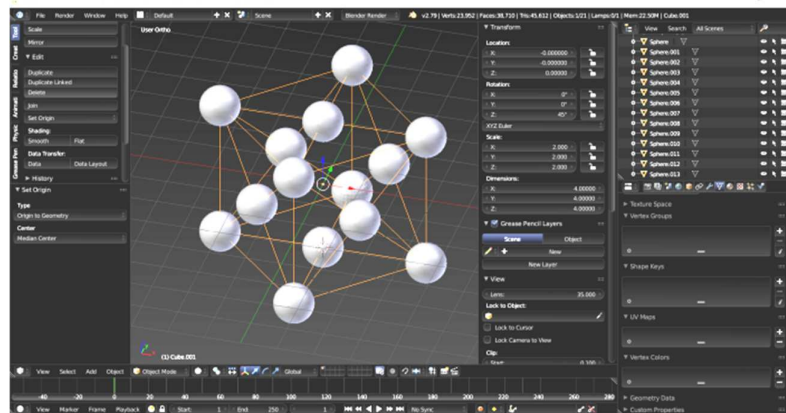


Fig. 5. Obtained variant of FCC construction + ready all 3D atoms.

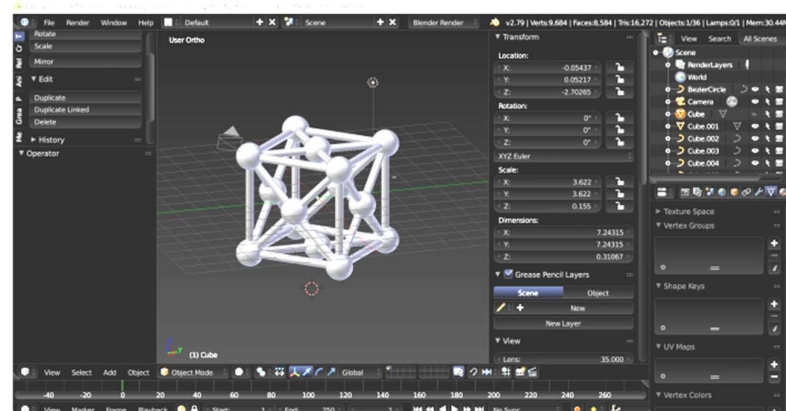


Fig. 6. Ready 3D model of FCC of Gold (Au 79) and Platinum (Pt 78) Crystal Structures.

The use of the capabilities of Bevel creates a volume of connecting elements that are converted into curves. Figure 6 shows the finished 3D model of FCC Crystal Structure (still not solid).

To create the visual realism of the precious metal, precise use of the material, stage and lighting is required, which is calculated by equation (Equation 1), [29]. Lamp / Point / Light Attenuation. Mixing “Linear” and “Quad”. If both values are greater than 0.0, the used formula to calculate the light is:

$$I = E \times (D / (D + L \times r)) \times (D^2 / (D^2 + Q \times r^2)) \quad (1)$$

Where I is the calculated Intensity of light;
 E - the current Energy slider setting;
 D - the current setting of the Distance field;
 L - the current setting of the Linear slider;
 Q - the current setting of the Quad slider;
 r - the distance from the lamp where the light intensity gets measured.

To create a 3D printed presentation model (Gold Crystal Structure selected), it is necessary to create a geometry density [30]. The 3D model has the following Vertices and Triangles parameters obtained in the following sequence of work situations as follows: model imported from Blender 3D in MeshMixer and Solid Transformed with values: Maximum Solid Accuracy 512 (Cell Size 0.02 mm) and maximum Mesh Density 512 (Cell Size 0.016 mm). Table 1 presents the Vertices and Triangles data of the presentation model.

Table 1

Mesh quality of the 3D model		
DIGITAL 3D PRESENTATION MODEL OF FCC GOLD (AU) CRYSTAL STRUCTURE /QUALITY OF THE MESH		
MeshMixer software calculation	Vertices	Triangles
Default Imported model from Blender 3D (no solid)	16828	23396
Accurate high-quality Solid calculation	1154273	2308650

Figure 7 shows fully ready Solid presentation of Gold (Au 79) Crystal Structure model. Figure 8 shows the quality of the three-dimensional model obtained after all the operations performed so far (Toggle Visibility). The clarity

and precision of the geometry can be seen without any inaccuracies. The finishing work on creating a real 3D presentation model is done by using XYZware software (Figure 9) related to the 3D printer XYZ [31]. For reference, the developed 3D digital models are versatile and can be adapted to other 3D printers and additive machines [32-37].

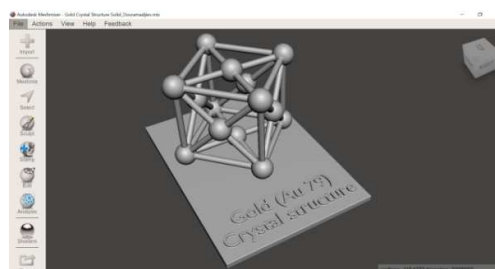


Fig. 7. Fully ready Solid presentation of Gold (Au 79) Crystal Structure model.

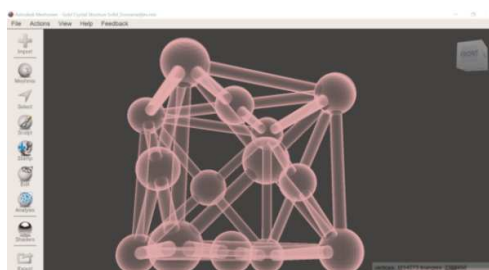


Fig. 8. Toggle Visibility (Autodesk MeshMixer software) shows the quality and precision of the resulting 3D model.

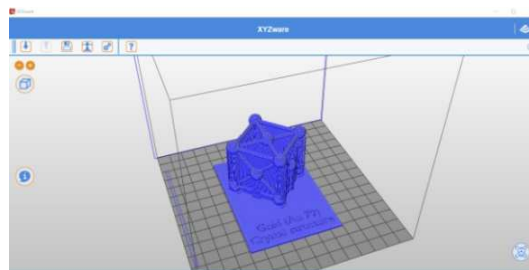


Fig. 9. The 3D model with supports in an environment of XYZware software.



Fig. 10. 3D printed model of Gold Crystal Structure / PLA material.

Figure 10 shows the actual presentation 3D model of Gold Crystal Structure materialized from PLA material (<https://www.youtube.com/watch?v=x00Oe09ZKrA>). The completed three-dimensional model has a stable construction and is presented in a form consistent with the needs of the study, combining the 3D geometry of FCC Gold Crystal Structure with 3D voluminous descriptive text.

4. RESULTS AND DISCUSSIONS

The obtained results are distinguished by the quality of execution. All set goals are achieved without the presence of inaccuracies in the developed models. The results are characterized as follows:

- Digital 3D FCC models have accuracy of values and parameters in accordance with the scientific requirements (Figure 6);
- Computer graphics have a clear vision, which makes them recognizable (Figure 7);
- Extremely high-quality three-dimensional geometry is obtained because of the transformation into solid of MeshMixer (Figure 7);
- There are no cracks, missing polygons/faces or deformed in the process of generating the final digital model with precisely connected geometry of different shapes (Figure 8);
- The printed 3D model confirms the good quality of the digital model, with no visible inaccuracies in the geometry (Figure 10).

5. CONCLUSION

In the present work, using advanced 3D technology, 3D digital models of Face Centered Cubic (FCC) Structures of precious metals are fully developed. With 3D printing, a model of Gold Crystal Structure is created. The use of advanced technological tools is a necessity for the development of 3D digital and real models by reference. Functional Python scripts are presented in this study to facilitate the generation of accurate three-dimensional geometry in terms of dimensions and precise

location in three-dimensional space. Practical skills for transforming digital surface geometry into solid are clearly demonstrated and the need to prototype real-world examples. In relation with the creation of three-dimensional invisible models for the human eye, models of Gold (Au 79) and Platinum (Pt 78) Crystal Structures are fully developed.

Fully accessible open-source software programs and software resources are provided, as well as free programs that create density for digital models designed for 3D printing. Gold Crystal Structure is real 3D printed.

The completed model is a clear example of Cubic Structure, which is publicly presented and accessible. The gained experience provides the necessary knowledge and practice through which similar types of models can be implemented, as well as others where hybrid programmatic and conventional design is required for maximum accuracy. The used optimized methodology gives a new approach and innovative vision for improved hybrid design, which is directly applied in practice to produce high-quality three-dimensional geometry and is for the benefit of specialists and students in the field of engineering, computer programming, 3D design and others.

Based on the 3D printed FCC final presentation model, the qualitative combination of the geometric elements is clearly shown. The multiplication of this type of FCC units in pure form in different lattice configurations is a prerequisite for the development of different applications for the needs of biomedicine and industrial practice, where this type of structures improve mechanical properties and strengthen and / or create conditions for integration between different materials.

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Proiectarea hibridului de computer folosirea scripturilor de pitone și modelarea convențională 3d pentru construcții (fcc) structuri cristale de metale precioase și prepararea lor pentru imprimarea 3D

Dezvoltarea unei geometrii 3D construite corespunzător este esențială pentru obținerea de modele 3D digitale și reale de înaltă calitate. În cadrul lucrării se prezintă modalitatea în care structurile de cristal din aur (Au 79) și platină (Pt 78), centrate pe față (FCC), sunt proiectate pentru a ilustra conținutul de formare a modelelor invizibile pentru ochiul uman. Prezentul studiu optimizează abordarea de proiectare prin aplicarea limbajului de programare Python direct în mediile Blender 3D, dezvoltându-l în continuare prin intermediul unei aplicații software compatibilă cu imprimantele 3D, în vederea realizării modelului final.

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