ANSYS Modeling for Bone Reconstruction by Using Hybrid Nano Bio Composite

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ABSTRACT

In the present work, an attempt has been made to study and improve the physical and biomechanical properties of adding Titanium dioxide (TiO\textsubscript{2}) and yttria stabilized zirconia (Y-PSZ) Nano fillers ceramic particles for reinforced the high density polyethylene (HDPE) matrix Nanocomposites for fabricated six bio nanocomposites hybrid by using hot pressing technique at different compounding temperature of (180, 190, and 200 °C) and compression pressures of (30, 60, and 90 MPa). The fabricated Nano systems were designed, produced and investigated for use in repairs and grafting of the human bones, which are exposed to accidents or life-threatening diseases. The main current research results show that with the increase of the TiO\textsubscript{2} filler contain from 0 to 10 %, the value bulk densities increase by 30.24 % and when adding 2% partial stabilized zirconia (Y-PSZ), this value was further increased by 13.91%. For the same conditions the value percentages true porosity decrease by 48.68 % and further by 84.85 %, respectively. For the same previous parametric values, it has also been accessed that the maximum compression strength for this study was increased by 33.34 % and then further by 22 %, where these values higher by 90.11% than the previous mentioned studies. The micro-Vickers Hardness increased by 30.11 % for the second manufacturing system comparing with the first one, while the maximum equivalent von–Misses Stresses obtained from the current work withstand higher stresses than the natural bone by 52.65 higher than the previous studies. The stress safety factors increase by 58.38 % and by 21.42 % for the first and second systems, respectively. The achieved results values for the modeled femur bone is equivalent to actual service of the activity during normal movement of the patient. These results give great the designers choices to use successful bio composites for in vivo tests according to the clinical situation, age and the static and dynamic loads when designing a material to repair the fractured bones due to different types of accidents.

Keywords: Femur bone ANSYS modeling; Nano HDPE /ceramic Bio-composites; Titanium Oxide; Yttria stabilized zirconia (Y-PSZ); Bone biomechanics.

1 INTRODUCTION

Bones in the human body are a living natural composite material, fractured due to impact stress and excessive loads [1-2]. They have a complex microstructural feature [3-4]. The effects of filler nanoparticles on these properties have been extensively investigated in recent years [5]. It has been found that the addition of a few

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percent of these nanoparticles can result in significant improvement in physical and chemical properties [6]. The main scaffolds materials can be categorized: polymeric, ceramic, composite, and metallic scaffolds [7-8]. The interaction of ceramic particulates with a thermoplastic high-density polyethylene (HDPE) material was considered as a very important factor influence on the tensile strength and fracture behavior of the HDPE- zirconia composites, which has formed the basis for selecting the Nano particles for bio-composite materials engineering [6]. In recent years, the adding small percentages of inorganic Zirconium dioxide (ZrO$_2$), also known as yttria (Y$_2$O$_3$), and titanium dioxide (TiO$_2$) with synthesized polymer Nano composites have been increasing due to their significant improvement in their thermal stability, electrical properties and mechanical performance [5, 9-11]. Titanium and its alloys, including the titanium oxide (TiO$_2$) are superior to many biomedical materials, such as stainless steel. They are widely used as orthopedic and implant materials for their biocompatibility and excellent mechanical properties, resistance to corrosion, absence of cytotoxicity, inertness and compatibility [12-13]. During melting, the polymerization process affected the polymer becomes viscous and its chains grow longitudinally and, the monomer remains relatively mobile due to the exothermic and the release of heat of the polymerization rate. The highly nonlinearity of the reaction rate during the process makes it difficult to capable of supporting stress. The problem is simplified if the mechanism of stress can be considered as a result of thermal deformations only. Results show maximum tensile stresses normal to the cracks directions, due to a link between residual stress and preload cracking [14]. To study the mechanical behaviour of biological structures, the finite element analysis (FEA) has been increasingly adopted [15-20], using the 3D finite element Analysis (FEA) to investigate the effect of daily living activity loading conditions on the mechanical strength in human bone [21-26].

The main objectives of this work were to predicted the influence of adding different concentrations of titanium dioxide and partial stabilized zirconia (PSZ) Nano ceramic fillers powders with at different compression pressures and compacting temperatures using the hot pressing fabricating technique on the physical and mechanical properties for TiO$_2$/ HDPE and Y$_2$O$_3$- partial stabilized zirconia (Y-PSZ)/ TiO$_2$/ HDPE Nano composites systems and to investigate the highest stress factors of safety to withstand the daily human activities loads. The SOLIDWORKS and ANSYS modeling were used to simulate and predicted the fracture mechanical behavior of the femur bone by develops a 3D solid numerical model, with the use of finite element method (FEM) for the human femur bone corresponding to the patient activities. The response surface methodology (RSM) technique and the Design Expert software program were used to improving and verifying the results, reaching and evaluated the optimal thermal and mechanical properties.

## 2 MATERIALS AND METHODS

### 2.1 Nano composites preparation method

Six Nano composites systems TiO$_2$/ HDPE and Y$_2$O$_3$- partial stabilized zirconia (Y-PSZ)/ TiO$_2$/ HDPE were fabricated in this study and used as bone grafting bio-composites. The used ceramic fillers are; the 99% purity titanium dioxide (TiO$_2$) with a particle density of 4.23 g/cm$^3$ and an average particle size of 40 nm, imported from M.K Nano (Canada, Toronto) and the 99.9% purity partially-stabilized zirconia (ZrO$_2$-PSZ), doped with 3 mol. % of yttria (Y$_2$O$_3$), of 5.91 g/cm$^3$ density and an average particle size of 40 nm, imported from M.K. Nano (Canada, Toronto). The particle size of 5 $\mu$m and density of 0.95 gm/cm$^3$ used high-density polyethylene (HDPE) biomaterial powder matrix was supplied by the Right Fortune Industrial Limited (China, Shanghai).

The prepared powders mixtures with each desired composition were dry mixed in a ball mill machine for 12 hrs, and then hot pressed at 180, 190, and 200 ºC and using a compounding pressure of 30, 60, and 90 MPa, respectively. The produced test samples were of a cylindrical shape with a height between 3 and 5 mm and 10 mm diameter. The main properties of the used nanomaterials are given in Table 1.

### Table 1

<table>
<thead>
<tr>
<th>Property</th>
<th>Titanium dioxide</th>
<th>Zirconium dioxide (Zirconia)</th>
<th>Yttrium oxide (Yttria) or Yttrium (III) oxide</th>
<th>High density polyethylene (HDPE) matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical formula</td>
<td>TiO$_2$</td>
<td>ZrO$_2$</td>
<td>Y$_2$O$_3$</td>
<td>C$_4$H$_8$</td>
</tr>
<tr>
<td>Molar mass (g/mol)</td>
<td>79.87</td>
<td>123.22</td>
<td>225.81</td>
<td>1000</td>
</tr>
<tr>
<td>Appearance</td>
<td>White solid</td>
<td>White powder</td>
<td>White solid</td>
<td>Translucent to White</td>
</tr>
<tr>
<td>Density (g/cm$^3$)</td>
<td>4.23</td>
<td>5.68</td>
<td>5.01, solid</td>
<td>0.94 - 0.97</td>
</tr>
<tr>
<td>Melting point (°C)</td>
<td>1843</td>
<td>2715</td>
<td>2425</td>
<td>126</td>
</tr>
<tr>
<td>Boiling point (°C)</td>
<td>2972</td>
<td>4300</td>
<td>4300</td>
<td>&gt; 300</td>
</tr>
<tr>
<td>Young's modulus (E) (GPa)</td>
<td>230-288</td>
<td>210</td>
<td>120</td>
<td>1.04</td>
</tr>
<tr>
<td>Property</td>
<td>Range</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------------------------------</td>
<td>----------------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tensile strength ($\sigma_t$) (MPa)</td>
<td>333.3-367.5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Endurance Limit (MPa)</td>
<td>283.5-330.7</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Compressive Strength (MPa)</td>
<td>660-3675</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Shear Modulus (GPa)</td>
<td>90-112.5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fracture Toughness (KIC)</td>
<td>2.4-3.3 MPa.m$^{1/2}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Poisson's Ratio</td>
<td>0.27-0.29</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal Expansion ($10^4$/K)</td>
<td>8.4-11.8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solubility</td>
<td>Not soluble in acidic; Soluble in HF, and hot H2SO4; Soluble in alcohol acid; Insoluble in most organic solvents</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solubility in water</td>
<td>Insoluble</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal conductivity (W/m.K)</td>
<td>4.8, 11.8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal conductivity (W/m.K)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.2 Physical and mechanical properties testing

A disk-shaped sample, were prepared for measured the fracture strengths by using the diametrical compression tests on the Instron tensile machine with a crosshead speed of 5 mm min$^{-1}$. In this test, a disk specimen is loaded along a diameter in compression edgewise. A biaxial stress state generates in the specimen with a transverse tensile stress and a compressive principal stress in the direction of loading. For a significant fraction of the test specimen, these stresses are nearly constant near the center of the disk. The following formula is used to calculate fracture strength [28]:

$$\sigma_f = \frac{2P}{\pi D t}$$

where: $\sigma_f$ is the tensile fracture strength (MPa); $P$ is the crosshead load (N); $D$ is the specimen diameter (mm) and $t$ is the specimen thickness (mm).

The Vickers micro-hardness tests were carried by using the Digital Micro Vickers Hardness Tester type TH714, manufactured by the Beijing TIME High Technology Ltd. /China) using a pyramid indenter with applied load of (50 gm). For all samples, the live bulk densities were done by using the Pycnometer instrument of sort AccuPyc1330 Pycnometer produced by the Micromeritics Instrument Corporation, Holland. The tests were performed after to remove moisture by drying the samples in oven for 48 hr at a temperature of 60 °C. Then the samples weighted by using 4-digit balances. The densities of the samples were calculated by using the Archimedes method and the following equations [28].

$$\text{Bulk density} = \frac{(W_a - W_b)}{W_D} \times D$$

$$\text{Bulk volume} = \frac{(W_a - W_b)}{W_D} \times D$$

$$\text{Apparent solid volume} = \frac{(W_a - W_b)}{D}$$

$$\text{Apparent solid density} = \frac{(W_a - W_b)}{W_D} \times D$$

where: $W_a$ is the weight of test piece soaked and suspended in air; $W_b$ is the weight of test piece soaked in water and suspended in distilled water and $W_D$ is the weight of test piece. The sintered samples are soaked in distilled water for 1 hr before measurement.

The True porosity was calculated using the following relation:

$$\text{True porosity (\%)} = \frac{[1-\text{bulk density/true density}]}{100}$$

2.3 Mathematical modeling

The governing equation used in the simulation of the femur bone consists of the geometric equation, the stress equilibrium equations, and constitutive equations. In index notation, these equations are [19]:
\[
\rho \frac{\partial^2 u_i}{\partial t^2} - \sigma_{ij,i} = f_i \quad (i=1,2)
\]  

(7)

\[
\varepsilon_{ij}(u) = \frac{1}{2}(u_{i,j} + u_{j,i})
\]  

(8)

\[
\sigma_{ij} = (C_{ep})_{ij} \varepsilon_{ij},
\]  

(9)

where; \(\sigma\) and \(\varepsilon\) denote the stress, and strain respectively, \(u\) is displacement, \(f_i\) represents body force, \(C_{ep}\) is the constitutive matrix. To solve the problem boundary value, the finite element analysis (FEA) is used. The standard weighted residual technique is applied and the typical domain is denoted by \(\Omega\). Eqs. (1), (2), and (3) can be written as:

\[
\rho \frac{\partial^2 u}{\partial t^2} - \left( \frac{\partial \sigma_x}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} \right) = f_x
\]  

(10)

\[
\rho \frac{\partial^2 v}{\partial t^2} - \left( \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} \right) = f_y
\]  

(11)

where,

\[
\varepsilon_x = \frac{\partial u}{\partial x}, \varepsilon_y = \frac{\partial v}{\partial y} \quad \text{and} \quad \varepsilon_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}
\]  

(12)

and,

\[
\begin{bmatrix}
\sigma_x \\
\sigma_y \\
\sigma_{xy}
\end{bmatrix} = \begin{bmatrix}
d_{11} & d_{12} & 0 \\
d_{21} & d_{22} & 0 \\
0 & 0 & d_{33}
\end{bmatrix} \begin{bmatrix}
\varepsilon_x \\
\varepsilon_y \\
2\varepsilon_{xy}
\end{bmatrix}
\]  

(13)

By using the terms of the displacements \(u\) and \(v\) in Eqs. (10) and (11) and by substituting Eq. (12) into (13) [24], then the result can be obtained in the following equations:

\[
-\frac{\partial}{\partial x} \left( d_{11} \frac{\partial u}{\partial x} + d_{12} \frac{\partial v}{\partial y} \right) - \frac{\partial}{\partial y} \left[ d_{33} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] = f_x - \rho \frac{\partial^2 u}{\partial t^2}
\]

(14)

\[
-\frac{\partial}{\partial x} \left( d_{33} \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) - \frac{\partial}{\partial y} \left[ d_{12} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] = f_y - \rho \frac{\partial^2 v}{\partial t^2}
\]

(15)

To develop a variational statement corresponding to the problem boundary value, we consider the following alternative problem. Form the governing differential equations, \(u\) and \(v \in H^1_t(\Omega)\) can be found for all the weights functions \(o_1\) and \(o_2 \in H^1_0(\Omega)\), then all the boundary conditions are satisfied, having:

\[
0 = \int_\Omega \left[ \frac{\partial o_1}{\partial x} \left( d_{11} \frac{\partial u}{\partial x} + d_{12} \frac{\partial v}{\partial y} \right) + \frac{\partial o_2}{\partial y} d_{33} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) - o_1 f_x + \rho o_1 \frac{\partial^2 u}{\partial t^2} \right] dx dy
\]

\[
-\phi_1 \int_\Omega o_1 \left[ \frac{\partial o_2}{\partial x} d_{11} \left( \frac{\partial u}{\partial x} + d_{12} \frac{\partial v}{\partial y} \right) n_x + d_{33} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) n_y \right] ds
\]

(16)
\[ 0 = \int_{\Omega} \left[ \frac{\partial \omega_2}{\partial x} d_{33} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \right) + \frac{\partial \omega_2}{\partial y} \left( d_{12} \frac{\partial u}{\partial x} + d_{22} \frac{\partial v}{\partial y} \right) - \omega_2 f_{y} + \rho \omega_2 \frac{\partial^2 \psi}{\partial t^2} \right] dx dy \]

\[-\phi_2 \omega_2 \left[ d_{33} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) n_x + \left( d_{12} \frac{\partial u}{\partial x} + d_{22} \frac{\partial v}{\partial y} \right) n_y \right] ds \]

The above numerical problem can be solved using the finite dimensional subspace. By choosing a N-dimensional subspace of \( H_h \in H_1 (\Omega) \) for \( u \) and \( v \) and the test functions \( \omega_1 \) and \( \omega_2 \). Let \( \{ \psi_j \}_{j=1}^{N} = 1 \) be the basis function of \( H_h \), then:

\[ u (x, u, t) = \sum_{j=1}^{N} \psi_j (x, y) u_j (t) \] (18)

\[ v (x, u, t) = \sum_{j=1}^{N} \psi_j (x, y) v_j (t) \] (19)

\[ \omega_1 (x, u, t) = \sum_{j=1}^{N} \psi_j (x, y) \omega_1_j (t) \] (20)

\[ \omega_2 (x, u, t) = \sum_{j=1}^{N} \psi_j (x, y) \omega_2_j (t) \] (21)

By substitute Eqs. (18) to (21) into Eqs. (16) to (17), and the resulting algebraic equations writing in the matrix form, then the system of ordinary differential equation obtained:

\[ M \ddot{U} + A (U) U = F \] (22)

Eq. (22) is a nonlinear system and can be solved by quasi-Newton method.

3 RESULTS AND DISCUSSION

3.1 Physical and mechanical properties

The physical and mechanical properties of the natural femur bone, which is contains of two composites; the outer cortical bone (compact) and the inner cancellous bone (trabecular) structure, are given in Table 2. [29] The effect of the fabrication input parameters i.e. the Nano ceramic filler Powder Compositions, the used compression pressures and hot-pressed temperatures on the mechanical and physical properties for the both fabricated two Nano composites systems TiO\(_2\) / HDPE and TiO\(_2\) / Y\(_2\)O\(_3\) - partial stabilized zirconia (Y-PSZ)/ HDPE are illustrating in Table 3 and 4, respectively.

In the present work, the experiments were designed by using the full factorial method (FFM), the response surface methodology (RSM) and the analysis of variance (ANOVA) technique to analyze the results. The three level factorial ANOVA analyses using the quadratic design model was implemented for analyzing the effect of input parameters on the compression fracture strength resulting for all the fabricated nanobiocomposites systems are given in Table 5. The model F-value of 143.38 and the \( P \)-values less than 0.0500 implies that the model is significant.

<table>
<thead>
<tr>
<th>Sp. composition</th>
<th>Density (g/cm(^3))</th>
<th>Modulus of elasticity (GPa)</th>
<th>Tensile strength (MPa)</th>
<th>Compressive strength (MPa)</th>
<th>Fracture strength (MPa)</th>
<th>Micro-Vickers Hardness Hv (kg/mm(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cortical bone (compact)</td>
<td>1.6</td>
<td>17.5</td>
<td>208</td>
<td>195</td>
<td>131-224</td>
<td>33</td>
</tr>
<tr>
<td>Cancellous bone (trabecular)</td>
<td>2.08</td>
<td>0.1</td>
<td>50–100</td>
<td>68</td>
<td>50–100</td>
<td>66</td>
</tr>
</tbody>
</table>

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Table 3
The effect of input parameters on the physical and mechanical properties of the fabricated Nano composites system TiO2/ Y2O3-
partially stabilized zirconia (Y-PSZ) HDPE.

<table>
<thead>
<tr>
<th>Exp. No.</th>
<th>Nano ceramic filler Powder Composition</th>
<th>Compounding pressure (MPa)</th>
<th>Hot pressed temperature (°C)</th>
<th>Compression fracture strength (MPa)</th>
<th>Micro-Vickers Hardness Hv (kg/mm²)</th>
<th>Bulk density (gm/mm³)</th>
<th>True porosity (%)</th>
<th>Stress Safety Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1% TiO2</td>
<td>30</td>
<td>180</td>
<td>28</td>
<td>90</td>
<td>1.022</td>
<td>13.53</td>
<td>0.5641</td>
</tr>
<tr>
<td>2</td>
<td>1% TiO2+2% ZrO2</td>
<td>30</td>
<td>190</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
<tr>
<td>3</td>
<td>1% TiO2+2% ZrO2</td>
<td>30</td>
<td>200</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
<tr>
<td>4</td>
<td>1% TiO2+2% ZrO2</td>
<td>60</td>
<td>180</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
<tr>
<td>5</td>
<td>1% TiO2+2% ZrO2</td>
<td>60</td>
<td>190</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
<tr>
<td>6</td>
<td>1% TiO2+2% ZrO2</td>
<td>60</td>
<td>200</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
<tr>
<td>7</td>
<td>1% TiO2+2% ZrO2</td>
<td>90</td>
<td>180</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
<tr>
<td>8</td>
<td>1% TiO2+2% ZrO2</td>
<td>90</td>
<td>190</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
<tr>
<td>9</td>
<td>1% TiO2+2% ZrO2</td>
<td>90</td>
<td>200</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
</tbody>
</table>

Table 4
The effect of input parameters on the physical and mechanical properties of the fabricated Nano composites system TiO2/ Y2O3-
partially stabilized zirconia (Y-PSZ) HDPE.

<table>
<thead>
<tr>
<th>Exp. No.</th>
<th>Nano ceramic fillers Powders Compositions</th>
<th>Compounding pressure (MPa)</th>
<th>Hot pressed temperature (°C)</th>
<th>Compression fracture strength (MPa)</th>
<th>Micro-Vickers Hardness Hv (kg/mm²)</th>
<th>Bulk density (gm/mm³)</th>
<th>True porosity (%)</th>
<th>Stress Safety Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1% TiO2+2% ZrO2</td>
<td>30</td>
<td>180</td>
<td>28</td>
<td>90</td>
<td>1.022</td>
<td>13.53</td>
<td>0.5641</td>
</tr>
<tr>
<td>2</td>
<td>1% TiO2+2% ZrO2</td>
<td>30</td>
<td>190</td>
<td>30</td>
<td>90.5</td>
<td>1.053</td>
<td>10.91</td>
<td>0.6044</td>
</tr>
<tr>
<td>3</td>
<td>1% TiO2+2% ZrO2</td>
<td>30</td>
<td>200</td>
<td>31</td>
<td>92</td>
<td>1.066</td>
<td>9.81</td>
<td>0.6245</td>
</tr>
<tr>
<td>4</td>
<td>1% TiO2+2% ZrO2</td>
<td>60</td>
<td>180</td>
<td>32</td>
<td>92.6</td>
<td>1.089</td>
<td>7.87</td>
<td>0.6447</td>
</tr>
<tr>
<td>5</td>
<td>1% TiO2+2% ZrO2</td>
<td>60</td>
<td>190</td>
<td>33</td>
<td>94</td>
<td>1.104</td>
<td>6.60</td>
<td>0.6648</td>
</tr>
<tr>
<td>6</td>
<td>1% TiO2+2% ZrO2</td>
<td>60</td>
<td>200</td>
<td>35</td>
<td>95</td>
<td>1.107</td>
<td>6.35</td>
<td>0.7051</td>
</tr>
<tr>
<td>7</td>
<td>1% TiO2+2% ZrO2</td>
<td>90</td>
<td>180</td>
<td>36</td>
<td>97</td>
<td>1.114</td>
<td>5.75</td>
<td>0.7253</td>
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<tr>
<td>8</td>
<td>1% TiO2+2% ZrO2</td>
<td>90</td>
<td>190</td>
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<td>98</td>
<td>1.116</td>
<td>5.58</td>
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<tr>
<td>9</td>
<td>1% TiO2+2% ZrO2</td>
<td>90</td>
<td>200</td>
<td>39</td>
<td>99</td>
<td>1.117</td>
<td>5.50</td>
<td>0.7857</td>
</tr>
<tr>
<td>10</td>
<td>5% TiO2+2% ZrO2</td>
<td>30</td>
<td>180</td>
<td>40</td>
<td>99.5</td>
<td>1.251</td>
<td>7.35</td>
<td>0.8059</td>
</tr>
<tr>
<td>11</td>
<td>5% TiO2+2% ZrO2</td>
<td>30</td>
<td>190</td>
<td>41</td>
<td>100</td>
<td>1.1233</td>
<td>7.41</td>
<td>0.8260</td>
</tr>
<tr>
<td>12</td>
<td>5% TiO2+2% ZrO2</td>
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<td>200</td>
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<td>1.125</td>
<td>7.27</td>
<td>0.8361</td>
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<tr>
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<td>180</td>
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<td>100.88</td>
<td>1.127</td>
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<td>0.8522</td>
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<td>60</td>
<td>190</td>
<td>43</td>
<td>101</td>
<td>1.129</td>
<td>6.94</td>
<td>0.8663</td>
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<tr>
<td>15</td>
<td>5% TiO2+2% ZrO2</td>
<td>60</td>
<td>200</td>
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<td>101.47</td>
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<td>6.61</td>
<td>0.8864</td>
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<tr>
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<td>5% TiO2+2% ZrO2</td>
<td>90</td>
<td>180</td>
<td>45.6</td>
<td>102</td>
<td>1.14</td>
<td>6.34</td>
<td>0.9187</td>
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<tr>
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<td>90</td>
<td>190</td>
<td>46.2</td>
<td>104</td>
<td>1.152</td>
<td>5.95</td>
<td>0.9308</td>
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<tr>
<td>18</td>
<td>5% TiO2+2% ZrO2</td>
<td>90</td>
<td>200</td>
<td>47</td>
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<td>1.157</td>
<td>4.63</td>
<td>0.9469</td>
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<tr>
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<td>10% TiO2+2% ZrO2</td>
<td>30</td>
<td>180</td>
<td>47.3</td>
<td>107</td>
<td>1.233</td>
<td>10.47</td>
<td>0.9529</td>
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<tr>
<td>20</td>
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<td>30</td>
<td>190</td>
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<td>1.245</td>
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<td>0.9630</td>
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<tr>
<td>21</td>
<td>10% TiO2+2% ZrO2</td>
<td>30</td>
<td>200</td>
<td>47.92</td>
<td>110</td>
<td>1.246</td>
<td>9.53</td>
<td>0.9655</td>
</tr>
<tr>
<td>22</td>
<td>10% TiO2+2% ZrO2</td>
<td>60</td>
<td>180</td>
<td>48</td>
<td>112</td>
<td>1.251</td>
<td>9.16</td>
<td>0.9670</td>
</tr>
<tr>
<td>23</td>
<td>10% TiO2+2% ZrO2</td>
<td>60</td>
<td>190</td>
<td>48.4</td>
<td>113</td>
<td>1.277</td>
<td>9.72</td>
<td>0.9791</td>
</tr>
<tr>
<td>24</td>
<td>10% TiO2+2% ZrO2</td>
<td>60</td>
<td>200</td>
<td>48.7</td>
<td>115</td>
<td>1.311</td>
<td>8.41</td>
<td>0.9811</td>
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<td>25</td>
<td>10% TiO2+2% ZrO2</td>
<td>90</td>
<td>180</td>
<td>49</td>
<td>117.5</td>
<td>1.323</td>
<td>3.94</td>
<td>0.9872</td>
</tr>
<tr>
<td>26</td>
<td>10% TiO2+2% ZrO2</td>
<td>90</td>
<td>190</td>
<td>49.45</td>
<td>118</td>
<td>1.344</td>
<td>2.41</td>
<td>0.9963</td>
</tr>
<tr>
<td>27</td>
<td>10% TiO2+2% ZrO2</td>
<td>90</td>
<td>200</td>
<td>50</td>
<td>120</td>
<td>1.352</td>
<td>1.83</td>
<td>1.0073</td>
</tr>
</tbody>
</table>

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Table 5
The ANOVA analysis of the compression fracture strength for all the fabricated nanobiocomposites system.

<table>
<thead>
<tr>
<th>Source</th>
<th>Sum of Squares</th>
<th>d自由度</th>
<th>Mean Square</th>
<th>F-value</th>
<th>P-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>463.61</td>
<td>3</td>
<td>154.54</td>
<td>143.38</td>
<td>&lt; 0.0001 significant</td>
</tr>
<tr>
<td>A-Nano ceramic filler Powder Composition</td>
<td>428.79</td>
<td>1</td>
<td>428.79</td>
<td>397.84</td>
<td>&lt; 0.0001</td>
</tr>
<tr>
<td>B-Compounding pressure</td>
<td>30.39</td>
<td>1</td>
<td>30.39</td>
<td>28.20</td>
<td>&lt; 0.0001</td>
</tr>
<tr>
<td>C-Hot pressed temperature</td>
<td>4.42</td>
<td>1</td>
<td>4.42</td>
<td>4.10</td>
<td>0.0546</td>
</tr>
<tr>
<td>Residual</td>
<td>24.79</td>
<td>23</td>
<td>1.08</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cor Total</td>
<td>488.39</td>
<td>26</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The ANOVA analyses used the quadratic design model for analyzing the effect of input parameters on the bulk densities responses values resulting for all the fabricated TiO2/HDPE Nanobiocomposites system as given in Table 6. The model F-value of 620.73 and the P-values less than 0.0500 implies that the model is also significant.

The final equations for prediction about the bulk density responses values without further experimental work in terms of actual factors for the both fabricated TiO2/HDPE and TiO2+2 % ZrO2/HDPE Nano ceramic fillers Compositions systems are:

Bulk density (I) = + 0.817720+0.083660* TiO2 Nano ceramic fillers contain (%) - 0.000109* Compounding pressure (MPa) - 0.001478* Hot pressed temperature (°C)  \[ (23) \]

Bulk density (II) = + 0.937383+0.022374 * TiO2+2% ZrO2 Nano filler contain (%) + 0.000835* Compounding pressure (MPa) + 0.000356 * Hot pressed temperature (°C)  \[ (24) \]

The effect of input parameters on the bulk densities values for all the fabricated TiO2/HDPE and TiO2+ 2 % ZrO2/HDPE Nano ceramic fillers Compositions systems are shown in the 3D graphs of Fig. 1. These graphs show that the bulk densities values were increased with increasing the process parameters, i.e. Nano ceramic filler contain, the compounding pressure and the hot-pressed temperature. With the increase of the TiO2 filler contain from 1% to 10 %, the value increase by 30.24 %. When using 10% TiO2 with adding 2% partial stabilized zirconia (Y-PSZ), hot pressed temperature of 200 °C and compounding pressure of 90 MPa, this value is further increase by 13.91%. The reasons for this increase in the bulk densities values is that the added ceramic Nano filler materials have four to five times the density of the high-density polyethylene (HDPE) matrix and the excellent bonding between their particles.

Table 6
The ANOVA analysis of the bulk densities responses for all the TiO2/HDPE Nanobiocomposites system.

<table>
<thead>
<tr>
<th>Source</th>
<th>Sum of Squares</th>
<th>d自由度</th>
<th>Mean Square</th>
<th>F-value</th>
<th>P-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>0.3983</td>
<td>9</td>
<td>0.0443</td>
<td>620.73</td>
<td>&lt; 0.0001 significant</td>
</tr>
<tr>
<td>A-TiO2 Nano ceramic fillers Powders</td>
<td>0.3747</td>
<td>1</td>
<td>0.3747</td>
<td>5254.80</td>
<td>&lt; 0.0001</td>
</tr>
<tr>
<td>Compositions</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B-Compounding pressure</td>
<td>0.0030</td>
<td>1</td>
<td>0.0030</td>
<td>41.51</td>
<td>&lt; 0.0001</td>
</tr>
<tr>
<td>C-Hot pressed temperature</td>
<td>0.0007</td>
<td>1</td>
<td>0.0007</td>
<td>9.65</td>
<td>0.0064</td>
</tr>
<tr>
<td>AB</td>
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<td>1</td>
<td>0.0005</td>
<td>6.56</td>
<td>0.0202</td>
</tr>
<tr>
<td>A²</td>
<td>0.0316</td>
<td>1</td>
<td>0.0316</td>
<td>443.79</td>
<td>&lt; 0.0001</td>
</tr>
<tr>
<td>Residual</td>
<td>0.0012</td>
<td>17</td>
<td>0.0001</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cor Total</td>
<td>0.3995</td>
<td>26</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(a) Hot pressed temperature (180 °C)  
(b) Hot pressed temperature (190 °C)
The effect of compression fracture strengths and the Nano ceramic fillers contents on the bulk densities values for the fabricated TiO$_2$/HDPE and TiO$_2$+2 % ZrO$_2$/HDPE Nano composites systems are shown in Fig. 2 (a) and (b), respectively. The bulk densities values were increased with increasing the compression fracture strength and the Nano ceramic filler contain, reached its maximum values as 1.164 kg/mm$^2$ for the first Nano Compositions system and with the adding of 2% partial stabilized zirconia (Y-PSZ) this value increased to 1.352, i.e. increased by 13.91 %.

(a) Fabricated system (I) / TiO$_2$/HDPE Nano composites
(b) Fabricated system (II) / TiO$_2$+2 % ZrO$_2$/HDPE Nano composites

The reason for this increase in the bulk densities values is the increase of the ceramic Nano filler contents added to the fabricated biomaterials systems. These Nano ceramic materials with their high densities values and their high correlation with the molecules of the matrix under high pressure and heat produced a high strengths and densities biocomposites materials closed to the specifications of human natural bone, making them at the forefront of materials in the processes of grafting and repair bones operations. The final prediction equations for the effect of
compression fracture strength and the Nano ceramic fillers contains on the bulk densities values for the both fabricated compositions systems are:

\[
\text{Bulk density (I)} = -0.975668 - 0.036289 \times \text{TiO}_2\text{ Nano ceramic filler Composition} + 0.113936 \times \text{TiO}_2\text{ Nano ceramic filler Composition}
\]
\[
\text{Compression fracture strength (MPa)}
\]

\[
\text{Bulk density (II)} = +0.986515 + 0.018955 \times \text{TiO}_2 +2\% \text{ ZrO}_2\text{ Nano filler contain} + 0.002076 \times \text{TiO}_2 +2\% \text{ ZrO}_2\text{ Nano filler contain}
\]
\[
\text{Compression fracture strength (MPa)}
\]

The final prediction equations for the true porosities responses values for the both fabricated TiO\(_2\)/HDPE and TiO\(_2\)+ 2 % ZrO\(_2\)/HDPE Nano ceramic fillers compositions systems are:

\[
\text{True porosity (I)} = + 21.50085 - 5.52285 \times \text{TiO}_2\text{ Nano ceramic fillers contain} - 0.027231 \times \text{Compounding pressure} + 0.080767 \times \text{Hot pressed temperature}
\]

\[
\text{True porosity (II)} = + 28.84149 - 0.152086 \times \text{TiO}_2 +2\% \text{ ZrO}_2\text{ Nano filler contain}-0.083056 \times \text{Compounding pressure} - 0.084333 \times \text{Hot pressed temperature}
\]

Fig. 3 shows the effect of input parameters on the percentages values of true porosity for all the fabricated TiO\(_2\)/HDPE and TiO\(_2\)+ 2 % ZrO\(_2\)/HDPE Nano bio compositions systems. These graphs show that the percentages true porosity values were decreased with increasing the process parameters, i.e. Nano ceramic filler contain, the compounding pressure and the hot-pressed temperature. With the increase of the TiO\(_2\) filler ceramic contain from 1% to 10 %, the value percentages true porosity decreases by 48.68 %. When using 10% titanium oxide Nano ceramic powder (TiO\(_2\)) with adding 2% partial stabilized zirconia (Y-PSZ), hot pressed temperature of 200 °C and compounding pressure of 90 MPa, this value is further decrease by 84.85 %, i.e. the percentages true porosity values were decreased from 17.38 % to the minimum value of 1.83 %. These figures show also that the addition of a small percentage of partial stabilized zirconia (Y-PSZ) led to stability of the true porosity values with increasing the TiO\(_2\) filler ceramic contain proportion as shown in the Fig. 3 (d), (e) and (f). These results are evidence of a remarkable degree of porosity of the produced Nano biomaterials for orthopedic that are appropriate to the various patient's clinical conditions and the degree of osteoporosis. The reason for this low degree of percentages values of true porosity obtained, which is very close to the natural human bones properties, is the use of nanomaterials in the fabricating and secondly in the same fabricating process by using the hot nanoparticles powder pressed method instead of the traditional melting methods.

Fig. 4 shows the effect of compression fracture strength obtained from experimental results and the Nano ceramic fillers contains on the percentages values of true porosity for all the fabricated Nano compositions systems. The percentages true porosity values were decreased with increasing the compounding pressure and the hot-pressed temperature. With the increase of the TiO\(_2\) filler ceramic contain from 1% to 10 %, the value percentages true porosity decreases by 33.34 %. When using 10% titanium oxide Nano ceramic powder (TiO\(_2\)) with adding 2% partial stabilized zirconia (Y-PSZ), hot pressed temperature of 200 °C and compounding pressure of 90 MPa, this value is further increased by 22 %. In a previous study on investigated the injection molded 5 % TiO\(_2\)/HDPE Nano ceramic compositions, the maximum compression strength it reached to 26.3 MPa [15], while for PEEK femoral component is 30 MPa [30], and equal to 12.5 MPa achieved when composite having composition of 70% LDPE+10% TiO\(_2\) +20% Al\(_2\)O\(_3\) was used [31], i.e. the maximum compression strength for this study is higher by 90.11% than the previous mentioned studies. The final prediction equations for the effect of compression fracture strength on the true porosities for the both fabricated compositions systems are:

\[
\text{True porosity (I)} = + 62.46377 + 1.73782 \times \text{TiO}_2\text{ Nano ceramic filler Composition} - 1.82694 \times \text{TiO}_2\text{ Nano ceramic filler Composition}
\]

\[
\text{Compression fracture strength (MPa)}
\]

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True porosity (II) = + 27.60304 + 0.834508 * TiO$_2$ + 2% ZrO$_2$ Nano filler contain - 0.599033 * Compressional fracture strength (MPa) 

(30)

Fig. 3
The 3D graphs for the effect of input parameters on the true porosities values for all the fabricated TiO$_2$/HDPE and TiO$_2$+2% ZrO$_2$/HDPE Nano ceramic fillers Compositions systems.

Fig. 4
The effect of compression fracture strength and the Nano ceramic fillers contains on the percentages values of true porosity.
The effect of compression fracture strength and the Nano ceramic fillers contains on the Vickers micro hardness values; (a) for the fabricated system (I) / TiO₂/HDPE Nano composites; (b) for the fabricated system (II) / TiO₂ +2% ZrO₂/HDPE Nano composites.

Fig. 5 (a) and (b) show the effect of compression fracture strengths and the Nano ceramic fillers contains on the micro-Vickers Hardness values for the both fabricated TiO₂/HDPE and TiO₂ +2% ZrO₂/HDPE Nano compositions systems, respectively. The micro-Vickers Hardness reached its maximum values with increasing the compression fracture strength and the Nano ceramic filler contain, as 92.23 gm/mm² for the first Nano Compositions system. With the adding of 2% partial stabilized zirconia (Y-PSZ) this value increased to 120 gm/mm², i.e. increased by 30.11%. The increase in the micro-Vickers Hardness values are due to the increase of the high strengths ceramic Nano filler contents added to the fabricated biomaterials systems. The final prediction equations for the effect of compression fracture strength and the Nano ceramic fillers contains on the micro-Vickers Hardness values for the both fabricated compositions systems are:

Micro-Vickers Hardness (I) = + 9.68811 - 5.47079 * TiO₂ Nano ceramic filler Composition + 4.71726 Compression fracture strength (MPa) (31)

Micro-Vickers Hardness (II) = + 70.94106 + 1.11439 * TiO₂+2% ZrO₂ Nano filler contain + 0.628565 * Compression fracture strength (MPa) (32)

Fig. 6
The boundary conditions for the femur bone ANSYS models for the bodies of patients weights with 70, 100 and 130 kg.
3.2 ANSYS modeling for stress distribution

The human femur bone 3D model to simulate the stress and strain fields corresponding to the patient activities was implemented by using the Solid works and analyzed by using the finite element module ANSYS workbench 15.7. The cortical bone is asymmetric and anisotropic in tension and compression. To predict bone failure and response, an orthotropic symmetric model was recommended utilizes the elastic-plastic constitutive, symmetric and isotropic models [32]. The femur bone mechanical properties for an adult human femur are; density =1.75 g/m³, Young’s modulus = 16.7 GPa, ultimate tensile strength = 43.5 MPa, ultimate compressive strength = 115.3 MPa and the Poisson’s ratio for both bone layers = 0.3 [1, 24].

The external loads applied at the head of the bone corresponding to periodic cycles of patient’s activities with 70, 100 and 130 kg body patient weights, respectively (or approximately two times normal body weight). The femur bone head-implant systems was loaded with 700, 1000 and 1300 N axial, lateral 100, 140 and 185 N loads and torsional moment of 10.0, 14.0 and 18.5 Nm. At the lower medial condyle surface of the fixed support is provided and the displacement is restricted in all directions [23-25, 33].

![Fig. 7](image)

**Fig. 7**
The maximum equivalent von-Misses Stresses obtained to withstand the patients body weights with 70, 100 and 130 kg.

The boundary conditions for the femur bone ANSYS models for the bodies of patients weights with 70, 100 and 130 kg are shown in Fig. 6 (a), (b) and (c), respectively. The maximum equivalent von-Misses stresses obtained to withstand the highest stresses producing during daily activities for prepared and fabricated Nano composites for bones repairs equal to 39.96, 56.30 and 74.01 MPa, which they represent the stresses resulting from the loads for the above three bodies of patients weights as shown in Fig. 7 (a), (b) and (c), respectively. The distribution of these stresses shows that the location of maximum equivalent von-Misses stresses, is in the middle portion of the bone with the lowest cross-sectional area where the fractures in various incidents are confirmed by most cases. In a previous study, the implemented femur bone maximum equivalent von-Misses Stresses obtained for axisymmetric loads natural femur bone equal to 29.64 MPa [21], and for natural femur bone ranged between 22 MPa and 26 MPa [9]. This means that the nanocomposites systems produced in the current work withstand higher stresses than the natural bone by 52.65 % and by 34.82 % higher than the previous study just mentioned.

Figs. 8 and 9 show the effect of input parameters for the fabricated Nano composites systems (I) and (II), respectively on the stress safety factors values for different Nano ceramic fillers Powders compositions according to the correspondents equivalent von-Misses stresses resulted from the external loads applied at the head of the bone for patient’s activities with 70, 100 and 130 kg body patient weights (at 90 MPa compounding pressure and 200 °C hot pressed temperature), respectively.
As shown in these figures, the value of the stress safety factors was increased with increasing the ceramic filler contains, the hot-pressed temperature and the compounding pressure. The results show that when increasing the Nano ceramic filler contains from 1% to 10 %, the stress safety factors increase by 58.38 %. When adding 2 % of zirconia (ZrO₂), the stress safety factors reached its maximum values, with an additional increase in its value by 21.42 % as shown on the 3D graphs Fig. 10 (a) and (b). The increase in the stress safety factors values can be returned to the adding of the high mechanical properties of the ceramic Nano filler materials and excellent bonding properties with the HDPE polymer matrix.

Fabricated Nano composites system (I)

Patient weights

70 kg

100 kg

130 kg

(a)

(b)

(c)

1 (%) TiO₂/ HDPE

(d)

(e)

(f)

5 (%) TiO₂/ HDPE

(g)

(h)

(i)

10 (%) TiO₂/ HDPE

Fig. 8

The effect of the input parameters for the fabricated Nano composites system (I) on the stress safety factors for different Nano ceramic fillers compositions and patient’s bodies weights (at 90 MPa compounding pressure and 200 °C hot pressed temperature).
Fig. 9
The effect of the input parameters for the fabricated Nano composites system (I) on the stress safety factors for different Nano ceramic fillers compositions and patient’s bodies weights (at 90 MPa compounding pressure and 200 °C hot pressed temperature).

The final prediction equations for the effect of process input parameters on the stress safety factors values for the both fabricated compositions systems are:

\[
\text{Stress safety factors (I)} = + 1.05751 + 0.015519 \times \text{TiO}_2 \text{Nano filler contain (%) } - 0.005765 \times \text{Patient weights}
\]  

(33)
Stress safety factors (II) = + 1.28882 +0.018082* TiO_2+2% ZrO_2 Nano filler contain (%) - 0.007003 * Patient weights

![Graphs](image)

**Fig.10**
The 3D graphs for the effect of the input parameters for the fabricated Nano composites systems on the stress safety factors values for different Nano ceramic fillers Powders compositions and patient’s weights.

## 4 CONCLUSIONS

After study and analysis of the effect of all parameters that influences the obtained qualities for the fabricated Nano biocomposites systems, the following conclusions can be drawn:

1- The results show that the bulk densities, the stress safety factors values for all the fabricated TiO_2/HDPE and TiO_2+ 2% ZrO_2/HDPE Nano ceramic fillers Compositions systems were increased with increasing the process parameters, while the percentages values of true porosity were decreased.

2- With the increase of the TiO_2 filler to 10 %, the value bulk densities increase by 30.24 % and when adding 2% partial stabilized zirconia (Y-PSZ), this value is further increase by 13.91%, i.e. reached its maximum values as 1.164 kg/mm² for the first Nano system and to1.352 for the second system, respectively.

3- The percentages true porosity values were decreased with increasing the compression fracture strength reached its minimum values as 8.92 % for the first TiO_2/HDPE Nano Compositions system. With the adding of 2% partial stabilized zirconia (Y-PSZ), this value was decreased to 1.83 %, i.e., these values were decreased by 48.68 % and by 84.85 %, respectively.

4- The obtained values of the compression fracture strength show that these values were increased with increasing the process parameters by 33.34 % for the first fabricated Nano system. When adding 2% partial stabilized zirconia this value is further increased by 22 %. The maximum compression strength for this study is higher by 90.11% than the previous mentioned studies.

5- The micro-Vickers Hardness reached its maximum values with increasing the compression fracture strength, reached 92.23 gm/mm³ for the first Nano Compositions system. With the adding of 2% partial stabilized zirconia (Y-PSZ) this value increased to120 gm/mm³, i.e. increased by 30.11 %.

6- The maximum equivalent von-Misses Stresses obtained from ANSYS models equal to 39.96, 56.30 and 74.01 MPa, resulting from the three bodies of patients weights and the nanocomposites systems produced in the current work withstand higher stresses than the natural bone by 52.65 higher than the previous studies.

7- The results show that when increasing the Nano ceramic filler contains from 1% to 10 %, the stress safety factors increase by 58.38 %. When adding 2 % of zirconia (ZrO_2), the stress safety factors reached its maximum values, with an additional increase in its value by 21.42 %.

## REFERENCES


