Research Article

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Structural, physical, and mechanical properties of the TiO₂ added hydroxyapatite composites

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Abstract: Composites are important as they have been used in a variety of different fields. Therefore, production and testing of composites have become one of the most popular topics for researchers. In this work, the physical, structural, and mechanical properties such as packing density (Vₚ), bond dissociation energy (Gᵢ), Young’s (E), bulk (B), shear (S), longitudinal (L), and indentation (E*) moduli, and Poisson’s ratio (ν) were obtained for (100 − x) HAP + xTiO₂ composite, where x = 0, 3, 7.5, and 10 wt%.

The variations in those properties with TiO₂ rate in HAP composites were tested.

Keywords: mechanical properties, hydroxyapatite composite, analytical method

1 Introduction

The composite materials which are composed of different components are recently the most popular materials and may be an effective material for many different purposes. Therefore, structural, physical, and mechanical properties of composites should be known as those parameters are vital in order to use these composites. It is also important to improve these properties by reinforcement of some other materials into composite [1–5]. Besides the other parameters, the physical parameters, dissociation energy, packing density and mechanical properties which are Young’s (E) modulus, bulk (B) modulus, shear (S) modulus, longitudinal (L) modulus, indentation (E*) modulus, and Poisson’s (ν) ratio are also important. There have been many different works done for this kind of purposes using different methods [6–35].

The main goal of this work is obtaining different types of materials by reinforcing different rates of TiO₂ into hydroxyapatite (HAP)-based composite materials and calculating some important physical and mechanical properties of these composites. This will also provide to test TiO₂ effect on these parameters. The calculations are done using Makishima and Mackenzie Model (MMM) via the analytical method.

2 Materials and methods

The physical, structural, and mechanical properties of four different types of HAP composite and the effect of TiO₂ on the properties of these composites have been investigated. HAP is one of the main inorganic components of bones and teeth which are important to human health. It is also utilized as an implant for bone substitute due to its excellent biocompatible properties [1–3]. Thus, HAP-based composite materials show significant properties in the field of biomedical applications. The chemical composition and also density of composite formulated as (100 − x)HAP + xTiO₂ is given in Table 1.

The mechanical properties of composites have been obtained using a model developed by Makishima and Mackenzie [39]. The model estimates the values of Young’s modulus (E, GPa), the bulk modulus (B, GPa), shear modulus (S, GPa), longitudinal modulus (L, GPa) Poisson’s ratio (ν), and indentation modulus (E*, GPa). In this model, with the help of the bond dissociation energy, Gᵢ (kJ cm⁻³) and the packing density (Vₚ, cm³ mol⁻¹) of the investigated materials, other structural and mechanical features are obtained. These characteristics are extracted through equations (1)–(9) [36–39]:

\[
G_i (kJ cm^{-3}) = \sum_i G_i x_i, \quad (1)
\]

\[
V_p (cm^3 mol^{-1}) = \frac{4\pi}{3} N_0 (XR_i^3 + YR_i^3), \quad (2)
\]

\[
V_f (cm^3 mol^{-1}) = \frac{\rho}{M} \sum_i V_i x_i, \quad (3)
\]

\[
E (GPa) = 2V_f G, \quad (4)
\]

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Table 1: The chemical components of (100 – x) HAP + xTiO2 composite

| Composite code | Chemical composition (wt%) | Density (g cm⁻³) |
|----------------|---------------------------|-----------------|
|                | HAP | TiO₂ |                |                |
| S1             | 100 | 0    | 3.140          |
| S2             | 97  | 3    | 3.192          |
| S3             | 92.5| 7.5  | 3.27           |
| S4             | 90  | 10   | 3.3133         |

(1) $B$ (GPa) = $1.2V\sigma$,  
(2) $S$ (GPa) = $\frac{3EB}{9B - E}$,  
(3) $L$ (GPa) = $B + \frac{3}{4}S$,  
(4) $\sigma = 0.5 - \frac{1}{7.2}V_t$,  
(5) $E^*$ (GPa) = $\frac{E}{1 - \sigma^2}$,  

where $N_A$, $R_A$, $R_O$, $X$, and $Y$ represent Avogadro’s number, ionic radius of the metal, ionic radius of oxygen, the number of metal atoms, and the number of oxygen atoms, respectively.

3 Results and discussions

Using MMM, the structural and mechanical features of the composite samples are extracted and the results were discussed. These parameters are obtained based on some mechanical components like packing density ($V_t$, cm³ mol⁻¹) and bond dissociation energy ($G_t$, kJ cm⁻³) which are listed in Table 2 for S1–S4 samples. The obtained structural, physical, and mechanical properties of the chosen samples are represented graphically in Figures 1–3.

Table 2: Some of the mechanical components of HAP + TiO₂ samples

| Sample code | $V_t$ (cm³ mol⁻¹) | $G_t$ (kJ cm⁻³) |
|-------------|------------------|-----------------|
| S1          | 0.755173         | 256.988         |
| S2          | 1.065676         | 190.000         |
| S3          | 1.51004          | 164.0664        |
| S4          | 1.748149         | 162.0022        |

Figure 1: Bond dissociation energy and packing density vs TiO₂ ratio for chosen HAP samples.

Figure 2: Mechanical moduli vs TiO₂ ratio for chosen HAP samples.
The obtained bond dissociation energy \( (G_t, \text{kJ cm}^{-3}) \) and packing density \( (V_t, \text{cm}^3\text{mol}^{-1}) \) vs TiO\(_2\) ratio are plotted in Figure 1. As it is seen from this figure that on increasing the rate of TiO\(_2\) from 0 to 10\%, a sharp reduction is reported for \( G_t \) from 256.988 (kJ cm\(^{-3}\)) to 162.0022 (kJ cm\(^{-3}\)). This may be due to replacing low \( G_t \) materials like TiO\(_2\) with high \( G_t \) materials. But a different trend is observed for \( V_t \) vs TiO\(_2\) ratio, which shows the strong linearity between TiO\(_2\) concentration and packing factor \( (V_t) \). In other words, increasing the rate of TiO\(_2\) causes an increase in the \( V_t \) values from 0.755173 (cm\(^3\) mol\(^{-1}\)) to 1.748149 (cm\(^3\) mol\(^{-1}\)) for S1–S4 samples.

The mechanical moduli such as \( E, B, S, L, E^*, \) and \( \sigma \) vs TiO\(_2\) ratio are represented in Figures 2 and 3. As expected, increasing the TiO\(_2\) concentration from 0–10\% causes an increase in the values of the \( E, B, S, L, E^*, \) and \( \sigma \) from 388.1408, 388.1408, 147.4606, 462.3315, 0.604885, and 612.0994 to 566.4078, 1188.198, 199.362, 199.362, 0.742798, and 1263.595, respectively. This means TiO\(_2\) is a positive material to enhance the shielding capacity of the studied HAP samples. Figure 4 shows the mechanical moduli vs density. From the obtained results it can be understood that by increasing the TiO\(_2\) concentration from S1 to S4 samples, the samples’ density
increases from 3.140 to 3.3133 g cm$^{-3}$. Any increase in the density value accounts for improvement in the stiffness of the S samples. Consequently, the mechanical moduli which is our main concern in this study.

4 Conclusion

The present study aims to investigate the physical, structural, and mechanical characteristics of the HAP + TiO$_2$ samples. These bio-composites are widely used in the human body as bone and teeth tissues. In order to enhance mechanical features, TiO$_2$ of different rates is inserted into HAP bio-composites. Outcomes show that TiO$_2$ is a positive material to improve the mechanical features of the S sample. This behavior may be due to the increase in the density of the S samples from S1 to S4, which improves the stiffness of the HAP samples, and consequently the mechanical moduli will enhance.

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