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Finite element modeling and simulation of the mechanical properties of chitin/graphene composite material and bone using ls-dyna software

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Abstract. The study uses LS-Dyna software to address the finite element modeling and simulation of the mechanical properties of chitin/graphene composite material and cortical bone. Properties such as density, Young's modulus, and tensile strength were characterized experimentally and compared with numerical simulations. CAD models were prepared for the pig bone and the chitin/graphene composite, applying uniaxial loading conditions and analyzing the stress distribution (Von Mises, Tresca) and plastic deformations. The results showed a significant discrepancy between the experimental and simulated values, with relative errors of 69.67% for bone and 97.36% for composite. Although the simulation identified critical fracture zones and nonlinear behavior, the simulated tensile strength values were lower than those of experiments and those reported in the literature, suggesting the need to optimize model parameters and the composition of the composite material.

Keywords: Ls Dyna, bone, Chitin-graphene, mechanical properties

1 Introduction

The high demand for advanced biomaterials with high-performance mechanical properties has driven research into polymer composites for biomedical applications, thanks to their biodegradability, biocompatibility, and antimicrobial properties. Chitin, which is a biodegradable polysaccharide [1] obtained from cellulose, is found in fungi, the exoskeleton of insects and the shells of crustaceans [2][3], such as shrimp and crabs [4], obtained by deproteinization and demineralization [5] However, its relatively low mechanical strength [6][7] limits biomedical applications around its tensile strength. To address this problem, the graphene solution has been explored as a reinforcement base thanks to its rigidity and its physicochemical properties, which includes Young's modulus, fracture resistance, thermal conductivity [8][4], thanks to its hexagonal structures to improve the load capacity. The reagents chosen to produce GO are concentrated H_2SO_4, nitric acid, hydrochloric acid, and graphite powder [9] by the Hummer method [10]. Chitin/graphene-based composite materials, which combine the distinctive properties of each component, offer innovative solutions in the field of regenerative medicine and tissue engineering [11].

Bone, a complex and dynamic tissue composed mainly of collagen and hydroxyapatite, with a hierarchical structure that gives it strength and toughness, plays an important role in the study of mechanical properties. Bone is a bone material that has complex structural characteristics, such as heterogeneity and hard fragility [12]. In the field of regenerative medicine, bone is a very interesting tissue [13] because it can regenerate and remodel itself throughout life. However, biomaterials emerge as a promising alternative for restoring bone function when a bone injury or disease compromises its natural repair capacity. Most of the scaffolds studied for bone regeneration include natural polymers, such as chitosan, hyaluronic acid (HyA), and collagen (COL) [14]. These biomaterials replicate the mechanical and biological properties of bone [14].

Chitin/graphene-based composite materials, which combine the distinctive properties of each component, this bio-based material were chosen as an alternative to synthetic polymers due to their competitive production cost, their non-toxicity, their solubility in water, their compatibility with nanomaterials, their biodegradability and bioadsorbability [15].

Despite the advances reported in the literature on chitin-graphene composites, predictive modeling of their mechanical properties under different loading conditions remains underexplored. Finite element analysis (FEA)

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with LS-DYNA provides advantages to experimental results by allowing numerical experimentation in a controlled virtual environment [16], a leading software in nonlinear dynamic simulations, offers a robust framework to optimize material composition, predict failure mechanisms, and reduce experimental costs before physical prototyping. By using finite element analysis, the strain rate can be increased, the yield strength as well as the tensile strength can be increased[17]. Therefore, numerical models are often introduced to comprehensively study the impact behavior of a composite structure. For comparison purposes, this work uses homogeneous finite element (FE) models to simulate the impact failure of the composite panels studied, ignoring the geometric characteristics of the fabric and focusing mainly on the effect of the effective properties [18].

2 Methodology

A comparative study was conducted between chitin/graphene and pig leg bones, which have a similar arrangement and shape to those of humans and are widely used in anatomical and medical studies. The mechanical properties of the chitin/graphene composite material, such as surface roughness (Ra), Vickers hardness (HV), apparent density (ρ), and tensile strength, were characterized experimentally. Chitin is obtained from the shell of brown shrimp by the chemical method of deproteinization and demineralization[19], graphene is obtained from pyrolytic graphite by spraying with strong acids (H2SO4, HNO3, HCl) [20], then the two obtained materials are mixed by stirring to form the chitin/graphene composite material.

For the preparation of the bone specimens [21], fresh bones were obtained from the pig's leg and then prepared using a bone preservation technique in hydrogen peroxide. The pig's leg is disarticulated using dissection equipment. Next, we remove the soft tissue, wash it with boiling water, and immerse the bones in 3% hydrogen peroxide for 24 hours. Then, we wash them again with boiling water until the remaining soft tissue is removed. We then wash them with boiling water, removing the remaining soft tissue. The bones are then placed in one part boiling water with two parts 5% acetic acid, and cooked for 5 hours, then washed with boiling water. Then, the bones are placed in 3% hydrogen peroxide for 1 hour and finally washed with boiling water and the bones are dried in an oven at 100° for 48 hours Fig. 1. Mechanical properties such as surface roughness (Ra), Vickers hardness (HV), apparent density (ρ) and tensile strength were experimentally characterized according to ASTM D638-10.

Fig. 1. a) Chitin/graphene samples. b) Bone samples

For the comparison study, the multi-scale method is developed. Generating the model with the help of CAD software and exporting it as a step or iges file, establishing a model and finite elements of the bone of the composite material. Within the control charts, the linear material with plastic characteristics is created with the experimental properties of each material analyzed, such as density, Young's modulus, Poisson's ratio, yield stress, and maximum deformation with their corresponding units. Next, in the Shell type materials section, with 2mm thicknesses, to obtain the stress vs. strain graphs. After that, assign the section and the material to the previously meshed model and apply the boundary conditions, with one end fixed and the other end moving on the X axis to apply a displacement speed. Establish the control charts to perform the simulation, including the simulation time and the data plotting time when being analyzed. The analysis is generated with the established conditions, observing the behavior and making the necessary corrections if necessaryFinally, export the data from the generated results, including the Von Mises stress and maximum unit strain graphs, to create the stress-strain curve with the generated simulation.

For the mechanical properties, the parameters obtained experimentally were assigned as indicated in Table 1. The model was analyzed as a Piecewise linear plasticity material, to which the mechanical properties of bone, detailed below, and the stress vs. deformation graph obtained experimentally were added.

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Table 1. Experimental parameters

Material	Density (Kg/mm^3)	Young's Modulus (GPa)	Poisson's ratio	Yield stress (GPa)	Hardness (HD)
Bone	1.159E-06	2.4316499	0.3	0.001258	88,6
Chitin/graphene	6.91E-07	0.74059	0.2	0.00201	76,69

Tensile test simulation in LS Dyna software - Preparation of the cortical bone model

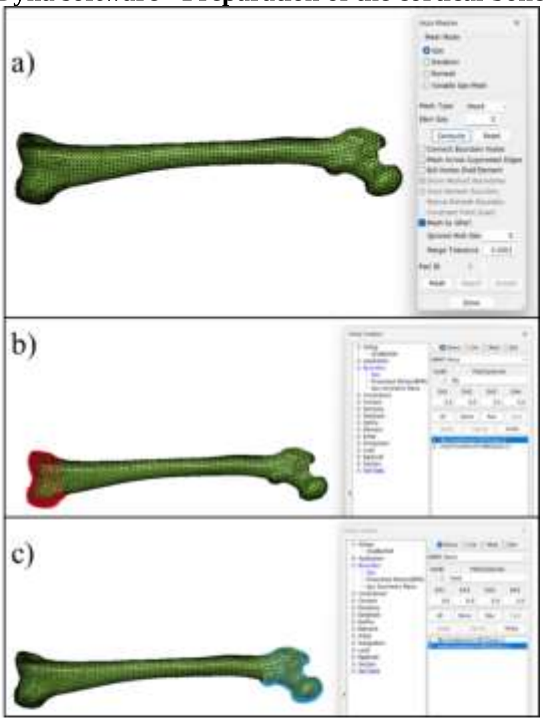

Fig. 2. a) Meshed cortical bone model. b) Nodes constrained in all degrees of freedom. c) Free nodes on the X axis

In Fig. 2a, the model was meshed with Shell-type elements combined between quadrilateral and triangular shapes, with a total of 6120 elements with sizes up to 5 mm. It has a 2 mm-thick section and an initial length of 361 mm.

Fig. 2 b shows the model graph and how the set of nodes was generated at each of the ends to be restricted and give degrees of freedom. On the far left, the nodes are fixed so that they do not move or rotate along the axes. On the right end, the displacement on the X axis is left free, and a speed of 1 mm/min was added to it, which was tested experimentally as indicated in Fig. 2c.

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Preparation of the ASTM D638 Type 1 specimen model with the Chitin/graphene composite material

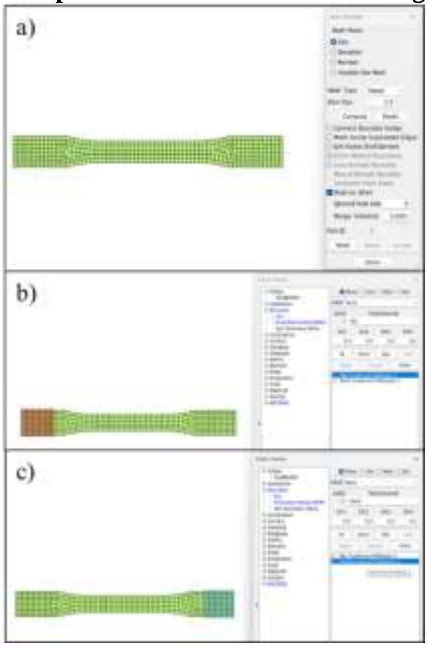

Fig. 3. a) Chitin/graphene mesh specimen. b) Nodes constrained in all degrees of freedom. c) Free nodes on the X axis

The test piece was meshed with combined shell-type elements combining quadrilateral and triangular shapes, with a total of 439 elements, with a size of up to 2.5 mm. It has a 2.5 mm-thick section, and an initial length of 165 mm as indicated in Fig. 3a.

The model graph is shown in Fig. 3 b), where a set of nodes was generated at each of the ends to be restricted and give degrees of freedom. On the far left, the nodes are fixed so that it does not move or rotate on the axes.

On the right end, the movement on the X axis is left free, and a speed of 1 mm/min is added to the speed that was experimentally tested (Fig. 3c).

3 Results

Bone simulation results

Once the analysis is performed, the effective Von Mises stress can be observed, obtaining a maximum stress of 6.52E-04 GPa in the fracture zone. The color transition (not shown but inferred) indicates a non-uniform distribution, typical of stress concentrations in complex geometries. Higher values (>5E-04) suggest critical areas where the material could fail. Low values (<2E-04) correspond to regions with minimal deformation or structural support (Fig. 4).

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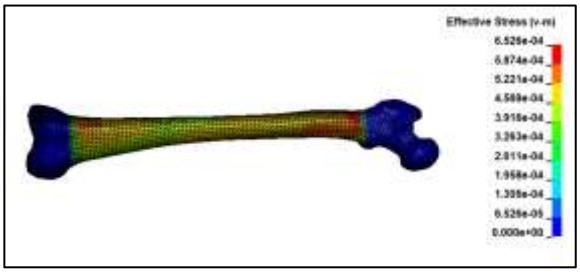

Fig. 4. Effective Von Mises stress in bone simulation

Finally, the bone breaks at the point of failure where the stress is concentrated.

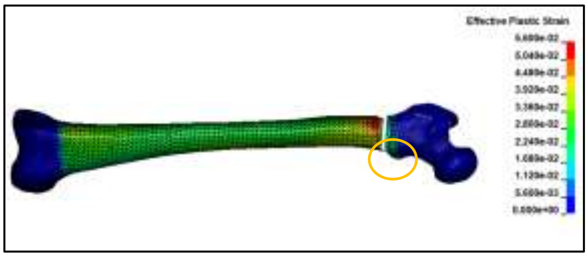

Fig. 5. Fracture in bone tensile simulation

Model Validation

After performing the simulation using finite element software, the stress-strain graphs generated experimentally are compared with those generated by the program (Fig. 6).

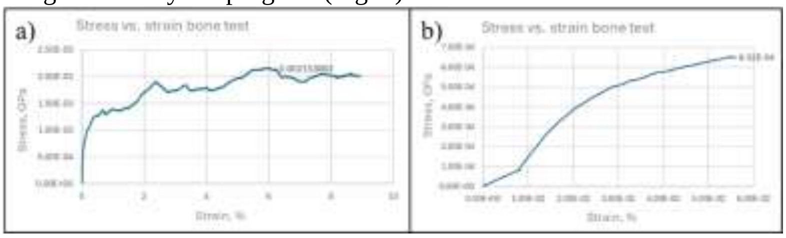

Fig. 6. a) Stress vs. strain curve of bone test. b) Stress vs. strain curve of bone simulation

In the curve in Fig. 6a, a maximum stress value of 2.15E-03 GPa can be observed, while the data generated by the simulation in Fig. 6 b show that the stress reaches a value of 6.52E-04.

The percentage of relative error is established:

$$\text{Percentage Error} = \frac{2.15\text{E}{-03} - 6.52\text{E}{-04}}{2.15\text{E}{-03}} * 100 = 69.67\% \qquad (1)$$

Results of the Chitin/Graphene Composite Material

After carrying out the analysis, the effective Von Mises stress can be observed in Fig. 7 with a maximum stress of 5.627e-05 GPa in the central area of the specimen. This provides a clear visual representation of the magnitude of the effective stresses at each point in the model.

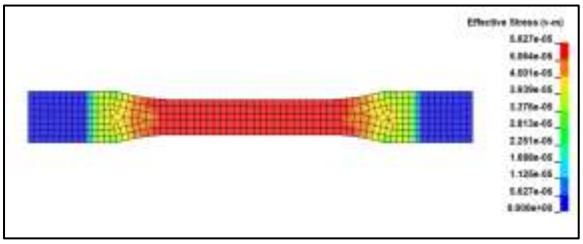

Fig. 7. Von Mises stress simulation of chitin-graphene specimen

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Finally, the ASTM D638 type 1 test piece breaks with the mechanical properties of the Chitin-graphene composite material.

Fig. 8. Fracture in the tensile simulation of the chitin-graphene specimen

Model Validation

After performing the simulation using finite element software, the stress-strain graphs generated experimentally are compared with those generated by the program.

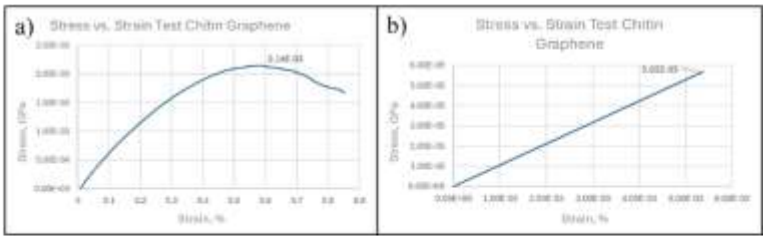

Fig. 9. a) Stress vs. strain curve of chitin-graphene test. b) Stress vs. strain curve of chitin-graphene simulation.

In the curve in Fig. 9a the maximum stress value is 2.14E-03 GPa, while in the data generated with the simulation shown in Fig. 9b the stress reaches a value of 5.65E-05. For which the percentage of relative error is determined:

$$\text{Percentage Error} = \frac{2.14\text{E}{-}03 - 5.65\text{E}{-}05}{2.14\text{E}{-}03} * 100 = 97.36\% \quad (2)$$

4 Discussions

According to the experimental data of the tensile strength of chitin/graphene composite, a maximum average value of 15.21 MPa was obtained with a 15 ml graphene solution about that obtained by the software, which obtained values between 0.0565 to 2.14 MPa. In the literature, experiments with chitin nanocrystals reached maximum values of 10.4 MPa [7]. The incorporation of certain compounds to optimize the mechanical resistance of chitin has been essential, given that the results range between 15 and 30 MPa [22]. These values show that by altering the percentages of composites about chitin, increasing these mechanical properties leads to experimenting with specific percentages of graphene that achieve better stability of the composite [23].

Simulations performed using LS-DYNA proved to be a valuable tool for modeling the mechanical behavior of both bone and composites. The software's ability to handle anisotropic and strain-rate-dependent material models is crucial to accurately represent bone response under various loading conditions. Modeling chitin-graphene composites in LS-DYNA requires careful selection of material models that can capture the interactions between the chitin matrix and the graphene reinforcement [21]. The study demonstrates that LS-DYNA simulation allows for the evaluation of how graphene reinforces the mechanical properties of chitin composites, bringing them closer to the strength of trabecular bone, combining biocompatibility and biodegradability for applications in bone substitutes. Although LS-DYNA facilitates modeling its behavior under load, there is a need to investigate its long-term performance in biological environments, optimize the chitin-graphene interface, analyze graphene dispersion in osseointegration, and develop more accurate constitutive models that improve the prediction of its clinical performance.

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5 Conclusions

Despite the differences, the material demonstrated promising mechanical properties, with experimental tensile strength of up to 15.21 MPa, comparable to existing biomaterials, although lower than theoretical values (30 MPa).

Simulations allowed for the visualization of stress concentrations and fracture points, useful for predicting structural failures and optimizing designs in biomedical applications.

The combined experimental-simulation approach highlights the importance of validating computational models with real-world data to improve their accuracy in biomechanical studies.

It is suggested that parameters such as the proportion of graphene, particle size, and loading conditions be adjusted in simulations to reduce errors and increase the mechanical strength of the composite, facilitating its application in regenerative medicine.

The relative error results (69.67% in bone and 97.36% in composite) are possibly attributable to simplifications in material properties or unrepresentative boundary conditions; these findings constitute a crucial opportunity to optimize future methodologies.

The study shows that chitin-graphene composites, enhanced by LS-DYNA simulations, represent a viable alternative for bone substitutes by combining mechanical strength comparable to bone with biocompatible and biodegradable properties.

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