Electroactive HA/BT Biocomposites for Bone Tissue Engineering: Synthesis, Dielectric Evaluation, and Computational Modeling

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I. Introduction

The dielectric behavior of bone, driven by Hydroxyapatite (HA) –collagen hydrogen bond separation under electric fields, is vital for cell regulation and repair[1]. Replicating this property is a key requirement in electroactive biomaterials for bone tissue engineering.

HA provides biocompatibility, osteoconductivity, and bioactivity, while lead-free barium titanate(BT) offers high dielectric coefficients, comparable to or exceeding those of hydrated bone, along with good cytocompatibility[2], [3]. Combining HA and BT yields composites that couple bioactivity with electromechanical responsiveness, thereby promoting osteointegration and electrical stimulation.

Computational modeling provides an efficient alternative to trial-and-error experiments in piezoelectric bone scaffold research, reducing costs, time, and ethical concerns while enabling optimized, patient-specific scaffold design for bone defect healing.[4]

While HA/BT composites have been previously explored, most solely focus on experimental dielectric characterization. In this work, HA and BT are synthesized, and HA/BT composites are fabricated to evaluate their dielectric properties experimentally. Finite element method (FEM) simulations are further employed to predict dielectric behavior, and the results are compared with experimental data.

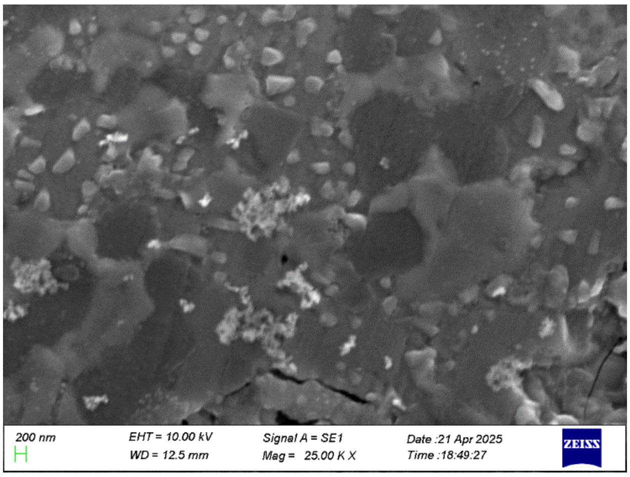

Fig. 1. SEM image of the HA/BT composite

II. Materials and Methods

A. Materials

Analytical grade Barium carbonate ($BaCO_3$), Analytical grade Titanium Dioxide (TiO_2), Polyvinyl alcohol (PVA), Analytical grade Ethanol, H_3PO_4 (88% GR, M 98.00gmol−1,1.75kg/l), $Ca(OH)_2$(minimum assay-96.09%), NH_4OH (Ammonia solution-25%).

B. Powder Synthesis

Barium Titanate was synthesized via a solid-state method using $BaCO_3$ and TiO_2 as starting materials. Equimolar $BaCO_3$ and TiO_2 were mixed in agate mortar and pestle, then calcined at 1200 °C for 3 h to drive the reaction.[2]

A standard wet chemical route was used to synthesize Hydroxyapatite. A 250 ml calcium hydroxide suspension was stirred for 1 h, then 250 ml orthophosphoric acid was added dropwise under stirring. The mixture was sonicated for 30 minutes, and NH_4OH was added to adjust the pH to 10, which was monitored until stable. The suspension was aged for 72 h, centrifuged, washed with deionized water, and the precipitate was oven-dried at 60 °C for 3 h.[5], [6]

C. Composite Fabrication

BT and HA powders were blended according to the HA:BT volume ratios 100:0, 70:30 and 50:50 with 3 wt % PVA binder, uniaxially pressed at 150 MPa into approximately 10 mm × 2 mm pellets and sintered at 1250 °C for 2 h followed by furnace cooling.[2]

D. Characterization of the Composite

Microstructural analysis of powders and the composite was performed using Scanning Electron Microscope (SEM), X-ray diffraction (XRD) analysis was done on HA, BT and the composite samples by employing "Rigaku Ultima IV" in the 2θ angle range of 0° to 65°.

The samples were polished, and thickness and diameter of the samples were precisely measured. The conductive silver paste applied samples were then connected to an LCR meter, and measurements of capacitance (C) were recorded at 1kHz. The relative permittivity (ε_r) was calculated using the following equation where d, A, and ε_r are thickness and surface area of the flat surface of the composite and the permittivity of air. [2]

$$\varepsilon_r = \frac{C \times d}{\varepsilon_0 \times A} \quad (1)$$

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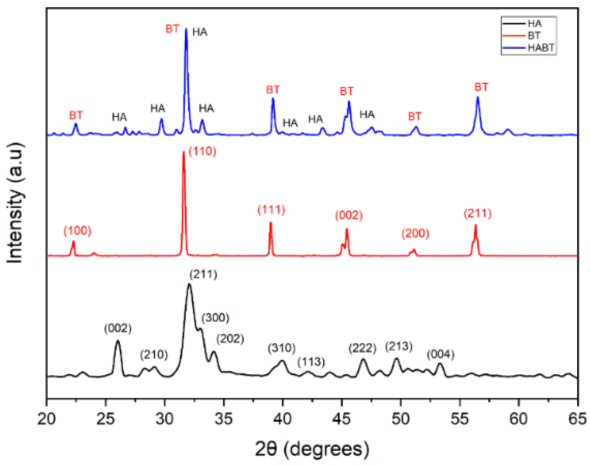

Fig. 2. XRD Spectrums of HA, BT and the composite

E. *Simulation Framework*

A 3D representative volume element (RVE) of a cubic HA matrix with a spherical BT inclusion was modeled in COMSOL 6.2 using periodic boundary conditions. BT was defined as transversely isotropic piezoelectric material, while HA was isotropic, linear-elastic, and non-piezoelectric material. The Solid Mechanics–Electrostatics coupling employed 10-node tetrahedral piezoelectric elements, with mesh convergence verified. Six mechanical and three electrical loading cases were simulated, and homogenized elastic and dielectric tensors were extracted from volume-averaged responses.

III. Results and Discussion

A. *Characterization of Barium Titanate*

SEM of BT showed irregular, rough-surfaced particles with an average size of ~400 nm. XRD in Fig. 2. revealed cubic perovskite structure of BT with peaks corresponding to (100), (110), (111), (200), (210), and (211) planes.

B. *Characterization of Hydroxyapatite*

SEM of HA showed rod-like particles with agglomeration and an average size of ~70 nm. XRD revealed characteristic HA peaks at 32°, 33°, and 34.2°, along with other standard reflections, confirming crystalline nano-HA formation.[5]

C. *Composite Characterization*

XRD confirmed high crystallinity and phase purity of the HA/BT composites, with clear HA and tetragonal BT reflections and no secondary phases. SEM in Fig. 1. revealed a granular, porous microstructure with dense packing and distinct HA and BT regions.

D. *Dielectric Property Evaluation*

The dielectric response of HA/BT composites was evaluated experimentally and compared with finite element method simulations. FEM predicted a continuous nonlinear rise of dielectric ε_{33} component, reflecting the percolation of high-permittivity BT within the HA matrix as in Fig. 3. Experimental results followed a similar trend but were slightly lower in magnitude with average deviation of 20%, likely due to processing-induced porosity, discrepancies between modeled and synthesized material properties, non-ideal phase interfaces, and grain boundary effects not fully represented in the simulations. These findings highlight good agreement

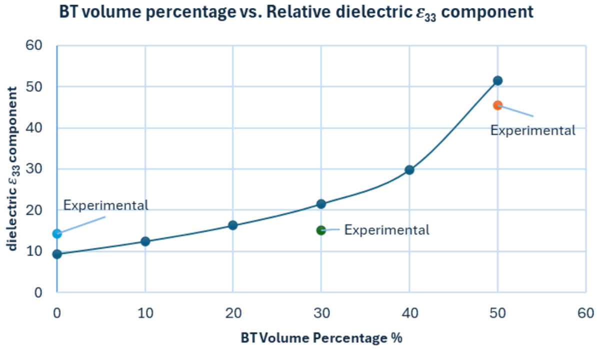

Fig. 3. FEM and experimental predictions of dielectric properties

between experimental data and computational predictions which can be used for early-stage predictions of dielectric properties.

IV. Conclusions

Barium titanate and hydroxyapatite were successfully synthesized, and the corresponding composites were fabricated. The experimentally measured and simulated dielectric permittivities across different BT volume fractions showed close agreement, indicating that the proposed model can reliably predict the dielectric properties of HA/BT composites at an early design stage of orthopedic implants. This accurate predictive capability is significant for optimizing the electroactive response of the material, which promotes better cell activity and bone regeneration at the implant interface. Ultimately, the ability to tailor dielectric behavior supports the development of implants with improved biological integration and long-term functional performance in load-bearing bone environments.

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