Impact of Transition Metal Ion Substitution on Physical, Mechanical, Electrical and Biological Characteristics of Bioactive Glasses

A thesis submitted in partial fulfillment for the Award of Degree

DOCTOR OF PHILOSOPHY

By

AKANKSHA SINGH

DEPARTMENT OF CERAMIC ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY
(BANARAS HINDU UNIVERSITY)
VARANASI – 221005
INDIA

ROLL No.: 17031002 **YEAR: 2024**

Dedicated to my Beloved son, husband, Parents and Family

Their blessings and
prayers accompany me in achieving
things in my life.

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It is further certified that the student has fulfilled all the requirements of the comprehensive examination, candidacy, and SOTA for the award of Ph.D. Degree.

10.10.2024

Dr. Preetam Singh
Supervisor
Associate Professor
Department of Ceramic Engineering
Indian Institute of Technology (BHU)
Varanasi - 221005, (U.P.), India

Dr. Preetam Singh
Associate Professor/सह–आचार्य
Department of Ceramic Engineering
सेरामिक अभियान्त्रिकी विभाग
Indian Institute of Technology (BHU)
भारतीय प्रौद्योगिकी संस्थान (का०हि०वि०वि०)
Varanasi-221005/वाराणसी-221005

Prof. Ram Pyare
Co-Supervisor
Professor (Rtd)
Department of Ceramic Engineering
Indian Institute of Technology (BHU)
Varanasi - 221005, (U.P.), India

Dr. Ashutosh Kumar Dubey
Head of Department
Department of Ceramic Engineering
Indian Institute of Technology (BHU)
Varanasi - 221005, (U.P.), India

विभागाध्यक्ष/HEAD
सिरामिक अभियान्त्रिकी विभाग
Department of Ceramic Engineering
भारतीय प्रौद्योगिकी संस्थान (का०हि०वि०वि०)
Indian Institute of Technology (B.H.U.)
Varanasi-221005/वाराणसी-221005

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BANARAS HINDU UNIVERSITY

DECLARATION BY THE CANDIDATE

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Akanksha Singh

Date: 10.10.2024

Place: IIT (BHU), Varanas

Signature of the student

(*Akanksha Singh*)

CERTIFICATE BY THE SUPERVISOR

It is certified that the above statement made by the student is correct to the best of my/our knowledge.

Preetam Singh 10.10.2024

Dr. Preetam Singh
Supervisor
Associate Professor
Department of Ceramic Engineering
Indian Institute of Technology (BHU)
Varanasi - 221005, (U.P.), India

Dr. Preetam Singh
Associate Professor
Department of Ceramic Engineering
सेरामिक अभियान्त्रिकी विभाग
Indian Institute of Technology (BHU)
भारतीय प्रौद्योगिकी संस्थान (काशी हिन्दू विश्वविद्यालय)
Varanasi-221005/वाराणसी-221005

Ram Pyare

Prof. Ram Pyare
Co-Supervisor
Professor (Rtd)
Department of Ceramic Engineering
Indian Institute of Technology (BHU)
Varanasi - 221005, (U.P.), India

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LIST OF ABBREVIATIONS

Notation	Abbreviations
et al.	et alia, Latin for “and others “
i.e.	That is
e.g.	Example
etc.	Et cetera, Latin for “and other similar things”
BG	Bioactive Glass
viz.	Namely
Mg	Milligram
G	Gram
Cm	Centimeter
Hz	Hertz
Min	Minute
Hr	Hour
s^{-1}	Per Second
IR	Infrared
BG	Bioactive Glass
BGs	Bioactive glass derivatives
XRD	X-ray diffractometer
SEM	Scanning electron microscopy
FTIR	Fourier Transform Infrared spectroscopy
EDS	Energy dispersive X-ray spectroscopy
SBF	Simulated Body Fluid
PBS	Phosphate-buffered saline
RBCs	Red Blood Cells
OD	Optical Density
RT or rt	Room temperature
MHz	Megahertz
PVA	Polyvinyl Alcohol
HA, Hap	Hydroxyapatite
HCA	Hydroxycarbonate apatite
MG-63	Human osteosarcoma cell line
DMEM	Dulbecco's Modified Eagle Medium
FBS	Fetal bovine serum
E	Applied Electric field
AFM	Atomic force microscopy
Tris buffer	Tris-hydroxymethyl aminomethane

T_c	Curie temperature
J	Leakage current density
P	Polarization vector
T	Temperature
R	Resistance
C	Capacitance
K	Kilo

Symbols used	
Symbols	**Full name**
K	Kelvin
°C	Degree Celsius
σ	Conductivity
χ^2	Chi square
δ	Delta
>	Greater than
<	Less than
Λ	Wavelength
Ω	Omega
E	Dielectric permittivity

This thesis describes the synthesis of transition metal ions like vanadium, titanium, zirconium and zinc ions substitution to bioactive glasses. Melt-quench technique was used to synthesize vanadium-substituted borosilicate glass, zirconium, vanadium, and titanium-substituted 1393-B3 borate glass and zinc substituted 45S5 glass. Characterization was achieved by both in vitro and in vivo experiments. Mechanical properties of the therapeutic ions-derived glass samples, along with parent glass-based glass samples, were examined by measuring the compressive strength, flexural strength and modulus of elasticity. Archimedes' principle analyzes physical property such as density. The characterization process includes in vitro bioactivity and cytocompatibility, hemocompatibility, as well as electrical performance. In vitro bioactivity was assessed using structural (XRD), functional (FTIR), and morphological (SEM-EDS) alterations caused by surface modification, as well as chemical behavioural (pH) changes induced by ion exchange in SBF (simulated bodily fluid). The hemocompatibility of materials is investigated using human blood red blood cells. The in vitro cytocompatibility of glass samples was investigated using MG-63 (Human osteosarcoma cell) to determine cellular viability, growth, and cytotoxicity. Bioactive glasses have medicinal applications in orthopaedic implants.

Chapter 1 presents the introduction of biomaterials and their application to modern medical techniques and a way forward to develop superior bioactive materials for different human body implants in case bone fractures and severe diseases.

Chapter 2 deals with synthesis and characterization techniques utilized in physico-chemical, mechanical, electrical properties, *in-vitro* study, hemocompatibility and the study of the MG-63 cell line growth to check the cellular compatibility of the materials.

Chapter 3 presents the investigation of bioactivity of borosilicate glass samples with the substitution of V_2O_5 (0-4 wt%). In-vitro bioactivity studied by FTIR, XRD, and SEM/EDS technique after SBF immersion. Physico-chemical, mechanical and electrical properties have been

studied. The results are studied considering the formation of HA layer on the glass surface. Hemocompatibility was tested with human blood, and cellular compatibility were performed on the MG-63 cell line.

Chapter 4 presents the investigation of bioactivity of 1393-B3 borate glass samples with the substitution of V_2O_5 (0-2.5 wt%). In-vitro bioactivity of the samples studied with FTIR, XRD, and SEM/EDS technique after SBF immersion. Hemocompatibility was assessed using human blood, while cellular compatibility was done using the MG-63 cell line.

Chapter 5 presents the investigation of bioactivity of 1393-B3 borate glass samples with the substitution of TiO_2 (0-2.5 wt%). Physical, mechanical and thermal properties were determined. The in-vitro bioactivity of the samples was examined using FTIR, XRD, and SEM/EDS techniques after SBF immersion. Hemocompatibility was determined using human blood, while cellular compatibility was determined using the MG-63 cell line.

Chapter 6 presents the investigation of bioactivity of 1393-B3 borate glass samples substituted with ZrO_2(0-2.5 wt%). Physical, mechanical and thermal properties are studied. After immersing the samples in SBF, in-vitro bioactivity was investigated using FTIR, XRD, and SEM/EDS techniques. Hemocompatibility and cellular compatibility were determined.

Chapter 7 presents the investigation of bioactivity of ZnO (0-3 mole %) substituted 45S5 glass before and after polarization process. In-vitro studied with the help of FTIR, XRD, SEM/EDS, and AFM techniques to find HA layer. Electrical properties of the samples were studied.

Chapter 8 provides the conclusion of the entire work. The future scope is also included in this chapter which is the proposal based on the results and explanation obtained in this thesis work.