Chapter 6

Conclusions and Future Scope

6.1. Conclusion

The electrical properties of living bone in combination with its functionally graded structure impart a unique set of properties to bone. This has tempted the present study to develop a material having property closely related to bone. In this perspective, present study is divided in two parts i.e.,

- (i) Modifying/developing the electrical equivalent circuit of a generalized living cell to get the additional insight into the interaction mechanism of E-field with the living cell, this further can be helpful in setting optimized E-field parameters for enhanced cell-material interaction.
- (ii) Development of a prosthetic implant material having inherent / induced electrical characteristics with better biocompatibility.

The present work comes up with the following conclusions:

- (i) From the electrical equivalent circuits of a living cell, the evaluated time constant is in the microsecond range, which suggests an immediate response of the cell towards E-field.
- (ii) Based on the electrical equivalent of the cell, the interaction of E-field is highly dependent on parameters such as cell size, capacitances and resistances of cell and nuclear membranes as well as resistances of cytoplasm and nucleoplasm.
- (iii) Using the developed/modified electrical equivalent models of living cell, the intensity of E-field required to electroporate a single living cell vary over a large range (0.1 600 kV/cm) depending on the cell size as well as pulse duration of the E-field. These values are in line with the experimental values where the electroporation is used for various

applications such as drug delivery etc. Therefore, the theoretical model is validated with the experimental studies.

- (iv) Simulation studies on electrical equivalent models depict that the current and voltage across various cellular compartments is highly dependent on pulse duration of applied Efield for similar intensity of voltage.
- (v) Dense hydroxyapatite (HA) compacts, developed via multistage spark plasma sintering route (950°C, 5 min; pressure: 80 MPa) and polarized under very high polarizing field (30 – 90 kV/cm) have been observed to accumulate the charge density from ~ 0.2 nC/cm^2 to ~ 2 $\mu C/cm^2$. Therefore, apart from temperature, formation of HA electret is highly dependent on polarizing field.
- (vi) Phase analyses reveal HA to be in hexagonal lattice. Microstructural analyses of fractured surfaces of SPSed HA reveal a dense microstructure.
- (vii) The activation energy for depolarization behaviour has been evaluated to be in the range of 0.4-0.7 eV. These values are associated with the reorientation of the OH^- dipoles as well as hopping of protons (H⁺) along columnar c-axis in HA.
- (viii) The dielectric (ε) as well as ac conductivity behaviour of unpolarized and polarized (90 kV/cm) HA depicts no significant change in dielectric and electrical response due to poling.
- (ix) The activation energy for polarized HA (0.65 eV) is slightly decreased as compared with that of unpolarized counterpart (0.71 eV). The associated mechanism of conduction remains same in both the samples i.e., conduction via proton (H^+) migration.
- (x) The X-ray photoelectron spectroscopy (XPS) analyses suggest that the polarization of HA at such a high field (90 kV/cm) does not alter its surface chemistry.
- (xi) Ferroelectric Na_{0.5}K_{0.5}NbO₃ (NKN), developed via multi stage spark plasma sintering route (950°C, 5 min; Pressure: 80 MPa), polarized under very high polarizing field (30 –

90 kV/cm) reveal a slight shift in the phase transition temperatures (T_{O-T} , T_C) towards higher temperature with increase in the polarizing field (30-90 kV/cm) as well as heating rate.

- (x) Phase analyses reveal NKN to be in orthorhombic lattice. Microstructural analyses of the fractured surfaces of SPSed NKN depict highly dense microstructure.
- (xii) The dielectric and ac conductivity measurements suggest that the polarization of NKN (90 kV/cm) slightly decreases T_{O-T} and T_C as compared to its unpolarized counterpart. The conductivity in NKN is mainly attributed to the migration of oxygen vacancies and n-type charge carriers.
- (xi) The HA-25 vol% NKN (HA-25 NKN) composite, developed via SPS route under similar parameters, polarized at 90 kV/cm, accumulates the charge density of 6.4 μ C/cm², which is significantly larger as compared with the charge density of monolithic HA, polarized and depolarized under similar parameters.
- (xii) Microstructural analyses of fractured surface of SPSed HA-25 NKN composite reveals the dense microstructure. Also, the phase analyses of HA-25 NKN composite reveals the presence of both, NKN and HA phases with no additional phase.
- (xi) The dielectric and ac conductivity behaviour for polarized (90 kV/cm) and unpolarized HA-25NKN composite suggests no degradation in the electrical properties and therefore sample chemistry.
- (xii) A significant increase in dielectric constant of HA-25NKN (~ 60) composite at room temperature has been observed as compared with that of pure HA (~ 25).
- (xiii) A slight increase in the ac conductivity of HA-25 NKN [$\sim 10^{-7}$ (ohm cm)⁻¹] composite has been observed as compared with that of pure HA [$\sim 10^{-8}$ (ohm cm)⁻¹]. Overall, the polarizability of the HA has increased with the addition of the piezoelectric NKN.

- (xii) Functionally graded materials (FGMs) of HA-BaTiO₃-HA and HA-CaTiO₃-HA were successfully developed via spark plasma sintering route (1100°C, 10 min; Pressure: 50 MPa) by inserting buffer interlayers of HA-BaTiO₃ and HA-CaTiO₃ for facilitating the gradual variation in thermal coefficient between the layers.
- (xiii) Microstructural analyses reveal that the layers of FGMs have been integrated well without any signature of delamination or crack formation at the interfaces.
- (xv) The dielectric constant of developed FGMs (~ 30) has almost increased two times with that of the pure HA (~ 15) at room temperature.
- (xvi) Slight increase in ac conductivity of FGMs $[\sim 10^{-8} \text{ (ohm cm)}^{-1}]$ was observed as compared with that for pure HA $[\sim 10^{-9} \text{ (ohm cm)}^{-1}]$ at room temperature.
- (xvii) Impedance spectroscopic study reveals additional electrical contribution of different layers, phases and constituents in the developed FGMs as compared with that of grain and grain boundaries in HA.

Overall, it is concluded that the polarizability of developed FGMs has increased significantly as compared with that of pure HA. Also, the surface chemistry of HA in the developed FGM has not been altered which in turn is associated with its excellent biocompatibility with the bone tissue. However, in case of HA-25NKN, although the polarizability has increased as compared with that of pure HA but with the addition of NKN reinforcement phase in HA, excellent surface chemistry of HA-25NKN composite has been altered and in turn, the excellent biocompatibility of HA might be influenced. Secondly, the E-field parameters evaluated from the electrical equivalents of cell can be utilized in the improvement of cell-material interaction under pulsed E-field.

6.2. Future Scope

- (i) As in the present study, the electrical equivalent circuit considers the nucleus as the only organelle inside the cell, the involvement of the electrical equivalents of other organelles such as, mitochondria etc. can further explore the analytical study of E-field interaction of living cell. In addition, the complex nature of cell as well as nuclear membrane also opens up the consideration of the inductive property of the living cell.
- (ii) As the grain size distribution affects the TSDC characteristics, it would be interesting to establish a correlation between grain size distribution and TSDC behaviour of such composite systems.
- (iii) The Antibacterial response as well as cellular viability of polarized HA, NKN and HA-25 NKN composite can be carried out in the subsequent study. Similar studies can also be carried out on the developed FGMs.
- (iv) As NKN is reported to be an excellent piezoelectric biocompatible material, its application in the development of FGM along with bioactive glass 1393 as well as 45S5 can be further explored for electroactive prosthetic implant.