ABSTRACT

Magnesium (Mg) alloys have emerged as promising candidates for resorbable implant applications due to their favorable mechanical compatibility with natural bone and inherent biodegradability. However, their rapid corrosion in physiological environments restricts their clinical translation. This thesis presents a comprehensive and eco-friendly surface engineering strategy integrating experimental development, computational modeling, and data-driven multi-objective optimization to enhance the corrosion resistance and biofunctional performance of Mg alloys for biomedical applications. The study initially focuses on the development of environmentally benign hydrophobic coatings based on stearic acid to mitigate early-stage corrosion. Systematic variation of the coating temperature enabled the formation of metal–stearate protective layers exhibiting improved surface hydrophobicity and reduced corrosion kinetics in simulated body fluid. Building upon this foundation, a hybrid multi-objective optimization framework was implemented to convert hydrophobic surfaces into superhydrophobic coatings using stearic acid and $ZnCl_2$. Response Surface Methodology (RSM-CCD), Artificial Neural Networks (ANN), and evolutionary optimization algorithms (NSGA-II, TLBO, and MOPSO) were integrated to simultaneously optimize the surface roughness, surface free energy, and corrosion resistance. The optimized coating achieved a water contact angle of 152° ± 1°, a corrosion inhibition efficiency exceeding 92%, and a significant reduction in degradation rate, demonstrating the effectiveness of data-driven material design. Subsequently, bioactive ceramic coatings consisting of hydroxyapatite (HA) and Zn-doped HA were developed via dip coating to further regulate the degradation behavior and enhance the biological response. Multiphysics simulations were employed to model flow-induced shear stress under dynamic simulated physiological conditions and correlate mechanical stimuli with corrosion behavior. Experimental electrochemical analysis confirmed substantial reductions in the corrosion rate, while comprehensive surface characterization and in vitro biological evaluations validated improved cytocompatibility and cellular adhesion. The influence of post-deposition heat treatment on chitosan/Zn-doped HA composite coatings was systematically investigated in this study. Controlled thermal processing optimized microstructural consolidation, phase purity, and interfacial integrity, leading to enhanced corrosion resistance and superior cellular response. Finally, finite element simulations further elucidated the relationship between surface stiffness, morphology, and mechanobiological interactions. Overall, this thesis establishes a scalable, eco-friendly, and data-integrated surface-engineering framework for Mg-based resorbable implants.