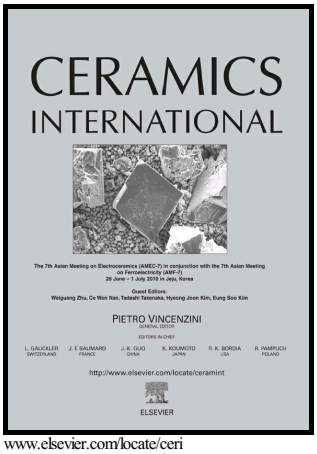

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Molecular Dynamics Simulation and Experimental Study of the Bonding Properties of Polymer Binders in 3D Powder Printed Hydroxyapatite Bioceramic Bone Scaffolds

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Abstract

Binder properties are a key factor affecting the quality of bone scaffolds produced using 3D powder printing. In this research, molecular dynamics simulation (MD) and experimental methods were applied to study the cohesive energy density, mechanical properties, bonding behavior, and surface morphology of three polymer binders (PVP, PAM, PVA) employed in the 3D fabrication of hydroxyapatite (HA) bone scaffolds. The bonding mechanisms of the three polymer binders were revealed by analyzing the interaction between the binders and the HA surface. The binding energies between the binders and HA are associated with the cohesive energy density and viscosity of each of the binders, which are attributed to functional groups in the binders. The mechanical properties determined experimentally for the bone scaffolds produced using each of the three polymer binders were in a different relative order than the engineering modulus of the binders and the interaction between the binders and HA calculated in simulations. This is a reflection of the mechanical properties of bone scaffolds being a comprehensive reflection of the basic materials and their bonding effect. Finally, SEM imaging indicated additional factors affecting the mechanical properties and degradation rate of the scaffolds. Conclusions from this work can be