Available online at www.sciencedirect.com

ScienceDirect

Ceramics International 40 (2014) 6631–6638

CERAMICS INTERNATIONAL

www.elsevier.com/locate/ceramint

Random stacking template of polymer spheres and water soluble particles to fabricate porous hydroxyapatite with interconnected pores

Yufei Tang[a,*], Qian Miao[a], Kang Zhao[a], Minke Zhu[a], Zixiang Wu[b]

[a]School of Materials Science and Engineering, Xi'an University of Technology, Xi'an 710048, PR China
[b]Institute of Orthopaedics, Xi'jing Hospital, The Fourth Military Medical University, Xi'an 710032, PR China

Received 3 October 2013; received in revised form 26 November 2013; accepted 26 November 2013
Available online 4 December 2013

Abstract

Particle stacking simulation is applied in the fabrication of porous hydroxyapatite (HA) ceramics to predict the relationship between the template preparation process and the porosity of porous ceramics. The stacking of multi-diameter spherical particles, such as polymer spheres and NaCl particles, in three-dimensional space is simulated by using continuous generation method. The porosity of porous HA is predicted by calculating the stacking density of large spheres (the ratio of large sphere volume and container volume). The model of three-dimensional random stacking spheres is implemented by using the C++ program. Porous HA ceramics with interconnected spherical pores were fabricated by slipcasting which the use of a polymer template. Templates were produced by randomly stacking polymer spheres and NaCl particles. The arithmetic average error between the porosity of porous HA ceramics and the stacking density of polymer spheres (large spheres) is 3.52%. Simulation results obtained by using the proposed method are consistent with the experimental results.

Keywords: B. Porosity; Interconnected pores; Porous ceramic; Random stacking

1. Introduction

Porous hydroxyapatite (HA) ceramics are the most promising bone implant material because its composition is similar to that of a natural bone, which promotes the growth of bone and soft tissues [1,2]. Addition of pore-forming agents, organic foam impregnation, and freeze casting are some methods of fabricating porous HA ceramics [3–5]. Porous HA ceramics with lamellar channels and spherical or mesh pores are obtained with the use of these methods. Studies on porous scaffolds with spherical pores focused on those prepared by using polymer spheres as the pore-forming agent, because their pore configuration can increase stress tolerance [6,7]. However, spherical pores with poor connectivity results in poor nutrient supply, metabolic waste removal, and cell attachment. Descamps et al. [8] reported the synthesis of macroporous β-tricalcium phosphate with a controlled porous architecture by using the template that resulted from a chemical reaction of polymer spheres. The compressive strength of fabricated samples is unimproved because of high porosity. Our research team developed a method that used a polymer template to fabricate porous HA scaffolds with interconnected spherical pores [9]. Porosity is a crucial factor in the mechanical properties of porous HA ceramics [10]. A large number of repeated experiments are necessary to determine the relationship between porosity and preparation, while precisely controlling porosity.

Particle stacking simulation is an extremely powerful tool for designing advanced materials [11,12]. The simulation is extensively utilized in powder metallurgy and cement applications to shorten the development cycle of materials [13]. Most simulation models are developed to solve particle size distribution issues. The model algorithm is complex, and the computation is large [14,15]. However, some applications aim to obtain the bulk density of particles and not to accumulate high density.

*Corresponding author. Tel./fax: +86 29 82312922.
E-mail address: yftang@xaut.edu.cn (Y. Tang).

0272-8842/$ - see front matter
http://dx.doi.org/10.1016/j.ceramint.2013.11.120

In this study, particle stacking simulation is applied to fabricate porous HA ceramics with interconnected spherical pores. We proposed a method that considers the random stacking of spheres from a particle motion perspective. The stacking process of multi-diameter spherical particles, such as polymer spheres and NaCl particles, in three-dimensional space is simulated by using the continuous generation method. The porosity of porous HA is predicted by calculating the stacking density of large spheres (the ratio of large sphere volume and container volume). The three-dimensional random stacking spheres model is implemented through the C++ program. Porous HA ceramics with interconnected spherical pores are fabricated by slipcasting with the use of a polymer template. Templates are produced by randomly stacking polymer spheres and NaCl particles. The simulation accuracy of the model is evaluated through experiments.

2. Simulation of random stacking

2.1. Design strategy

The design strategy of the polymer template and the process for HA ceramics with interconnected pores involves five steps (Fig. 1): (1) distribution of random water soluble particles in the gaps between polymer spheres to prevent contact among spheres; (2) formation of an adhesive area across the polymer spheres by adding an adhesive; (3) removal of water soluble particles through washing in deionized water and then drying; (4) the use of ceramic slurry for slipcasting, and (5) sintering. Pores possess interconnectivity with their neighbors from the polymer template made by the random stacking of polymer spheres and water soluble particles, and fixed by an adhesive. The coordination number and stacking density of the polymer spheres are determined by the diameter and number ratios between polymer spheres and water soluble particles. Pore connectivity and porosity of sintered porous ceramics are affected by the coordination number and stacking density of polymer spheres in the template. The coordination number and the porosity greatly affect the properties of fabricated porous ceramics.

2.2. The model

A model that simulates the random stacking of spheres in a three-dimensional space is developed in this paper to serve as a guide for the polymer template process. Spheres with two sizes are assumed to be rigid to simplify the algorithm in sphere contact. Large spheres refer to polymer spheres, whereas small spheres refer to water soluble particles. With the inclusion of the diameter and number ratios between large spheres and small spheres as well as the container size, the geometry of accumulated spheres was obtained by simulating the

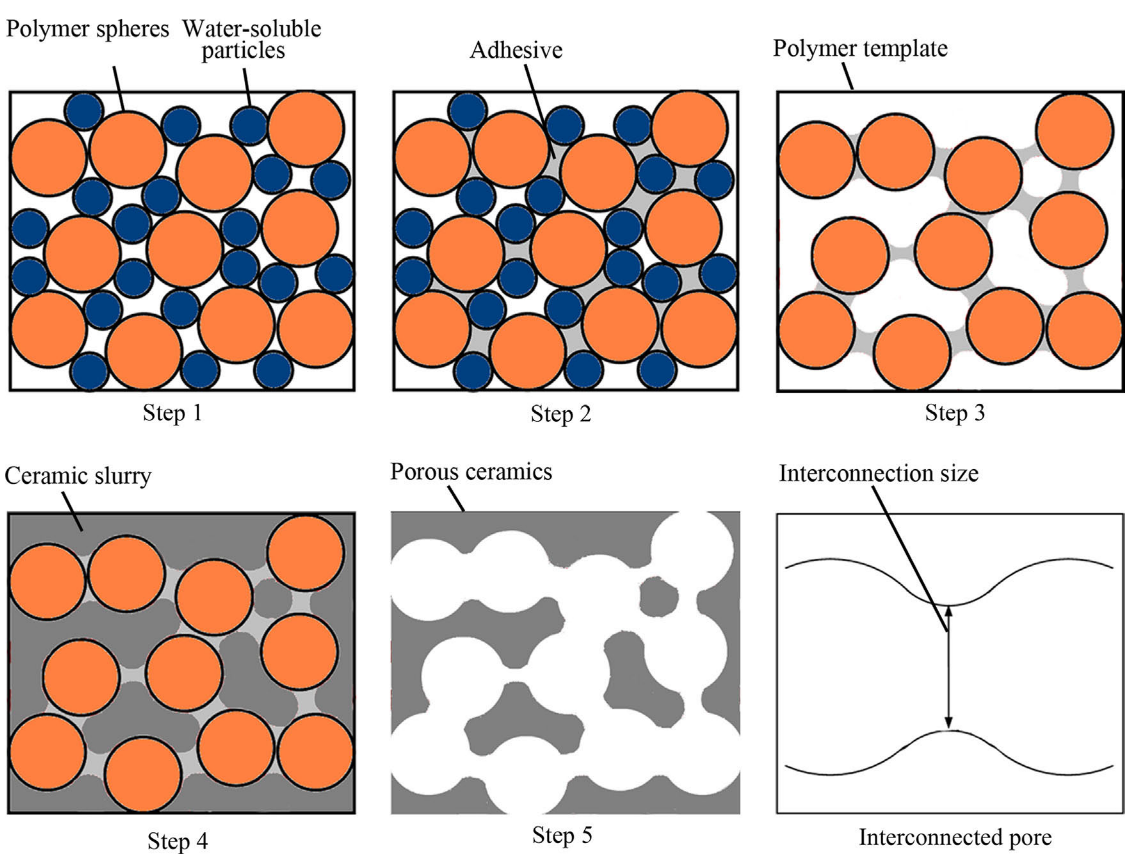

Fig. 1. Plan view of the design principle for porous ceramics with interconnected pores. Step 1: random stacking of polymer spheres and water-soluble particles, Step 2: formation of an adhesive area among the polymer spheres by adding adhesive, Step 3: removal of NaCl particles by washing and drying, Step 4: slipcasting, and Step 5: sintering.