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Three-dimensional real structure-based finite element analysis of mechanical behavior for porous titanium manufactured by a space holder method

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ABSTRACT

In this study, porous titanium samples were manufactured by a space holder method with sodium chloride. Each porous titanium sample contained two types of pores based on their sizes: macropores and micropores. Macropores were those emerged from removing the space holder, whereas micropores were voids created during powder compaction. The porous titanium exhibited low elastic modulus close to that of the human bone. Computed tomography (CT) was employed to examine the porous structure of the Ti samples. The CT results were then used in finite element simulations for analysis of the mechanical behavior of the porous titanium. The CT-based finite element model was found to give better results compared to the unit-cell finite element model in terms of agreement with the experimental data. The CT model combined with the strain hardening behavior of Ti having micropores prescribed to the matrix allowed for accurate predictions of elastic modulus, yield strength, and flow stress. These results signify the importance of taking into account pores at different scales as well as their morphology and distribution at least at macroscale.

1. Introduction

Titanium and its alloys have received much attention due to their excellent mechanical and chemical properties [1–5]. They have been extensively investigated, in particular, for biomedical applications because of their exceptional biocompatibility and chemical stability in a human body environment [6,7]. However, elastic moduli of Ti and its alloys are higher than those of human bones and this difference of elastic modulus between implant materials and human bones causes bone degradation due to a stress-shielding effect [8–11]. Porous materials are strong candidates for resolving the problem of bone degradation caused by implants. The porous materials exhibit different yield, compressive and creep behavior [12–16], and reduced mechanical properties such as elastic modulus and yield strength [17–19] compared to those of their nonporous counterpart. Powder metallurgy with a space holder method, first developed by Wen et al. [20], is an effective process in manufacturing porous materials because the pore size and porosity can be controlled by tuning the space holder material. For example, an earlier study [21] showed that using sodium chloride and irregular urea is advantageous for improving the overall mechanical performance of porous Ti.

The finite element method (FEM) combined with computed tomography (CT)-based modeling is a powerful tool for the analysis of mechanical properties of porous materials [22,23], metal foams [24–26], and composites [27], and the effects of structural features such as irregular morphology and spatial distribution of second-phase particles or pores. There are several methods to access three-dimensional (3D) information on the inner structure of the material, such as serial sectioning with microscopy [28], X-ray imaging [22–24], and 3D electron backscatter diffraction (EBSD) [27]. Among these techniques, the X-ray imaging is a nondestructive method, which provides a distinct advantage in linking microstructural features to the mechanical behavior of a material since the same specimen can be used for both X-ray imaging and mechanical testing.

In this study, porous Ti was manufactured from pure Ti powders and sodium chloride (NaCl) particles using the space holder

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method. The mechanical behavior of the porous Ti was investigated both experimentally and numerically through uniaxial compression tests. In the numerical uniaxial compression test, two different 3D FEM models, unit-cell model and CT-based model, were employed to investigate the effect of pore shape and distribution on mechanical behavior of porous Ti. Furthermore, each 3D FEM model used three different matrix properties to analyze the effects of matrix properties on the mechanical behavior of the porous Ti.

2. Experimental procedure

Pure Ti powders with an average particle size of 45 μm (Ti–0.003Al–0.003Cr–0.02Fe–0.028Ni in wt.%) were used to manufacture the matrix of the porous samples (Fig. 1a). Sodium chloride (NaCl) was selected as a space holder because our previous study has shown that, among several space holding materials, NaCl yields the best overall mechanical performance of the resulting porous Ti [21]. The NaCl particles selected for this study were cubic shaped with an average size of 200–400 μm (Fig. 1b). The Ti powders were mixed with the NaCl particles at a volume ratio of 7:3 for 12 h. The resulting mixture of the powders was compacted under a pressure of 120 MPa. The dimensions of a green compact were 14 mm in diameter and 12 mm in height. In order to remove NaCl after the compaction process, the green compact was put into water for 24 h. The density of the green compact after removing NaCl was 0.46. Subsequently, the green compact was sintered at 1000 °C for 2 h with the heating and cooling rates of 5 °C/min under vacuum (10^{-1}–10^{-2} Pa). In addition, a sample containing only Ti powders (i.e. no space holder) was prepared in the same manner. The CT was employed in order to obtain information on 3D porous structure of the Ti specimens. An industrial CT machine (RayScan 250, RayScan Technologies GmbH, Germany) with 3 μm resolution capable of analyzing samples with dimensions in a range of 3–600 mm was used in this study.

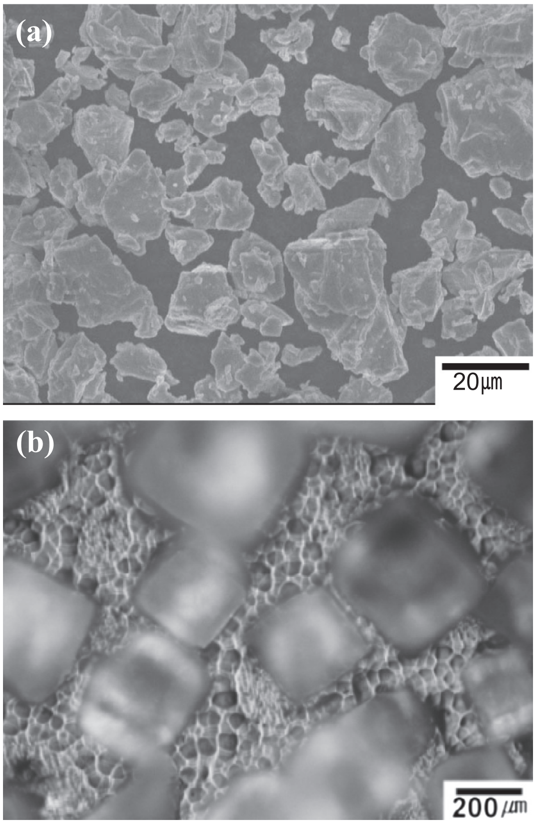

Fig. 1. Scanning electron microscope images for (a) pure Ti powder and (b) sodium chloride.

For compression tests, the consolidated samples were cut to 10 mm in diameter and 10 mm in height. Compression tests were performed using an INSTRON 8862 machine with a strain rate of 10^{-3} s^{-1}. A digital image correlation (DIC) method was employed during compression tests to accurately measure the strain using ARAMIS 5 M optical system (GOM mbH, Germany). The detailed procedure of DIC strain measurements is described elsewhere [29,30]. A Teflon tape and MoS_2 lubricant were used during the compression tests to reduce friction between the specimens and the compression dies. The same compression tests were performed with pure Ti grade 2 and 4 in order to acquire input data for the FEM simulations.

3. Numerical procedure

3D FEM models were constructed for analyses of the mechanical behavior of the porous Ti. Two types of FEM models were developed in the present study. In the first model, the real structure of the porous specimen was reconstructed from 330 images obtained using CT. Commercial image-processing software AMIRA 5.2 (FEI, USA) was employed to reconstruct a 3D configuration from a series of 2D images. Since simulations with the whole specimen used in the compression experiments would result in an excessive computational cost due to a large number of elements, a representative volume having 2 mm in diameter and 2 mm in height (Fig. 4) was taken from the reconstructed 3D configuration. The second model of the porous Ti was a simple cubic unit-cell model with a centered spherical pore and 30 vol.% porosity.

For simulating compression tests, a displacement boundary condition (up to 15% engineering strain) was prescribed on the top nodes of the sample mesh, whereas the bottom nodes were fixed. For the unit-cell model, 1/8 of the unit cell was considered with corresponding symmetry boundary conditions applied.

In both models described above, the matrix was assigned an elastoplastic material model with isotropic hardening. In order to describe the mechanical behavior of the matrix, three sets of elastic and plastic properties were used. In the first two sets, reference values of Poisson ratio, 0.32, and elastic modulus, 110 GPa, known for bulk Ti grade 2 or grade 4 were taken. The strain hardening behavior of the matrix was described by stress–strain data obtained from uniaxial compression of bulk Ti grade 2 and grade 4. In the third set, both elastic modulus and strain hardening behavior were obtained from uniaxial compression of the microporous Ti consolidated from pure Ti powders without a space holder. All simulations were performed using the commercial finite element code ABAQUS/Standard (Dassault Systèmes).

4. Results

4.1. The structure of porous Ti

The porous structure of the Ti specimen obtained with 30 vol.% NaCl is presented in Fig. 2. The morphology and size of pores are similar to those of the precursor NaCl particles (Fig. 1b). These pores generated by the space holder are referred to as macropores in the present paper. In addition to the macropores, there also exist smaller pores that originate from voids between the Ti powder particles. The size of these pores is in the order of 1 μm and we refer to these pores as micropores.

Fig. 3 exhibits cross-sectional images of the porous Ti specimen obtained through CT. Good detection of macropores is supported by calculation of the relative density based on the CT data. The