Finite element simulation on mechanical properties of zeolite as a potential cellular structure

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Abstract. The mechanical properties of the zeolite model with cellular structure as a unit cell were studied via simulation. Four zeolite models were selected, and the mechanical properties of zeolite and traditional cellular structure were compared by mechanical finite element analysis. The results demonstrate that the zeolite structures possess better mechanical behavior under loading, accompany with uniform distribution of structural stress and less stress concentration. In addition, the effect of porosity on mechanical properties of zeolite model was studied. The results demonstrate that both yield strength and elastic modulus for zeolite decrease with the increase of porosity.

1. Introduction
Introducing cellular structure into biomedical β-type titanium alloys for bearing implants can effectively reduce the elastic modulus and the "stress shielding" effect caused by the mismatch between the high elastic modulus of titanium alloy and human bone tissue[1], and enhance the fixation of implants in the human body. Besides, the cellular structures with interconnected pores are also conducive to biological cell behaviors such as cell adhesion, proliferation and bone tissue regeneration[2,3], resulting in greater biological bonding between implants and tissues. Additive Manufacturing (AM) technologies, such as Selective Laser Melting (SLM) and Electron Beam Melting (EBM)[4], can manufacture cellular structures with complicated shapes. Therefore, the preparation of cellular structures using AM has attracted extensive attention in the field of biomedical implants.

Nowadays, most cellular structures are based on struts with straight edges and sharp turns or those derived from Boolean intersections of geometric primitives, such as Tetrahedron lattices and Octet truss[5]. These cellular structures with straight edges and sharp turns usually contain stress concentrations inside struts, which is harmful to load-bearing orthopedics implants. In addition, these cellular structures could hardly provide a suitable environment for cell attachment, migration and proliferation, because some cells will be naturally isolated by curved partitions from the aggregates of cells in foam/extracellular matrix[6,7].

Zeolite is a kind of micro-nano material with regular and uniform pore structure. There are many advantages for zeolite structures, such as no fatigue stress nodes, large specific surface area, and multi-scale pore size, which makes them have strong adsorption capacity via reversibly adsorbing and releasing functional ions and drug molecules. Resultantly, these advantages of zeolite can promote the implants to obtain better bone integration and antibacterial properties[8,9]. Therefore, zeolite structure is
one of the most potential candidates for cellular structures implants. However, to our best knowledge, no studies have been devoted to zeolite as cellular structure so far.

Based on the above, this paper focuses on the design and optimization of zeolite structure. Several zeolite models suitable for unit cell were selected and then modeled in three dimensions. Their mechanical properties were compared by finite element analysis at the same porosity. By changing the strut thickness, the Zeolite model with different porosity, pore structure and pore size was designed to meet the human bone performance.

2. Materials and Methods
At present, there are more than 200 known zeolite structures. Their structure shape is different, complex and variable, which make it impossible to study each one of them. For the sake of simplicity, we choose several zeolites suitable as unit cell for research. Before that, suitable zeolites should meet the following conditions: (1) The unit cell structure of zeolite should not be too complex to array and modeling, such as the ERI in Fig. 1; (2) The difference of pore size should be as small as possible. If the large pore size of the structure is much larger than the small one, it will be limited by AM. For example, the large pore size of SAF in Fig. 1 is almost 6 times of the small one, suggesting that this zeolite cannot be prepared by AM. Based on the above discussions, four zeolite structures were selected for study, namely SOD, DFT, BCT and ATN. Because these four zeolites have simpler unit cells, and the difference between large and small pores is smaller. In addition, Tetrahedron lattices (TET) and Octet Truss (OCT) were chosen to compare the mechanical property between zeolite and traditional cellular unit cell. The unit cell models of these six structures were shown in Fig. 2. These models are modeled by commercial modeling software SolidWorks 2016. To compare the mechanical properties of these six models, static finite element analysis method was used for compression simulation by the commercial simulation software ABAQUS.

The guideline of simulation is as follow: the porosity of these four models is equal. Normal human cancellous bone porosity ranges from 50% to 90%, here the porosity of four models was set to 80%. The model was endowed with the material properties of biomedical β-type titanium alloy Ti-35NB-7Zr-5Ta. The elastic modulus is 22.95Gpa and the Poisson’s ratio is 0.315. The bottom surface of the model was completely fixed. A press plate with vertical downward movement was added to the top surface of the model. The contact type between the plate and the top surface of the model was set as Tie. The plate displacement was set to 20% of the model height. In the visualization module, the stress value is obtained by dividing the support force in the Z direction of the plate bottom surface by the cross-sectional area of the model top surface, the strain value is obtained by dividing the Z direction displacement of the plate by the model height. Subsequently, the stress-strain curves of zeolite during compression simulation can be obtained. Then one of the zeolite structures was selected for study. By changing porosity, the relationship between mechanical property and porosity of zeolite was explored.
3. Results & Discussion
To compare the mechanical property of the zeolite and traditional cellular structures, these six models were set to the same porosity, which was 80%. According to the compression simulation results, stress concentration occurs in traditional cellular structures, especially for TET. Some struts of the TET are subjected to excessive stress, which means that severe deformation is more likely to occur in these positions. On the contrary, the stress distribution of zeolite is relatively uniform, and no obvious stress concentration phenomenon is observed. Among them, the stress distribution of SOD is more uniform, as shown in Fig. 3.
Fig. 3 Equivalent stress nephogram of (a) SOD, (b) DFT, (c) BCT, (d) ATN, (e) TET and (f) OCT after compression.

Fig. 4 shows the simulated stress-strain curves of these six different structures under the same porosity. It can be seen that the compressive stress-strain curves of various zeolite models can be divided into two stages: (I) the linear elastic stage and (II) the plastic deformation stage. In the linear elastic stage, the stress of materials follows a linear relation with the strain, and the elastic modulus of zeolite structure is calculated with the slope of this stage. Once the elastic limit is reached, plastic deformation begins as the cellular unit cell begins to yield or bend. The yield strength and elastic modulus can be calculated from the stress-strain curves and the results are shown in Tab. 1. It is not difficult to see that the mechanical properties of zeolite structures are better than that of traditional cellular structures, except for BCT.

Fig. 4 Stress-strain curves of SOD, DFT, BCT, ATN, OCT and TET, respectively.

Tab. 1 The yield strength and elastic modulus of SOD, DFT, BCT, ATN, OCT and TET, respectively.

| Mechanical Properties    | SOD  | DFT  | BCT  | ATN  | OCT  | TET  |
|--------------------------|------|------|------|------|------|------|
| Yield Strength (Mpa)     | 42.5 | 46.1 | 32.0 | 56.0 | 39.1 | 23.9 |
| Elastic Modulus (Gpa)    | 0.95 | 0.95 | 0.81 | 1.73 | 0.93 | 0.93 |

Among these four zeolite structures, the comprehensive mechanical properties and symmetry of SOD are the best, without anisotropy, so SOD model was selected to investigate the relationship between the porosity and mechanical properties of zeolite. In the SOD model, the porosity of the
model was adjusted by changing the strut thickness. Specifically, the porosity of the model was reduced by increasing the strut thickness, and the corresponding porosity is 70%, 75%, 80%, 85% and 90%, respectively, as shown in Fig. 5. Fig. 6 shows the stress-strain curves of the SOD model with porosity from 70% to 90% after compression simulation. As can be seen from the Fig. 6, the models with porosity of 70% and 75% show the obvious strain hardening, while the models with porosity of 80% to 90% almost remained unchanged after reaching the yield point, showing a long stress plateau. With the increase of porosity, the yield strength and elastic modulus of the model decrease regularly, especially for the yield strength.

Fig. 5 Different porosity models of SOD.

Fig. 6 Stress-strain curves of SOD models with different porosity

4. Conclusions
In this paper, zeolite was introduced as a unit cell model of cellular structure, which was reconstructed and used for statics finite element analysis. Four types of zeolites were selected for study, and the stress-strain curves of each model were obtained by compression simulation. The mechanical properties of the four zeolite structures and two traditional cellular structures under loading were compared. The simulation results indicate that the four zeolites show better mechanical behaviors under loading, with uniform distribution of structural stress and less stress concentration, which satisfy the feasibility of additive manufacturing. The SOD structure was taken out, and the porosity was adjusted by changing the strut thickness to explore the effect of structural porosity on mechanical properties. The results demonstrate that the yield strength and elastic modulus decrease with the increase of porosity.
Acknowledgments
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