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Impact of bone geometry on effective properties of bone scaffolds

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Abstract

The characterization of bone/scaffold composite mechanical properties is essential for translation to the clinic, but in vivo studies require resources and personnel not available to many investigators. Therefore, the ability to predict composite properties could facilitate scaffold evaluation and reduce the number of in vivo studies required. To date, there have been no studies that have used experimental data to formulate a model of bone morphology or that have examined morphology as a variable in composite properties. In this study, a simple model was developed to predict the effective elastic properties of hydroxyapatite (HA) scaffold/bone composites using representative volume elements (RVE) and finite element analysis. While the RVE for the scaffold is clear, the choice of RVE for bone is not. Two bone geometries were generated for the RVE based on data from an in vivo study: a uniform coating and bridges in pores. Three scaffolds were evaluated in order to consider the effects of scaffold material modulus and porosity. Results showed that the bone geometry had little influence on composite elastic properties when compared to experimental error from the in vivo study. The implication is that such properties can be estimated by measuring the volume fraction of bone using a non-destructive method like microcomputerized tomography and the simple RVE model.
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1. Introduction

Research in bone tissue engineering has made significant progress in determining appropriate scaffold materials, pore sizes and pore fractions that result in bone formation in vivo [1–4]. Work has also been done in the area of optimization of scaffold architectures to fulfill mechanical and transport requirements [5,6]. Despite these efforts, little work has been done to characterize the mechanical behavior of scaffold/bone composites either experimentally or computationally. Characterization of composite behavior throughout the healing period is essential in order for synthetic scaffolds to replace autografts and allografts, each of which have major disadvantages, in the clinic [7,8]. This is particularly true for the case of large and load-bearing defect repair.

Numerous challenges are associated with the mechanical property characterization of bone/scaffold composites. The need for large animal models tops the list. Animal studies are expensive and require facilities, resources and personnel that are not available to all investigators. In addition, implanting samples with suitable geometry for mechanical testing is complicated by the complex geometry of whole bones, and retrieving samples for testing is difficult. It is perhaps because of these limiting factors that few researchers have characterized the properties after bone growth in vivo. The lack of experimental data also precludes the development of accurate computational models that can be used to predict composite behavior.

Biodegradable polymers, such as polylactic acid [9], poly(lactic-*co*-glycolic acid) [10] and poly(ε-caprolactone) [3,9,11], and calcium phosphate ceramics, like hydroxyapatite (HA) [4,12–14], the material system of interest here, and tricalcium phosphate [15], which degrade more slowly in vivo as compared to polymers, have been studied as

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bone replacement materials. Researchers study periodic, porous scaffolds (PPS) for bone tissue engineering because of the ease with which the structures can be fabricated and modeled. They are typically modeled as simple square, cylindrical or spherical pore geometries [5,16–18], but in some cases, more sophisticated pore shapes have been studied [6].

The use of the representative volume element (RVE) is a common way in which to model the mechanical behavior of PPSs [5,16,18]. The RVE is a volume of heterogeneous material that is large enough to represent the bulk. This concept originated in composites literature and it is generally accepted that models that use periodic boundary conditions give the most accurate results [19,20]. With the application of periodic boundary conditions, the RVE is equivalent to one unit cell, which makes this method a simple and efficient way to determine effective properties of PPSs.

While periodic scaffolds can be accurately modeled, the choice of an appropriate geometry for bone in a scaffold/bone composite RVE is unclear. The dependence of the specific bone morphology on scaffold permeability, local mechanical environment, anatomical site, host species and state of healing in vivo has not been established. Thus the lack of a clear rationale for the choice of the bone geometry when modeling bone/scaffold composites may be another reason for the lack of research in this area.

Hollister et al. [5] optimized the microstructure of polymer scaffolds, as well as the bone that would replace the scaffold, to match target tissue moduli. They assumed that the bone would exactly fill the scaffold pores and examined the properties of the RVE at the initial time point, when there was no bone, and at the end point, when the scaffold had completely degraded, leaving only bone in the shape of the pore space. While the optimization was sophisticated and elegant, there is no experimental evidence to support that particular morphology of ingrown bone. Perhaps the most detailed analysis of composite scaffolds to date is by Adachi et al., who simulated bone growth and scaffold degradation for two different scaffold unit cell models. The polymer and bone evolved according to degradation of the scaffold by hydrolysis and bone ingrowth according to the uniform stress hypothesis [16], respectively. The boundary condition of applied load on two opposing surfaces resulted in columnar bone aligned in the loading direction. Again, this bone morphology has not been observed in vivo.

The purpose of this study was to develop a simple model that can be used to predict the effective elastic properties of PPS/bone composites with varying degrees of bone growth within a slowly degrading scaffold. The main question to be addressed was how to represent the bone in an RVE in a simple finite element (FE) model. Does the geometry used to represent bone morphology in the RVE play an important role in the resulting composite effective elastic properties? The scaffold structure evaluated has been shown to support bone ingrowth in vivo [4]. Furthermore, both the microstructure and the structure of the scaffold can be tailored to meet property requirements of host bone using directed deposition [13,14], a direct-write fabrication technique, which would allow it to replace a range of bone and defect types.

In this study, two idealized bone geometries were generated based on quantitative characterization of bone morphologies present in scaffold pores after a recent in vivo study [4]. One consisted of a uniform coating of bone while the other consisted of cylindrical struts that bridged the scaffold pores. These were then incorporated into three different idealized monolithic scaffold RVEs and an FE-based numerical homogenization technique and periodic boundary conditions were used to calculate the effective elastic properties of the composite. The three scaffolds include one based on measurements from the in vivo study, one with the same architecture but a smaller rod diameter, and one with simply a lower material Young's modulus. The impact of bone growth on effective properties was predicted for and compared between the three scaffolds.

This work is one of few that considers properties of the scaffold/bone composites; most compare properties of just the scaffolds [6,17,21] or properties of the bone that replaces the scaffolds [5]. There are no studies, to our knowledge, that represent bone morphology based on experimental data or that compare models with multiple bone morphologies. Unlike other work thus far, the geometries and volumes of bone used were based on quantitative evaluation of in vivo data [4] and represent stages of early and intermediate bone growth rather than just an initial stage with no bone and an end point.

2. Methods

2.1. Scaffold fabrication

HA scaffolds were fabricated using a directed deposition technique [13,14] and consisted of alternating layers of porous orthogonal rods that formed a periodic structure with orthotropic symmetry. The periodicity allowed for reduction of the scaffold to a simple and accurate RVE.

Details of HA ink preparation and deposition have been described in detail elsewhere [22]. Briefly, the colloidal ink used to fabricate the scaffolds contained 50% by volume of polymethylmethacrylate (PMMA) microspheres. Following deposition, PMMA microspheres and other organic additives were burned out and then were sintered for 2 h at 1300 °C, leaving behind interconnected micropores that ranged from 2 to 8 μm in diameter. The microporosity was believed to enhance osteoconductivity in vivo [4] and can be used to tune the mechanical properties and permeability of the material from which the scaffold is made.

2.2. Measurement of the elastic properties of microporous HA

Bulk properties of microporous HA were determined using pulse transmission ultrasound following the ASTM

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