Fracture Toughness of Carbon Nanotube Reinforced Artificial Bone Tissue

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Abstract: The idea of hydroxyapatite (HAp) precipitation on functionalized carbon nanotubes (CNTs) introduces a new aspect of bone tissue engineering. Based on this idea, a mechanical model is developed for predicting effective Young's modulus and tensile strength of a representative volume element of a tip-functionalized CNT reinforced HAp. Results of this study show that there is an increase in fracture toughness of the HAp-CNT composite compared to that of HAp-collagen, i.e. natural bone. However, natural bone, showing quasi-brittle behaviour, undergoes microcracking under everyday normal physiological load which stimulate bone remodeling process to stop propagation of microcracks and finally make new bones at the affected areas, as a toughening mechanism. Knowing that CNT reinforcement increases bone fracture toughness and so would decrease microcracks production, another aspect of this research is addressing if the CNT-HAp composite is better than HAp-collagen from a bone remodeling point of view.

Keywords: carbon nanotube, bone, fracture toughness, microcrack, remodeling

1. INTRODUCTION:

Carbon nanotubes (CNTs) are considered as biocompatible materials and many studies are going toward their usage in tissue engineering, biosensors, drug delivery agents, and other aspects in biomedical engineering. (CNTs) have been presented as ideal biocompatible scaffolds for the growth of living tissues [1-5]. This can find a wide range of applications in tissue engineering, since CNTs show extraordinary electrical, chemical and mechanical properties [6].

Recent experimental studies have promised the use of CNTs as templates for bone material regeneration [7]. It is shown that CNTs provide a suitable environment for adhesion and proliferation of bone cells [8]. On the other hand, nucleation of bone mineral ions is an interesting phenomenon observed in chemically functionalized CNTs [9,10]. The functional group attached to the CNT acts as a

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substratum which can attract the calcium ions and subsequently by exposure to phosphate ions, it is feasible to form a bioceramic similar to bone tissue mineral phase, namely hydroxyapatite (HAp), over the CNT [9,10]. Therefore, a composite material tends to form consisting of CNTs (which act as the reinforcement phase) and HAp (which acts as the matrix).

This kind of artificial bone can be considered, to some extent, as an imitation of natural bone tissue, since CNT takes the role of collagen fibers (organic phase) as the template for mineralization of HAp [11]. CNT also can provide tensile strength for the matrix just like what collagen fiber does in hierarchical structure of bone [12]. The concept is even justifiable from the point that the geometric dimensions of both CNTs and collagen fibers are approximately in a closely comparable range.

The differences between the mechanical properties of CNTs and those of collagen fibers can most likely lead to significant alterations in the mechanical behavior of the artificial bone compared with normal bone tissue; and this, in turn, will have a definite effect on the rate of bone remodeling and turnover which ultimately dictate the mechanical properties of the bone tissue. In this research, we try to shed some light on the important question of: “How the changes in the material properties of artificial bone tissue (compared to a natural bone) can affect the functions of bone as a living tissue and its adaptation process”. So, a simple model of a representative volume element (RVE) of the CNT-HAp composite is presented here in order to predict the fracture toughness of the artificial bone as a key quantity for its adaptation process, and also fracture behavior.

2. METHOD:

2.1 Building the RVE:

The RVE is composed of two phases: CNT and HAp. CNT is assumed to be tip-functionalized with carboxyl groups (-COOH). This chemical group leads to the formation of homogeneous HAp matrix surrounding the CNT [9,10]. A solid cylinder represents the CNT [13], and a hollow cylinder stands for the HAp matrix surrounding the CNT. The linkage between these two phases is made by a beam element connecting the corresponding heads of the CNT and matrix. This beam represents the covalent bond between a carbon atom on the CNT head and the carbon atom in the carboxyl group. The total strain energy of the beam is taken equal to the carbon-carbon (C-C) bonding energy, so that mechanical constants of such a beam element can be obtained [14]. So the RVE can be illustrated as shown in Fig. 1.

Figure 1: RVE of HAp on tip-functionalized CNT

2.2 Obtaining the composite material properties:

Once the RVE model is built as a combination of elastic elements, the problem can be solved for axial loading conditions to determine the mechanical response of the RVE in the form of elastic deformation. This yields the effective axial Young's modulus of the RVE.

A criterion can be assumed for the determination of the axial tensile strength of the RVE. In this approach, the axial tensile stress applied on the RVE cross-section leads to a combination of stresses within each element, since the linking beam element transfers stresses from the matrix to the reinforcement. The resulting stresses in either HAp matrix or the C-C bond representing element may exceed the ultimate value, i.e., defined tensile strength for that element, and cause failure. Therefore, the value of axial tensile stress which causes failure in either HAp or C-C bond can be calculated as the tensile strength of the RVE. Here, failure of the RVE is supposed to occur without any non-linear deformations.

The effective Young's modulus defines the slope of the stress-strain curve, when neglecting the non-linear response of the chemical bonding and assuming overall linear elastic behavior for the RVE. On the other hand, the same assumption leads to the determination of the fracture strain at the point in which fracture strength is known. As a result, the area under the stress-strain curve, up to the fracture point, can be obtained as fracture toughness. This is a critical parameter which describes the energy dissipated prior to fracture.

3. RESULTS:

The effective Young's modulus of the RVE is shown in Fig. 2 for different CNT aspect ratios (the ratio of CNT length to its diameter) as a function of CNT volume fraction. The figure includes the results of Voigt [15] and Reuss [16] models, which consider isostrain and isostress configurations of elements, respectively. When CNT aspect ratio is near to 100, or higher, this model is approximately set on the Voigt's prediction which is illustrated as a straight line.

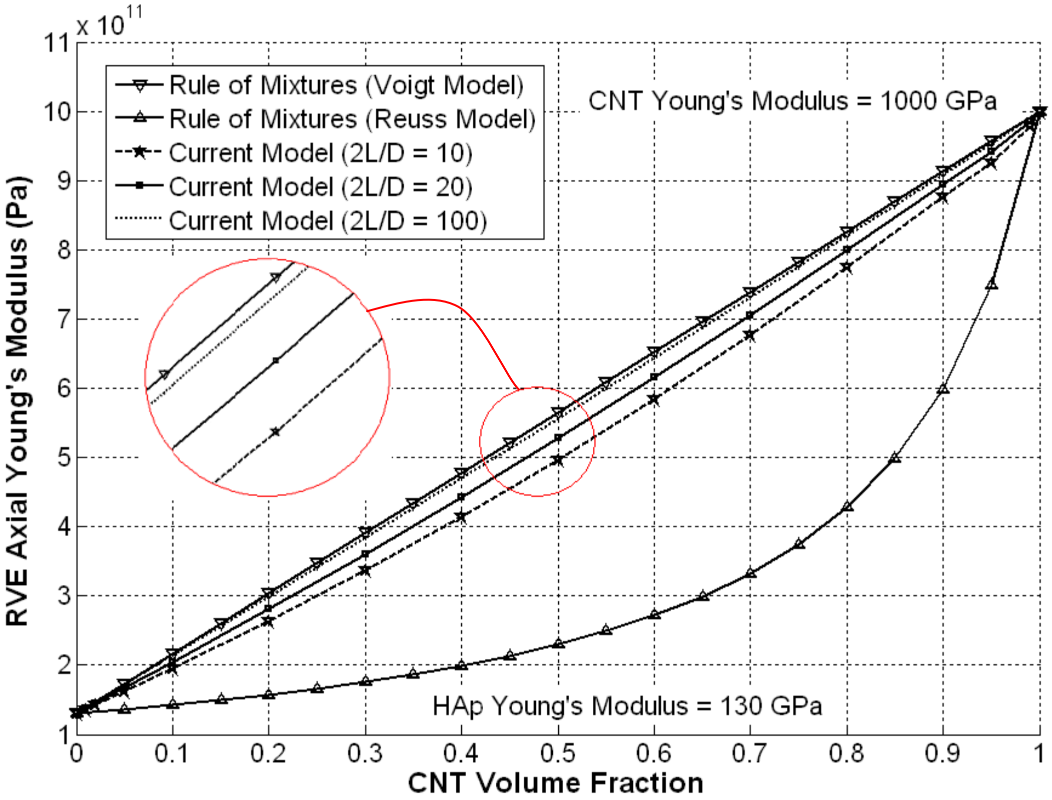

Figure 2: Axial Young's modulus versus CNT volume fraction

The predicted tensile strength of the RVE is shown in Fig. 3 for different CNT aspect ratios as a function of CNT volume fraction. This figure shows that reinforcing mechanism acts more effectively to increase the tensile strength, when there is an increase in CNT volume fraction and/or aspect ratio. This is in agreement with results by previous studies [17-19].

Our results also show a significant increase in both axial Young's modulus and tensile strength of the HAp when reinforced by CNT. A simple comparison leads to the understanding that fracture toughness of the synthesized HAp-CNT is several times higher than that of the natural bone (HAp+collagen) (see Fig. 4).

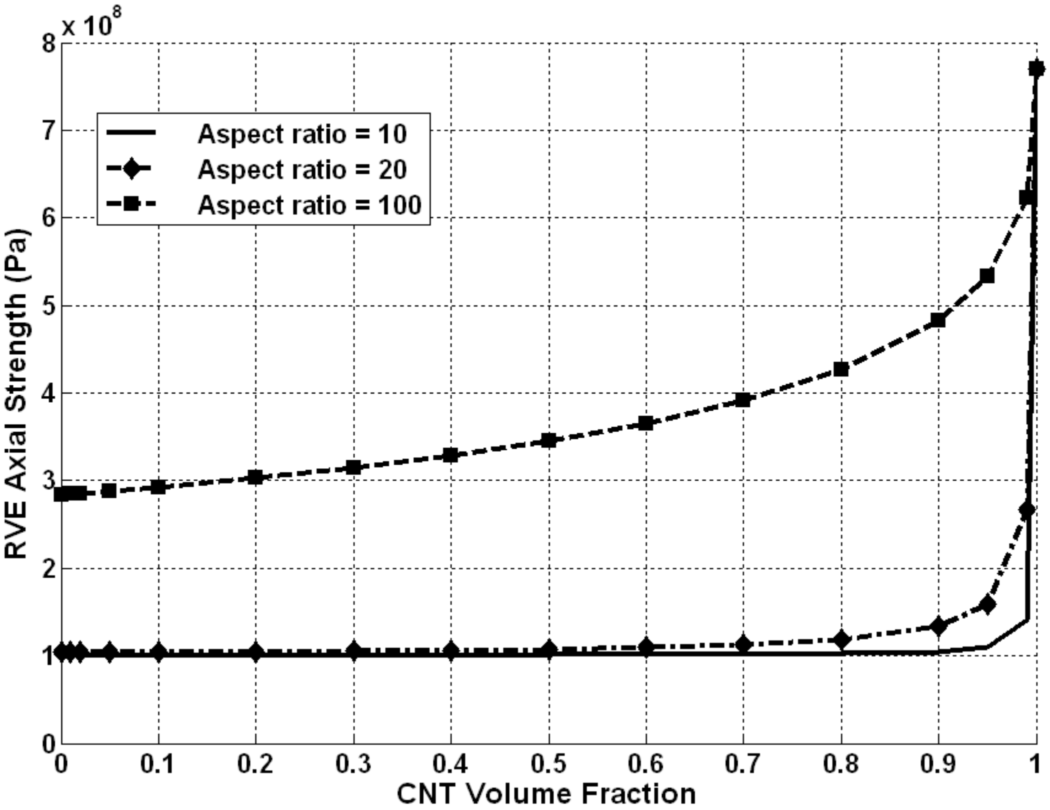

Figure 3: Axial tensile strength versus CNT volume fraction

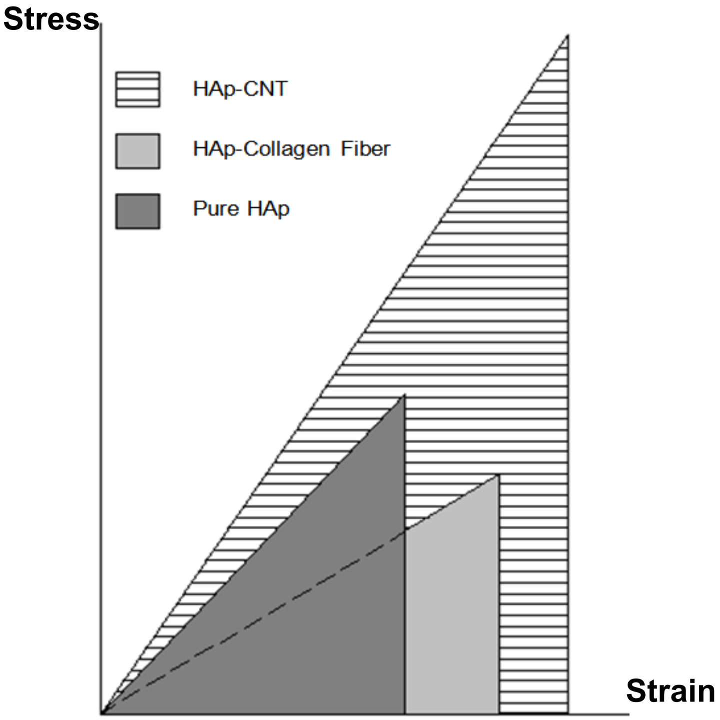

Figure 4: Schematic stress-strain curves for HAp-CNT, HAp-Collagen Fiber, and Pure HAp

4. DISCUSSIONS:

Our predicted RVE Young's modulus lies between two limits given by Voigt and Reuss models. Voigt, assuming perfect bonding between matrix and reinforcement, considers isostrain condition in which elements deformations are equal at every contact point between two phases. Perfect bonding assumption in such situation, gives the uppermost limit of effective properties of a RVE of the composite. However, the current model presents the interphase interaction only at functional sites which results in a considerable deviation from the Voigt's prediction (see Fig. 2). Knowing that the strength of a fiber composite material is a function of the strength of interface between the matrix and fibers, among other factors, it makes a very good physicals sense that the Young's modulus of Voigt model should be the most compared to others (Fig. 2). There is a jump in initial values of strength, from the aspect ratio of 20 to 100 (see Fig. 3). It, perhaps, shows a critical aspect ratio for CNT between these two values in which the load transfers completely from matrix to the linkage. Thus, the results see, to suggest that the failure at such or higher aspect ratios occurs at the C-C bond, but not in the HAp matrix.

Fracture toughness as a measure and indicator of the capacity of a material to resist failure, is an important parameter that can be used to determine to which category of materials, a material belongs to. It is well known that pure HAp is a brittle material, while bone tissue behaves in a quasi-brittle manner [20-22], and this is due to the collagen inclusion as a flexible phase which can increase bone toughness. The enhanced elastic properties of CNTs in the HAp matrix, however, introduce the doubt on change of the material behavior as to ductile. Microcracking is a common toughening mechanism in bone, as a quasi-brittle material, which occurs near the main crack tip to resist the crack growth [20-22]. Moreover, it is well accepted that microcracks can initiate and also accelerate bone remodeling process in which there will be a break for the crack propagation and can encourage making new bony material at the deteriorated sites [23-26]. It seems reasonable, by considering the differences between the mechanical properties of the natural and artificial bone (HAp+CNTs), to assume that the rate of bone remodeling process will be altered, and possibly disturbed when CNTs replace the collagen fibers in natural bone tissue.

Although promising results are shown in initial steps toward the bio-applications of CNTs as scaffolds for bone growth, more investigations need to be done to address the question of: "Is replacing collagen fibers by CNTs beneficial for bone from the bone adaptation point of view or can be seen as a disturbing factor in the remodeling process?"

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