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Nano finite element modeling of the mechanical behavior of biocomposites using multi-scale (virtual internal bond) material models

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Abstract

It is evident that biocomposites, specifically mineralized Type-I collagen fibrils, have strong mechanical properties, such as a desirable combination of elastic modulus, fracture toughness, and fracture strength. The mineral Hydroxyapatite [Hap] by itself is stiffer, and it is not clear whether a collagen fiber by itself has a lower breaking strength than the mineralized fiber. Hence, the objective of this paper is to develop, outline, apply, and demonstrate issues involving a new nano explicit finite element based framework, by which the mechanical behavior of mineralized collagen fibrils and their constituents can be studied. A multi-scale virtual internal bond model is used to model the material behavior and failure of such biocomposites. In this research two models have been studied. The first model attempts to illustrate the hypothesis that materials are less sensitive to flaws at nanoscale and the second model studies the mechanical behavior of a nano sized dahlite mineral crystal commonly found in collagen fibril. Two important implementation characteristics have been introduced and illustrated, namely that scaled properties can be used at the micro and nano length scales along with scaled dimensions and secondly the loading time can be appropriately scaled without the loading becoming a dynamic loading.

Keywords

finite element analysis; collagen; nanomechanical behavior; biomineralization; dentin

INTRODUCTION

There is a great need for research into the mechanical behavior of biological materials in order to attempt to correlate the development of biological tissues and the proclivity and progression of certain diseases to the mechanical behavior. Such a correlation would involve a combination of development in experimental, theoretical and computational areas. Experimental capabilities, at the micrometer and nanometer levels, have made significant advances in studies of the behavior of biological tissues. For instance, the atomic force microscope (AFM) can be used to obtain images of the structure of the material at the nanoscale level. Mechanical properties also are being studied at the micro- and near-nano-scale levels by the use of the scanning acoustic microscope (SAM), which can be used to determine the elastic modulus of substrates in the order of 0.5 μm using the very high frequency (2 GHz) lens. Thus, these

experimental advances have provided the motivation to develop mechanical behavior models using a bottom up approach.

It is fairly well established that certain biological materials, such as bone, exhibit a hierarchical structure consisting of several levels.^{1–3} Weiner and Traub⁴ have outlined that the fundamental level bone consists of plate-shaped crystals of carbonated apatite (also known as dahlite) 2–4-nm thick and few tens of nanometers wide, now known to be 10-nm wide and 0.61-nm thick.⁵ These crystals are arranged in parallel arrays in a collagenous framework to form mineralized collagen fibrils. The mineralized collagen fibril is the basic building block of biocomposites such as bone. Other biological tissues that contain mineralized collagen fibrils include dentin, cementum, mineralized tendons etc. There are three major components of the mineralized collagen fibril; the collagen molecule, minerals, and water.³ The proportion of the three components varies for different tissue types. The collagen molecule in these fibrils are predominantly Type I collagen, which is made up of three polypeptide chains of about ~1000 amino acids wound together to form a triple helix. The triple helix has an average diameter of 1.23 nm, possibly less as the measurement made by diffraction probably includes the presence of water molecules, and is about 300-nm long.⁶ The diameter of the mineralized fibril itself is of the order of 80–100 nm. The collagen molecule is the major protein component of the fibril.

The organization and structure of mineralized collagenous fibril is not simple and many known forms have been proposed. The 300 nm sized collagen molecules show quasi-hexagonal packing with periodicity of 67 nm (the D period), which is due to the molecules being staggered in axial direction by 67 nm with respect to each other, according to the Hodge–Petruska scheme.⁷ Since the length of the molecule is $4.46D$, there are gap regions of $0.54D$. Each collagen molecule is divided into four segments of length D and the fifth segment of length $0.46D$. The 67-nm periodicity of the collagen molecule comprises of a 40-nm hole region and 27-nm overlap region.⁶

Mineralization of collagen fibrils

The processes of mineralization as well as the arrangement of minerals in collagen fibrils and fibers are areas of extensive ongoing research. Veis⁸ has outlined that the mineralization process can either be "biologically induced" (in corals) wherein the crystals have random orientations or can be "matrix-mediated" wherein shape, orientation and nature of crystals is confined to closed spaces or channels defined by the collagen molecule orientations. Du et al.⁹ have shown that in tooth enamel highly ordered apatite crystals are formed. Studies of crystal growth in collagen fibril shows that the mineral crystals are initially formed in the hole zone and during the first stage they are confined to this zone. Crystals accommodated within the internal hole zone are oriented with their crystallographic c-axes generally parallel to the long axis of collagen and their planes approximately parallel to each other.⁶ The collagen molecules form channels at the hole region, transverse to the c-axis of the collagen fibril for a distance of at least 10 nm.¹⁰ The hole expands upon mineralization, but all the minerals cannot be accommodated in this region. Veis⁸ has further outlined the differences in the mineralization process in the dentin and enamel regions. Jager and Fratzl¹¹ have stated that in a typical bone remodeling event, the collagen matrix is deposited first and the thin mineral particles are nucleated in the gap region and grow without a change in the overall volume, essentially replacing the water. In general, the mineralization process is an area that is still not very well understood.

Tong et al.¹⁰ have noted that in young postnatal bovine bone the mineralites formed are shorter and narrower, $9 \pm 3 \text{ nm} \times 6 \pm 2 \text{ nm}$, but thicker, $2 \pm 1.2 \text{ nm}$, than the mineralites. Eppell et al.⁵ have described the mineral geometric properties by performing AFM studies on mature bovine cortical bone mineralites. They have suggested that the minerals are plate like in shape with a thickness ranging from 12 to 115 nm (mean of 37 nm), width ranging from 27 to 172

nm (mean 64 nm) and length ranging from 43 to 226 (mean 90 nm). In addition, they also pointed out that the large mineralites could be located at the outer surface of the fibrils and the minerals (98%) have a mean dimension of $12 \times 10 \times 0.61 \text{ nm}^3$. They have also suggested that the binding strength of the collagen molecule to the mineralites may be maximized when the mineral length takes on a particular value. Landis et al.⁶ demonstrated for the first time platelet shaped crystals on the surface of collagen fibrils in turkey leg tendons. Balooch et al.¹² investigated the intrafibrillar (within the fibrils) demineralization of single human dentin collagen fibrils using AFM. Kinney et al.¹³ used small angle X-ray scattering (SAXS) technique and suggested the thickness of the mineralite crystals in human tooth, in general, was ~5 nm.

Structure–mechanical relations at lower levels of hierarchy

Mechanical models to study the relationship between the structure and the mechanical behavior at lower levels of hierarchy have been proposed in the recent past. Currey¹⁴ suggested that the elastic modulus increases with increasing mineralization. Mineral crystals in collagen have the effect of increasing the stiffness and fracture stress but reducing the fracture strain.¹¹ It has been suggested that two main factors that must be considered to describe the mechanical behavior at the fibril level are (a) mineral density in the fibril and (b) arrangement of mineral particles in the collagen matrix of the fibril.^{3,15} The reduced presence or absence of intrafibrillar mineral in dentinogenesis imperfecta type II (DI–II) teeth is known to cause defective mechanical properties.¹³ The lack of the intrafibrillar minerals results in drastically reduced elastic modulus and hardness of dentin.¹³

Mineralization geometry models—In the axial direction there is good long-range order of collagen molecules. However in the lateral direction the geometric pattern for mineralization of collagen fibrils is complex and not very well understood. It is known to vary depending on the source of the tissue. Mineralization is known to initiate primarily in the gap regions. Hence, the geometric order of the gaps in the lateral direction is important in determining the mineralization pattern and geometry. It is hypothesized that in the lateral direction only short range order exists. Two hypothesis of the manner in which the channels are formed are (a) concentric channel arrangement¹⁶ and (b) three dimensional packing models that arranges gaps as lateral channels or holes that are one molecule thick (~15 Å) and extending to unknown distances in the transverse direction.⁴ Tong et al.¹⁰ have suggested that the channels run for a distance of at least 10 nm in the transverse direction. Hulmes et al.¹⁶ have discussed radial packing and order arrangements in collagen fibril and had proposed that the gaps in the collagen fibril run as concentric channels around a central fibril core. Jager and Fratzl¹¹ have discussed three possible arrangements of minerals in the fibril namely (a) crystals occupying only the gap zones (b) crystals growing into the overlap zone and (c) longer crystal sizes (~100 nm) extending beyond the overlap zone as well and having a staggered arrangement. It appears that the Jager and Fratzl models are based on the model proposed by Hulmes et al.¹⁶

MATERIALS AND METHODS

Biocomposites, specifically Type-I collagen fibrils, have good mechanical properties, such as a desirable combination of elastic modulus, fracture toughness and fracture strength. The mineral Hydroxyapatite [Hap] by itself is stiffer, and it is not clear whether a collagen fiber by itself has a lower breaking strength than the mineralized fiber. Hence, the overall objective of this research is to develop a new finite element based framework by which the mechanical behavior of mineralized collagen fibrils can be studied.

The primary motivation to develop a new framework arises from the fact that collagen and minerals have elastic moduli that vary by two to three orders in magnitude. Traditional material

models that are based on elasticity, plasticity and fracture based theories may not be directly suitable. There are at least three requirements that have to be addressed, namely (a) the protein component is expected to undergo high strains while the mineral component is expected to be in low strain regions at the same time (b) the high strains in the protein regions could lead to a number of localized fracture spots, which must be seamlessly modeled and (c) the components are themselves nanometers in size, which must be modeled in finite elements without a loss of stability and accuracy from a computational perspective. At the nanometer scale the primary problem arises due to the mesh size. The FE code exits with an error stating that elements have zero or negative volume. Using double precision in computational strategies is not the only answer. These issues and others, as outlined below, are addressed in this paper by (a) the development and implementation of a multi-scale virtual internal bond (VIB) model suitable for this application and (b) addressing many of the implementation issues of the proposed nano finite element (nanoFE) framework in detail.

The first major goal of modeling collagen fibers, which are composed of many collagen fibrils, is sought to be achieved in four stages. Firstly, the nature and issues pertaining to the modeling of nano sized mineral platelets must be addressed, to be followed by the modeling of tissues that contain only type I collagen such as the rat tail tendon; the third step would be to develop models for a collagen fibril and finally the collagen fibril model would be statistically combined to develop the finite element framework for collagen fibers. The development and studies using the nanoFE model could lead to addressing a broader question namely, how does the degree of mineralization affect the mechanical properties of collagen fibers? How does the mechanical property of mineralized collagen fibril depend on the amount of mineral particles and their arrangement within the fibril? This paper addresses the first stage of this process, namely the aspects and issues related to the modeling of a single mineral platelet.

Virtual internal bond model basics

The VIB model is a multi-scale model as it combines the behavior at two length scales, namely the atomistic and the continuum levels. The basic premise of the VIB model^{17–19} is that the body can be considered as a spatial distribution of material points at the continuum level, which is represented by the integration points in a finite element scheme (Fig. 1). Each individual material point F_1 can be thought of to represent collectively the behavior of underlying atoms. At the atomistic level the interaction between the atoms is represented by two body pair potential based cohesive bonds, which results in a cohesive type interaction between material points at the continuum level.

The Cauchy–Born rule of crystal elasticity relates the motion of atoms to the continuum deformation process and its measures. This rule assumes that the atomic motion, from the undeformed to the deformed configuration, under a homogeneous deformation, can be defined as a single mapping. At the continuum level, the deformation gradient $\mathbf{F}$ defines such a mapping. The interaction at the atomistic level may be described through interaction potentials. In a polycrystalline material, the material behavior is isotropic because of the random crystallographic orientation of grains. Such behavior can be modeled by a random spatial distribution of cohesive bonds using the VIB model. While it is recognized that biocomposites is a complex material, it is reasonably assumed in this study that it can be modeled as material points interconnected by cohesive bonds. Further details of the implementation of the VIB model can be found in Thiagarajan et al.^{20,21}

VIB model framework and its suitability

The VIB model is described within the framework of hyper-elastic continuum mechanics. The initial and the deformed configurations are defined using the Lagrangian coordinates $X = X_I$ and the Eulerian coordinates $x = x(X, t) = x_i(X_I, t)$, respectively. In this paper, capital letter

subscripts are used for the initial configuration while lower case subscripts are used for the deformed configuration. In the Lagrangian description the deformation gradient can be expressed as follows

$$F = \frac{\partial x}{\partial X} \text{ or } F_{ii} = \frac{\partial x_i}{\partial X_i} \quad (1)$$

and the Green–Lagrange strain tensor may then be defined as

$$E = \frac{1}{2}(F^T F - I) \quad (2)$$

where, I is the second order identity tensor.

In the atomistic framework, the bond can be described by a potential energy function $U(l)$ where l is the bond length. Consider an arbitrary micro-structural bond at an angle θ and φ , where θ is the angle of the bond orientation with respect to the vertical positive 2-axis, and φ is the angle in the horizontal plane with respect to the positive 1-axis, respectively. The unit vector along this direction is given as $\xi = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ with respect to the undeformed configuration. The stretch of this bond can be related to the continuous deformation as follows

$$l = l_0 \sqrt{1 + 2\xi_i E_{ij} \xi_j} \quad (3)$$

The macroscopic strain energy density function is derived using the Cauchy–Born rule as follows, thus linking the two scales.

$$\Phi(E_{ij}) = \langle U(l) \rangle \quad (4)$$

where, $\langle \rangle$ represents the weighted average with respect to the bond density function D_d and $U(l)$ is the bond potential energy function. Assuming that all bonds have the same initial length l_0 , for the general case the weighted average is given as,

$$\langle \dots \rangle = \int_0^{2\pi} \int_0^\pi \dots D_d(\theta, \varphi) \sin \theta d\theta d\varphi \quad (5)$$

The term $D_d(\theta, \varphi) \sin \theta d\theta d\varphi$ represents the number of bonds per unit volume between the bond angles $(\theta, \theta + d\theta)$ and $(\varphi, \varphi + d\varphi)$.

Constitutive equations and cohesive force law

From the strain energy density function Φ given in Eq. (4), the symmetric second Piola Kirchhoff stress S_{ij} and the elastic modulus C_{ijkl} can be derived as follows

$$S = \frac{\partial \Phi}{\partial E} \text{ or } S_{ij} = \frac{\partial \Phi}{\partial E_{ij}} \\ C_{ijkl} = \frac{\partial^2 \Phi}{\partial E_{ij} \partial E_{kl}} \quad (6)$$

The modulus derived from this potential satisfies the major and minor symmetries, $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$ as well as the Cauchy symmetry, $C_{ijkl} = C_{ikjl}$. For isotropic material this results in only one independent elastic constant due to the fact that the Cauchy symmetry is satisfied by the fourth order isotropic elasticity tensor only for the case of $\lambda = \mu$, where λ and μ are the two Lamé's constants. Consequently, the VIB model as used in this work represents a Poisson's ratio of 0.25. The Poisson's ratio value of the VIB model suits well with the

analytical modeling effort by Jager and Fratzl¹¹ in their development of a mechanical model for mineralized collagen fibrils, wherein they also replaced the anisotropic nonlinear collagen by an effective elastic material with a Poisson's ratio of 0.25, as also done by Akiva et al.²²

To represent the potential $U(l)$, in this paper the two parameter cohesive force law, based on the Smith–Ferrant potential function is chosen and can be expressed as follows

$$U'(l) = A(l - l_0)e^{\frac{l-l_0}{B}} \quad (7)$$

The form of the function is shown in Figure 2. Figure 2(a) shows the bond interaction potential $U(l)$ function. $U'(l)$ is the cohesive force and is the derivative of the bond potential energy with respect to the bond length l . The constant A can be related to the material shear modulus by Eq. (7) and represents the initial slope of the curve in Figure 2(b). The parameter B is related to the strain at which the cohesive stress is reached.

VIB and nano-FE modeling

Modeling the behavior of nano structures using traditional finite elements necessitates the usage of material models that appropriately represent the behavior at the nano scales. Hence, traditional elasticity, plasticity, fracture and damage based constitutive models may not be suitable. There are a number of requirements. For example, it has been hypothesized^{23,24} that failure of nano structural materials is governed by critical surface energy and not necessarily by stress concentrations at crack tips. It is difficult for regular FE material models to incorporate this feature. This paper attempts to demonstrate that the VIB material model is better suited for this purpose.

To address the issues a new framework of nano finite element modeling effort a new way to address them is presented here by using scaled property values at the different scales studied.

Scaling issues—The numerical values of the geometry for the finite element model can be represented in two ways.

1. Firstly, the nano scale model could be represented by giving nanometer dimensions to the geometry and using the material property values identical to that of the continuum scale model. The approach suffers from two major drawbacks namely
 2. The element sizes are very small resulting in very small incremental time steps with ABAQUS/Explicit. For instance the nanometer sized element could result in time steps of 10^{-12} s which would make real time, for example 1 s, simulation prohibitively expensive if not impossible.
- a. Using continuum properties such as $E = 100$ GPa with nanometer dimensions (10^{-9}) creates numerical issues in FE programs even with using double precision.
- b. Secondly, a set of scaled SI units can be used to represent the nanometer and micrometer dimensions. Scaling the dimensions should be accompanied by appropriately scaling the material properties as well. This approach results in using reasonable numerical values to represent the geometry. For example, if a scaled meter represents 10^{-9} m, then the geometry of 25×50 nm² can be represented in the FE model as a solid of 25×50 units, which avoids any associated numerical issues. Three sets of scales are used in this study namely (a) millimeter (mm), (b) micrometer (μm) and (c) nanometer (nm).

Scaling adopted—For the nanometer and micrometer studies, both the mass and the length values are scaled. The scaled dimensions, for the nanometer scale, used in this study are as follows

- a. 10^{-9} m = 1 scaled meter (sm).
- b. 10^{-3} kg = 1 scaled kg (skg).

The scaling of the length and mass values results in the scaling of associated properties. For example $1 \text{ Pa} = 10^6 \text{ sPa}$; the density of $3180 \text{ kg/m}^3 = 3.18 \times 10^{-21} \text{ skg/sm}^3$ at nm scale. For the micrometer studies a scaled meter represents 10^{-6} m and the scaled kg is the same as that for the nanometer scale. It can be shown that for the micrometer scaled study a stress value $1 \text{ Pa} = 10^3 \text{ sPa}$. For the centimeter scale study both the geometric and material properties were given in kg and cm units, which results in $1 \text{ Pa} = 10^2 \text{ sPa}$. Table I outlines the dimension and material property conversions.

Another major advantage of dimension scaling is that in simulations using ABAQUS/Explicit, the solution results in more reasonable simulation times. For example, the speed of longitudinal wave c in a solid is given in terms of its elastic modulus E and its density ρ as $c = \sqrt{E/\rho}$. As the density, modulus and length values are scaled; the wave speed in scaled dimensions are significantly higher, which results in the stresses reaching the center of the plate much faster. Consequently, it is hypothesized that quasi-static simulations can be run for significantly shorter times without the loading becoming dynamic. In fact, it can be expected that as scales decrease the simulation times will also decrease. This outcome, termed as *scaled time* quasi-static studies, is explained in detail later.

Models studied

To demonstrate the hypothesis of materials being insensitive to flaws at the nanoscale and to study the mechanical behavior of mineral platelets, new and appropriate multi-scale models, such as the Virtual Internal Bond (VIB) model is proposed in this research study. The implementation of these models in a numerical scheme, using finite elements, is outlined in this section. The study will be useful in defining and setting up a framework for nano FE simulations. Two different models, as described below, are used to study the fracture toughness and flaw resistance of nano sized mineral platelets.

- Model I is set up to study the effect of varying thickness on a nano sized platelet with a flaw in the form of a thumb nail crack. The objective of this model study is to demonstrate that as the thickness tends to drop below a critical thickness the failure may not be governed by stress concentrations at the crack tip.
- Model II is set up to study the effect of *dimension* and *time* scaling on the behavior of nano sized mineral particles. The objective of this model study is to demonstrate the implementation aspects of the framework of nano FE studies using the VIB model and to address some of the issues that arise.

Model I—Thumb nail crack model—The failure behavior of nano sized platelets with two identical planar dimensions but of different thicknesses is studied by modeling a central thumbnail crack enclosed in a mineral platelet as shown in Figure 3. From Griffith's criterion the fracture strength of a mineral platelet can be determined as follows

$$\sigma_m^f = \alpha E_m \psi = \sigma_{th}$$

$$\psi = \sqrt{\frac{\gamma}{E_m h}}$$
(8)

where, γ is the surface energy and h is the thickness of the mineral crystal. For a thumb nail crack in the middle of a platelet, defined as a crack depth equal to half the depth of the plate, the geometric parameter α has an approximate value of $\sqrt{\pi}$. Hence, the critical thickness below, which flaws do not effect failure $h = h^*$ can be determined from the following expression as

$$h^* \approx \alpha^2 \frac{\gamma E_m}{\sigma_{th}^2} \quad (9)$$

For a mineral platelet the elastic modulus is in the range of 100 GPa. Assuming²⁴ $\gamma = 1\text{J/m}^2$ and a σ_{th} value of $E_m/30$ [Ji and Gao, 2004] the value of h^* comes to about thirty nanometers. The thickness effect was studied, in this study, by varying the thickness h at nanoscale and the thickness studied were $h = h^*$, $2h^*$, and $10h^*$. The plate dimensions modeled are $10\text{ }\mu\text{m} \times 10\text{ }\mu\text{m} \times h$ and the loading applied is uniaxial and in vertical direction. The density of the platelet was taken as 3.18 gm/cc.

VIB model parameters: As outlined in Thiagarajan et al.,²⁰ the parameter A is representative of the initial bond density and can be determined from the shear modulus of $G = 40\text{GPa}$, from ($E = 100\text{ GPa}$) of the mineral as shown below,

$$A = \frac{4G}{\pi D_o^2 l_o} = \frac{4 * 40\text{GPa}}{\pi} = 50.9\text{ Gpa}$$

D_o and l_o can be considered as unity without any loss of generality. As seen in Figure 2(a), which is related to the initial tangent of the two parameter cohesive force law, represents the initial elastic modulus of the material.

The second parameter B of the cohesive force law, which represents the strain at the cohesive stress, is now determined as follows. Gao and Ji²³ had shown that the size of the localization zone can be expressed as

$$h = - \frac{J_1}{\pi D_o U(l_o^*)}$$

where, J_1 is the J -integral expressed in Lagrangian terms, and $U(l_o^*)$ is the bond potential energy at the initial unstrained length. Using the two parameter phenomenological cohesive force law the expression for h can be rewritten as follows from which an estimate of the parameter B can be made as shown below for the nanometer model study (thickness $h = 4\text{ nm}$).

$$h = \frac{2\gamma}{\pi D_o A B^2} \\ B = \sqrt{\frac{2\gamma}{\pi D_o A h}} = \sqrt{\frac{2(1\text{J/m}^2)}{\pi(1)(50.9\text{e}9\text{N/m}^2)(4\text{e}-9\text{m})}} = 0.055$$

For the micrometer ($h = 4\text{ }\mu\text{m}$) and millimeter ($h = 4\text{ mm}$) studies it can be shown from the above equation that the values of B should be of the order of 0.0018 and 0.000056 respectively. Alternatively, this implies that the values of B used, to insure failure by surface energy separation rather than crack tip stress concentration, should be higher for lower scales although the same material is used. As the exact surface energy and σ_{th} are not known, after a few trials the effect of the parameter B is studied here by trying two different values of B , namely $B = 0.005$ and $B = 0.0005$.

Mass scaling factor: In explicit dynamic finite element analysis the mass scaling factor plays a very important role in the simulations. It artificially increases the mass density with a

consequent reduction in the step time required. The step time reduction is directly proportional to the square root of the density. For example, the scaling factor of 10,000 reduces the simulation time by 100. It is to be noted that the scaling factor changes the stress values also by the square root of scaling factor value. In the thumb nail crack simulation, which represents a quasi-static loading, a scaling factor of 10,000 was chosen to achieve all the solutions in a computational time of few hours. All computations have been carried out using IBM p-Series 690 machine, which has an IBM Power4 processor running at 1.3 GHz (5.2 GFLOPS). A detailed study of scaling factor issues is presented in the notch model (Model II) study section.

Model II—Dahlite crystal study—The objective of this model study is to establish the implementation framework for nano sized material behavior in an Explicit finite element environment. Two aspects of implementation namely, the effect of scaled properties and scaled time are studied in detail.

In this model notched specimen of different length scales, namely millimeters, micrometers and nanometers are studied using the properties of Dahlite mineral crystal of matured bone. A notch is considered to study the effect of flaw at the nanoscale. The geometric dimensions of $50 \times 25 \times 4 \text{ nm}^3$ (Fig. 4) chosen for this study reflect a probable actual size of a mineral platelet in a mature bone.³ In this property and time scaling study the stress pattern at the "mm", " μm ", and "nm" scales are compared.

Mass scaling factor: In the Dahlite model, it is important to choose an appropriate mass scaling factor. As seen in the earlier section the mass scaling factor increases the stress values, but decreases the simulation time. A parametric study was conducted on the thumb nail crack specimen. All the variables except the scaling factor were kept constant and the stresses at the crack tip at different time steps were observed. Table II shows the comparison of the stress values.

In Table II column two represents the stresses at the top of the plate at the end of the first time step. It can be seen that the stress values increases by the square root of the mass density factor. The stresses (S_{22}) and strains (LE_{22}) at a later stage ($t = 2.4 \times 10^{-9} \text{ s}$), shown in columns three and four, well after the stresses reaches the crack tip. For MSF of ten and hundred there was no change in the stress value and the variation in stresses at higher MSF, while increasing, could not be predicted. On the basis of this important observation a MSF of one hundred (highest value chosen to minimize simulation times) was picked for Model II studies.

RESULTS AND DISCUSSIONS

Model I

Figure 5 shows the axial stress contour (S_{22}) of the three models studied, namely $h = h^*$ [Fig. 5(a)], $h = 2h^*$ [Fig. 5(b)] and $h = 10h^*$ [Fig. 5(c)]. From the figure (Fig. 5) it can be seen that as the thickness increases the stress concentration is localized near the crack tip. At low thicknesses, $h = h^*$, there is greater uniformity in stress distribution, as seen from a wider area over which peak stresses occurs [Fig. 5(a)], which would lend to a conclusion that the failure due to flaws are not necessarily due to stress concentrations. From Figure 5(c) ($h = h^*$) it can be seen that the possibility of failure due to stress concentration is greater at larger thicknesses as the stresses are high only near the flaw tip.

Figure 6 shows the graph of the variation of the axial stress (S_{22}) in the element adjacent to the crack tip for the three thicknesses studied. From Figure 6 it can be seen that at $h = h^*$ the stress at the crack tip reaches a high value and continues to increase as loading increases. For $h = 2h^*$ and $h = 10h^*$ the stress at the crack tip reaches a peak value and then continues to experience a post peak softening indicated by a decrease in stress value indicates failure at

crack tip. In other words the ability to withstand greater stress at crack tip increases with decrease in the thickness of the material. As the thickness decreases the failure is of a more general (not caused due to the crack) character and the axial stress near the crack tip decreases at failure.

Other observations that can be made from Figure 6 are that as the thickness of the material increases; (a) the time of failure increases, (b) the peak axial stress at failure decreases and (c) the displacement taken to failure increases.

Model II: Dahlite model study

Figure 7 shows the axial strain (LE_{22}) contours for the three models studied. The models represent the behavior of the three length scales namely, millimeter [Fig. 7(a)], micrometer [Fig. 7(b)] and nanometer [Fig. 7(c)] respectively. The crack propagation and branching can be clearly seen in the millimeter scale model. At the lower scales a more general failure can be seen. This suggests that at the lower scales, the structural failure occurs due to overall failure of all the elements and not due to stress concentration at the crack tip, whereas in larger sized object the failure is due the stress concentration at the crack tip

Quasi-static loading and time scaling

A natural question that arises is that in an explicit finite element environment, how one ensures that the loading applied is a quasi-static one, since it is well known that explicit FE modeling is ideally suited only for dynamic loading situations. To establish this, two types of studies were conducted. The first involves the study of the *energy variation* of the element adjacent to the crack tip and the second study involved *the scaling of the time parameter* itself.

Energy study—In a dynamic problem the total work done in the body is given as

$$WK=IE+KE+AE$$

Where IE represents the internal energy due to strains, KE represents the kinetic energy and AE is the artificial energy due to spurious hour glass modes. This check is made since ABAQUS/Explicit uses the reduced integration order elements only. Here, the C3D4R element is used, which uses a first order integration. For the loading to be classified on quasi-static the major percentage of the work done must be transferred as the IE of the system. The kinetic energy and the artificial must represent a very small percentage of the total energy (5–10%). To study this energy plot for the nanometer study is shown in Figure 8, from which it can be seen that the total work done is equal to the internal energy in the initial time phase and the kinetic energy remains under 10–15% of the total work done for the rest of the time.

Scaled time study—Even with scaled dimension the stable step time increment for the three scales are vastly different. For example, the initial step time increment values were 8×10^{-6} , 7.7×10^{-10} , and 1.8×10^{-12} s for the millimeter, micrometer and nanometer scales. To apply an equal displacement (0.5 units) on each of the models in the same real time, it is clear that the nanometer model would require approximately a million times more CPU time for the simulation—a simulation that is prohibitively expensive if not impossible. Hence, a study was conducted as described below to scale down the applied displacement time and see if the results showed a dynamic effect.

For the "mm" scale the displacement was applied over a real time of 1 s while in micrometer and nanometer study the same displacement unit was applied over 10^{-4} and 10^{-7} s, in effect reflecting the dimension scaling to the lower levels. Figure 9(a–c) shows the axial stress S_{22}

for the three models at times of 1.2e^{-2} , 1.2e^{-6} , and 1.2e^{-9} s, which represents a scaled time of 0.012 in each case or at 1.2% of the total displacement applied.

The following observation and conclusions are made from Figure 9(a–c). The maximum S_{22} values, which occurs in the crack tip element are 66.4, 67.42, and 67.64 MPa for the cm, μm , and nm scales respectively. These numbers have been converted, from the values shown in Figure 9, to MPa units by appropriately scaling them, as explained in Table I.

The most significant conclusion that can be made from the observation of equal stress values at the same scaled time is that *time scaling can also be effected without the loading becoming a dynamic one*. This observation implies that nano FE simulations using Explicit FE method can be scaled for time also thereby significantly (order of 10^9 times) reducing simulation times. The CPU times for "mm," " μm ," and "nm" scales were 1 h 03 min, 1 h 22 min, and 26 min respectively. The nanometer simulations, in fact, took only about half to third of the upper scale simulation times.

Hence, Model II studies clearly show that nano FE simulations can be effectively achieved in reasonable real time by scaling dimensions material properties as well as time without losing the quasi-static nature of the loading. If time alone were scaled without scaling dimensions and material properties the loading would become a dynamic one.

CONCLUSIONS

This paper has described a novel methodology, outlined, applied and demonstrated issues involving nano FE VIB modeling in an explicit finite element framework. Two very important characteristics have been illustrated in the implementation, namely that scaled properties can be used at the lower levels along with scaled dimensions and secondly the loading time can be appropriately scaled without the loading becoming a dynamic loading. The scaled time aspect is very significant as it allows for computations to be completed in real times, which are about a three to six orders less than the traditional frameworks.

The FE modeling demonstrates that nano structural behavior characteristics—namely—failure at the nano level is not necessarily due to stress concentration. From the first model study it can be seen that at lower thickness levels, there is greater uniformity in stress distribution, as seen from a wider area over which peak stresses occur. From model two studies it can be seen that smaller scaled materials have a greater ability to withstand stress concentrations at the crack tip, resulting in the failure occurring due to the theoretical stress limit being reached elsewhere before the cohesive stress at the crack tip being reached, suggesting that nano scale materials are possibly more resistant to flaws

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Figure 1. Conceptual representation of the Virtual Internal Bond Model showing the FE mesh and the atomistic representation of each integration/material point.

Figure 2.
Graphical forms of the Interaction Potential and the Cohesive Force Function.

Figure 3. Schematic of thumb nail crack model. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Figure 4.
Schematic of dahlite crystal model.

(a) $h = h^*$ (b) $h = 2h^*$ (c) $h = 10h^*$ **Figure 5.**

Axial stress contours for the thicknesses of the thumb nail model for plate thicknesses of (a) $h = h^*$ (b) $h = 2h^*$ (c) $h = 10h^*$. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Figure 6.

Axial stress variation at a crack tip element for the thumb nail model for the three thicknesses $h = h^*$, $h = 2h^*$, $h = 10h^*$. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Figure 7.

Failure patterns, shown using axial strain contours, for the three scales in the dahlite crystal model (a) mm (b) μm (c) nm. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Figure 8.

Energy plots for nanometer study. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Figure 9.

Axial stress contours at a specified scaled time of 0.012, for the three scales in the dahlite crystal model (a) mm (b) μm (c) nm. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

TABLE I

Scaling Conversions for the Scales Studied

Scale	Length (sm)	Mass (skg)	Density (skg/sm ³)	Stress/Modulus (sPa=skg/sm ³ -s ²)
Nanometer	10 ⁻⁹ m	10 ⁻³ kg	10 ⁻²⁴	10 ⁻⁶ Pa
Micrometer	10 ⁻⁶ m	10 ⁻³ kg	10 ⁻¹⁵	10 ⁻³ Pa
Millimeter	10 ⁻³ m	1 kg	10 ⁻⁹	10 ⁻³ Pa
Centimeter	10 ⁻² m	1 kg	10 ⁻⁶	10 ⁻² Pa

TABLE II

Comparison of Stress Values for Different Mass Scaling Factors

Mass scaling factor	S_{22} Initial	S_{22} @ $t = 2.4\text{e-}9$	LE_{22} @ $t = 2.4\text{e-}9$
10	*	230	0.00082
100	34	230	0.00082
1,000		375	0.00125
10,000	350	—	—
100,000	1017	—	—

* Indicates the stress have reached the crack tip within the first time step.