Nonlinear homogenisation of trabecular bone: effect of solid phase constitutive model

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Abstract

Micro-finite element models have been extensively employed to evaluate the elastic properties of trabecular bone and, to a limited extent, its yield behaviour. The macroscopic stiffness tensor and yield surface are of special interest since they are essential in the prediction of bone strength and stability of implants at the whole bone level. While macroscopic elastic properties are now well understood, yield and post-yield properties are not. The aim of this study is to shed some light on what the effect of the solid phase yield criterion is on the macroscopic yield of trabecular bone for samples with different microstructure. Three samples with very different density were subjected to a large set of apparent load cases (which is important since physiological loading is complex and can have multiple components in stress or strain space) with two different solid phase yield criteria: Drucker-Prager and Eccentric-Ellipsoid. The study found that these two criteria led to small differences in the macroscopic yield strains for most load cases except for those that were compression-dominated; in these load cases the yield strains for the Drucker-Prager criterion were significantly higher. Higher density samples resulted in higher differences between the two criteria. This work provides a comprehensive assessment of the effect of two different solid phase yield criteria on the macroscopic yield strains of trabecular bone, for a wide range of load cases, and for samples with different morphology.

Keywords: Finite element, bone biomechanics, micro-architecture, constitutive models, multiscale modelling
Introduction

With the exponential growth of older population, problems associated with the load bearing capacity of trabecular bone need urgent attention. Thus, a deeper understanding of how the microstructure of bone, the material properties of the solid phase, and its macroscopic mechanical properties are related is needed in order to examine the response of musculoskeletal systems.

Trabecular bone is a highly heterogeneous material that resembles open-cell foams and its properties depend on the considered working scale. While trabecular bone at the macroscale is highly anisotropic, trabecular bone at the microscale is usually modelled as an isotropic material although it is recognised that trabecular bone at this level is transverse isotropic or orthotropic. However, as Cowin pointed out, since the axis of the trabecula is the same as the loading axis, a beam made of orthotropic material can be reduced to a beam made of isotropic material. Although trabecular bone elastic properties are well established, its nonlinear behaviour is not fully understood.

The cellular structure of trabecular bone endows it with complex failure mechanisms. These mechanisms are known to depend on trabecular bone microstructure, and while high density bone tends to fail due to tissue yielding, low density bone is inclined to fail due to a combination of tissue yielding and large deformation mechanisms, i.e. bending and buckling of trabeculae. Therefore, in numerical simulations using micro-finite element models (µFE) both material and geometric nonlinearities need to be included in order to capture the correct behaviour of a trabecular bone specimen.

Porosity is a key feature of bone, which is reported to be present at every hierarchical scale. Tai, Ulm showed that bone behaves like a cohesive-frictional material and that the increased yield properties in compression may be explained by the friction between the mineral components, and that cohesion is provided by the organic matrix. Several computational studies on the nanoindentation behaviour of bone tissue have successfully modelled the mechanical response found in nanoindentation experiments by
using a Mohr-Coulomb 17 or a Drucker-Prager 18 (DP) yield surfaces. Maghous, Dormieux 19 showed that an eccentric-ellipsoid (EE) is the yield surface of an isotropic porous material the matrix of which is modelled with a DP yield surface. Consequently, Schwiedrzik and Zysset 20 reported that EE could effectively approximate the yield behaviour of bone tissue. Data on post-yield hardening behaviour of the solid phase of bone is not readily available and most of the simulations for nonlinear homogenisation use a 5% of the elastic slope as the linear hardening slope. 5, 21-23 Some experimental studies have measured the hardening behaviour of the extracellular matrix 24, 25, but this cannot be directly employed for representing the solid phase of trabecular bone due to the difference in scale.

Homogenisation techniques to obtain the macroscopic response of bone from its microstructure have been successfully employed for determining bone apparent anisotropic elastic properties 11, 12, 26. Links have also been established to relate elastic properties with bone volume over total volume fraction (BV/TV) and fabric tensors 3, 27, 28. However, homogenisation procedures to find yield and post-yield properties of bone are much more computationally expensive since they require evaluation of multiple load cases to assess multiaxial behaviour. Additionally, in order to capture nonlinear phenomena, FE meshes need to be finer and each load step may require a number of iterations to obtain a converged solution if an implicit time integration scheme is used. Only few studies have attempted nonlinear homogenisation techniques on trabecular bone 5, 21-23, 29. In these studies, only Panyasantisuk, Pahr 21 and Levrero-Florencio, Margetts 29 used a DP criterion, while the others used a simple bilinear criterion to represent the solid phase of bone. Results of these studies indicate that the macroscopic yield surface of trabecular bone can be effectively approximated by an isotropic criterion in strain space.

To our knowledge there is only one previous study that has examined the effect of different solid phase yield criteria on the macroscopic yield response of bone 30. However, this study only considered two simple load cases, unconfined uniaxial compression and pure shear, and concluded that the differences
between macroscopic yield with different solid phase criteria were small and any solid phase criterion with strength asymmetry will perform reasonably well. The aim of this study is to evaluate the effect of two different solid phase yield surfaces with the same uniaxial strength asymmetry, DP and EE, on the yield strains at the macroscopic level by using a nonlinear homogenisation approach, derived from multiscale theory \(^\text{31-33}\), by applying a large range of load cases, including complex normal and shear scenarios.
Materials and methods

Sample extraction and imaging

Three cylindrical specimens of bovine trabecular bone (young cattle, <2.5 years old) were extracted from bovine trochanters. The extracted specimens had approximate dimensions of 10.7 mm diameter and 30 mm length. Diamond-tipped cores (Starlite Industries, Rosemont PA, USA) were used in the extraction of the specimens and the edges were cut with a slow speed saw (Isomet 1000, Buehler, Düsseldorf, Germany) by using a diamond wafering blade designed for bone; all these operations were performed under constant irrigation to avoid excessive abrasion and overheating. After coring, the specimens were submerged in phosphate buffered saline (PBS) and scanned using a µCT device (Skyscan 1172, Bruker, Zaventern, Belgium) with a resolution of 17.22 µm. The scanning parameters were 94 kV, 136 mA and 200 ms integration time; four scans in 720 equiangular radial positions. Binarisation of the grey scale images was performed with an automatic thresholding algorithm 34.

Three virtual cubes of 5 mm length were extracted from each of the previously mentioned cylinders; this length has been previously considered appropriate to capture the features of trabecular bone 23, 26, 35. Figure 1 shows the geometry of these specimens and Table 1 shows their morphological indices. The Mean Intercept Length (MIL) fabric tensor 36 was evaluated using BoneJ 37 and then used to align the coordinate axes of the images with the fabric. This approach has been recently employed by Wolfram, Gross 22 and Leverero-Florencio, Margetts 29. After the 5 mm cubes were cropped, the alignment was rechecked to ensure that no misalignment larger than 8° was found 22, 23, 29. MIL is known to approximate the macroscopic elastic orthotropy of trabecular bone 4 and thus the samples can be considered to be aligned with these axes.

[insert Figure 1.]

Figure 1. The three used specimens ordered in increasing density from left to right.
Table 1. Morphological indices of the three used specimens.

<table>
<thead>
<tr>
<th></th>
<th>Porous sample</th>
<th>Medium sample</th>
<th>Dense sample</th>
</tr>
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<tbody>
<tr>
<td>BV/TV (%)</td>
<td>14.8</td>
<td>23.1</td>
<td>30.3</td>
</tr>
<tr>
<td>Degree of Anisotropy</td>
<td>2.65</td>
<td>2.09</td>
<td>2.67</td>
</tr>
<tr>
<td>Structure model index</td>
<td>1.59</td>
<td>0.98</td>
<td>0.52</td>
</tr>
<tr>
<td>Trabecular thickness (µm)</td>
<td>221.8</td>
<td>183.6</td>
<td>175.3</td>
</tr>
<tr>
<td>Connectivity</td>
<td>209</td>
<td>813</td>
<td>1059</td>
</tr>
</tbody>
</table>

**Constitutive models**

The solid phase was assumed to be a homogeneous isotropic elastoplastic material, although it is recognised that bone at the tissue level is actually transverse isotropic or orthotropic \(^7\)\(^9\) and heterogeneous \(^38\)\(^39\). However, as Cowin \(^10\) pointed out, there is little to no error in assuming tissue isotropy. This is because trabecula are composed of laminated material about their axes, which implies anisotropy, as in lack of isotropy; but since the axis of a trabecula is the same as its loading axis, a beam made of orthotropic material can be reduced to a beam made of isotropic material. Further, it has been argued that the solid phase of bone is not homogeneous; Renders, Mulder \(^39\) found a decrease of 21% in apparent stiffness when considering a heterogeneous solid phase. Since we wanted to be able to validate our results with previously published data, we kept our solid phase properties as homogeneous \(^22\)\(^23\). Moreover, since the aim of this study was to compare two different constitutive models, this assumption of solid phase homogeneity was not expected to change trends.

The notation used in this section follows the notation used by Schwiedrzik, Wolfram \(^40\) and Leverero-Florencio, Margetts \(^29\). The elastic regime of the solid phase was modelled by using a Hencky’s
hyperelastic model, with a Poisson ratio of 0.3 and a Young’s Modulus of 12700 MPa. A quadric yield surface is given by

\[ G(\tau) = \sqrt{\tau: \mathbb{G}: \tau + \mathbb{G}: \mu - 1 = 0} \quad (1) \]

where \( \tau \) is the Kirchhoff stress, \( \mathbb{G} \) and \( \mathbb{G} \) are, respectively, a fourth-order tensor and a second-order tensor defined by

\[ \mathbb{G} = -\zeta_0 \mathbb{G}_0^2 (I \otimes I) + (\zeta_0 + 1) \mathbb{G}_0^2 (I \otimes I) \quad (2) \]

and

\[ \mathbb{G} = \frac{1}{2} \left( \frac{1}{\sigma_0^+} - \frac{1}{\sigma_0^-} \right) I \quad (3) \]

where
\[ G_0 = \frac{\sigma_0^+ + \sigma_0^-}{2\sigma_0^+ \sigma_0^-} \] (4)

**I** is the second-order unit tensor, \( \sigma_0^+ \) and \( \sigma_0^- \) are the tensile and compressive yield stresses, respectively, and \( \zeta_0 \) is a parameter which defines the general shape of the surface.

Equation 1 approximates the DP criterion when \( \zeta_0=0.49 \) (Figure 2(a)) and we chose an arbitrary \( \zeta_0=0.2 \), which defines an EE (Figure 2(b)); both yield surfaces are defined in stress space and have the same uniaxial yield values. Uniaxial yield strains of 0.41% in tension and 0.83% in compression \(^41\) were converted to yield stresses by using the approach described in Schwiedrzik, Gross \(^42\). We assumed a linear hardening of 5% of the elastic slope \(^22,41,43\). In order to ensure global convergence of the plasticity update Newton-CPPM scheme, a line search procedure as in the primal-CPPM algorithm described in Perez-Foguet and Armero \(^44\) was implemented.

**Figure 2.** (a) Approximated Drucker-Prager. (b) Eccentric-Ellipsoid. Both of these surfaces are defined in a six-dimensional stress space, but their shapes can be illustrated in principal stress space as shown.

**Computational methods**

The three cubic specimens were meshed with a voxelised mesh by using trilinear hexahedra, with the largest mesh having around nine million nodes. The applied boundary conditions used to constrain the cubic volume elements (VE) were kinematic uniform boundary conditions, as described by Wang, Feng \(^45\). These boundary conditions provide an upper bound for trabecular bone stiffness \(^45\) and also for yield \(^21\).
Each VE was subjected to 144 strain load cases, which is a slightly reduced number from Leverero-
Florecio, Margetts 29, as listed in Table 2.

<table>
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<tr>
<th>Type of analysis</th>
<th>Number of analyses</th>
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<tr>
<td><strong>Uniaxial normal</strong></td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{ii} \neq 0 )</td>
<td>3 tensile and 3 compressive</td>
</tr>
<tr>
<td>( \varepsilon_{jj} = \varepsilon_{kk} = 0 )</td>
<td>6</td>
</tr>
<tr>
<td>( \gamma_{lm} = \gamma_{ln} = \gamma_{mn} = 0 )</td>
<td></td>
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<tr>
<td><strong>Biaxial normal</strong></td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{ii} = \varepsilon_{ij} \neq 0 )</td>
<td>3 planes, 1 analysis per quadrant</td>
</tr>
<tr>
<td>( \varepsilon_{kk} = 0 )</td>
<td>12</td>
</tr>
<tr>
<td>( \gamma_{lm} = \gamma_{ln} = \gamma_{mn} = 0 )</td>
<td></td>
</tr>
<tr>
<td><strong>Uniaxial shear</strong></td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{ii} = \varepsilon_{jj} = \varepsilon_{kk} = 0 )</td>
<td>3 clockwise and 3 counter-clockwise</td>
</tr>
<tr>
<td>( \gamma_{lm} \neq 0 )</td>
<td>6</td>
</tr>
<tr>
<td>( \gamma_{ln} = \gamma_{mn} = 0 )</td>
<td></td>
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<tr>
<td><strong>Biaxial shear</strong></td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{ii} = \varepsilon_{ij} = \varepsilon_{kk} = 0 )</td>
<td>3 planes, 1 analysis per quadrant</td>
</tr>
<tr>
<td>( \gamma_{lm} = \gamma_{in} \neq 0 )</td>
<td>12</td>
</tr>
<tr>
<td>( \gamma_{mn} = 0 )</td>
<td></td>
</tr>
<tr>
<td><strong>Biaxial normal-shear</strong></td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_{ii} \neq 0 )</td>
<td>9 planes, 3 analysis per quadrant</td>
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<tr>
<td>( \varepsilon_{jj} = \varepsilon_{kk} = 0 )</td>
<td>108</td>
</tr>
<tr>
<td>( \gamma_{lm} \neq 0 )</td>
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<tr>
<td>( \gamma_{ln} = \gamma_{mn} = 0 )</td>
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</tr>
<tr>
<td>( \forall i,j,k,l,m,n = 1,2,3 )</td>
<td>Total</td>
</tr>
<tr>
<td>( \forall i \neq j \neq k )</td>
<td>144</td>
</tr>
<tr>
<td>( \forall l \neq m \neq n )</td>
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</table>

The simulations were performed on a Cray XC30, hosted by ARCHER (UK National Supercomputing Service). The FE analyses were carried out with an in-house developed parallel implicit finite strain solver, within the context of ParaFEM 46,47. This code uses Message Passing Interface (MPI) to perform the parallelisation 48,49 and its scalability has already been shown in previous studies 50,51. To solve the
global FE system, a Newton-Raphson scheme was used as the solution tracking technique and a preconditioned conjugated gradient solver was used as the linear algebraic solver. The initial load increment size corresponded to 0.1% macroscopic strain norm and could decrease to a minimum of 0.001% if global convergence was not achieved. However, no convergence problems occurred in our simulations.

**Macroscopic yield**

Although a finite strain formulation needs to be taken into account when performing the simulations involving the microstructure, strains at the macroscopic level can be considered small due to their relatively small norms, and thus a linear kinematic formulation can be used. The yield points were described in the plane where the abscissa is the Frobenius norm of the applied macroscopic strain and the ordinate is the Frobenius norm of the homogenised stress, described by

\[
\sigma_{\text{hom}} = \frac{1}{V_0} \sum_{i=1}^{\text{nel}} \sum_{j=1}^{\text{nip}} w_i \det \mathbf{J}_{ij} \sigma_{ij}
\]

(5)

where there is no summation implied on repeated indices, \(V_0\) is the initial volume of the VE, \(\text{nel}\) is the number of elements in the FE system, \(\text{nip}\) is the number of Gauss integration points in a trilinear hexahedron, \(\mathbf{J}\) is the Jacobian, \(\sigma\) is the stress at the solid phase, and \(w\) are the weights corresponding to the specific Gauss integration point. The 0.2% criterion was used to define the yield points.
Results
The samples have been labelled as Low density, Medium density and High density for BV/TV of 14.8%, 23.1% and 30.3%, respectively. The macroscopic yield strains for the three samples considered for the uniaxial normal and biaxial normal cases (row 1 and 2 of Table 2) are shown in Figure 3. Further, since strain-based yield criteria have been previously shown to be approximately isotropic, we use yield points in strain space.

Figure 3. Yield strains in normal-normal planes. The axes have been rearranged so that the orthotropic Young’s Moduli are descending (E_{11}>E_{22}>E_{33}).

In normal-normal planes it can be seen that differences between yield strains when considering these two different yield surfaces for the solid phase are not significant in tension-tension quadrants (Figure 3(a) to (c), upper right quadrant), or even in tension-compression quadrants (Figure 3(a) to (c), upper left and lower right quadrants). However, they become distinguishable in compression-compression quadrants (Figure 3(a) to (c), lower left quadrants).

The macroscopic yield strains for the three samples considered in uniaxial and biaxial shear cases (row 3 and 4 of Table 2) are shown in Figure 4 (a) to (c). It can be seen that there are no significant differences in the macroscopic shear yield strains when using these two different yield criteria for the solid phase.

Figure 4. Yield strains in shear-shear planes.

Yield strain norms were evaluated separately for load cases with only: normal compressive components; normal tensile components; and shear components, for both material models and all three samples. These
are shown in Figure 5. It can be seen that the yield strain norm for tension-only and shear-only load cases is almost the same, but differs by around 13% for compression-only load cases.

[insert Figure 5.]

**Figure 5.** Bar plot showing the average of the macroscopic yield strain norm for load cases that contain only: compressive components, tensile components, and shear components, for both EE and DP. The error bars are the SD of the macroscopic yield strain norms.

Macroscopic yield strains in normal-shear planes are shown in Figure 6(a) to (i) (rows 5 and 6 of Table 2). This figure shows that these yield strains differ for load cases which have compressive components when considering these two different material properties, and this difference increases as the considered load case becomes more compression-dominated (i.e. the load case has a higher proportion of compression over shear) (Figure 7). Figure 7 shows that this effect is also more prominent for the higher density samples. This effect was also found to occur in normal-normal planes (Figure 3) (not illustrated here).

[insert Figure 6.]

**Figure 6.** Yield strains in normal-shear planes, with the normal component in the X-axis and the shear component in the Y-axis.

[insert Figure 7.]

**Figure 7.** Difference in macroscopic yield strain norm between DP and EE, for cases in normal-shear planes with a compressive component. The strain norm corresponding to DP is consistently higher. The first number in the proportion on the X-axis corresponds to the normal component, and the second to the shear component.
Discussion

Our study shows that the effect of hydrostatic yield in the solid phase constitutive model is significant for compression-dominated load cases and that this effect is larger for high density samples. Our findings agree with Baumann, Shi\(^30\) who only considered uniaxial unconfined compression and pure shear and consequently concluded that solid phase strength asymmetry dominates the macroscopic mechanical response.

Macroscopic yield strain results in normal-normal planes show that the effects of the two solid phase yield surfaces on the macroscopic behaviour is minimal except for cases containing only compressive components (Figure 3(a) to (c), lower left quadrants). When comparing the macroscopic yield strain norms for the two material models, it can be seen that DP results in a norm which is around 13% larger than when using EE (Figure 5). The highly aligned structure of trabecular bone is likely to partially reflect features of the solid phase yield surface, which in this case is a lack of hydrostatic compression yielding, resulting in an increase of the macroscopic yield strain norms in compression-dominated load cases. Figure 3 also shows that tension-dominated load cases are not affected by the different solid phase yield surfaces.

When considering shear load cases, it can be seen that there are no differences in macroscopic yield strains when using these two different solid phase yield criteria (Figure 4 and 5). This is consistent with Sanyal, Gupta\(^43\) in that tensile microscopic strains predominate in macroscopic shear loading, which results in these load cases being unaffected when using these different solid phase yield surfaces. However, it is important to point out that shear load cases in clockwise and counter-clockwise directions can have different yield strains, especially in low BV/TV samples, as has been shown previously\(^29\).

In normal-shear planes (Figure 6, upper and lower left quadrants), the macroscopic yield strains follow a similar pattern to those in normal-normal planes (Figure 3). Specifically, the two solid phase yield criteria
result in greater differences as the load case becomes more compression-dominated, which is shown graphically in Figure 7. This figure shows the difference in macroscopic yield strains between the DP and EE solid phase yield surfaces in the load cases which are pure shear, or compression-shear. This difference increases as the compression/shear proportion increases and also as density increases; this means that higher density samples, which are more continuum-like, demonstrate a greater difference between the two solid phase material properties, as these properties are more directly mirrored at the macroscale.

As mentioned earlier, to the best of our knowledge, only one previous study has assessed the effect of different solid phase yield criteria on the macroscopic yield strains. The load cases considered in this study were limited to unconfined compression and shear. As we consider a large number of complex load cases, our study could be considered as a possible extension of the above cited study. Although our material properties are different and the way of assessing macroscopic yield is different, it can be seen that our shear strains are not very dissimilar (our uniaxial shear strains in Figure 4 need to be scaled by \( \sqrt{2} \) to be comparable to those in Baumann, Shi, because these are shown as tensorial components; compression strains cannot be compared because our uniaxial compression cases are confined and theirs are unconfined)

Our study has some limitations. Validation for all the macroscopic yield strains is not possible as these are very complex load cases which cannot be tested experimentally and samples tested once cannot be retested. There have been some attempts to perform complex load cases, such as multiaxial compression, on trabecular bone samples. For our solid phase properties, we considered homogeneous tissue properties, which may result in an overestimation of the macroscopic yield values, but the effects are likely to be similar for both the solid phase models. We also assumed that the solid phase can be modelled with plasticity, which may not be true as localised tissue strains can cause microcracks, possibly leading
to an eventual fracture; these are effects that plasticity models are not readily able to capture.\textsuperscript{55,56} Furthermore, although our meshes were extremely detailed, and thus these simulations were computationally expensive, we only considered three samples, which, it can be argued, may not deliver statistically conclusive results.

This study provides a comprehensive understanding of how the yield surface at the microscopic level affects the homogenised yield strains at the macroscopic level. Yield strain of high density samples is affected more by the choice of the solid phase criteria. The strain norms associated to the use of DP, which has no yielding in hydrostatic compression, were found to be consistently higher than when using EE for compression-dominated load cases; a difference of up to 20\% in some cases. It can be argued that most physiological activities result in compression-dominated loading states in trabecular bone; consequently the choice of the solid phase criterion is of great importance in the development of macroscopic yield criterion.
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Conflict of interests
The authors declare that there is no conflict of interest.
References


Notation

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<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$\mathbf{A}$</td>
<td>A second-order tensor</td>
</tr>
<tr>
<td>$\mathbb{A}$</td>
<td>A fourth-order tensor</td>
</tr>
<tr>
<td>$\boldsymbol{\sigma}$</td>
<td>Infinitesimal stress tensor</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Kirchhoff stress tensor</td>
</tr>
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<td>$A_{ij} B_{ij}$ in indicial notation</td>
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<td>$\mathbf{A} \otimes \mathbf{B}$</td>
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Abbreviations

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<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>BV/TV</td>
<td>Bone Volume over Total Volume</td>
</tr>
<tr>
<td>DP</td>
<td>Drucker-Prager yield criterion</td>
</tr>
<tr>
<td>EE</td>
<td>Eccentric-ellipsoid yield criterion</td>
</tr>
<tr>
<td>MIL</td>
<td>Mean Intercept Length</td>
</tr>
<tr>
<td>MPI</td>
<td>Message Passing Interface</td>
</tr>
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<td>VE</td>
<td>Volume Element</td>
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<td>$\mu$CT</td>
<td>Micro computed tomography</td>
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