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The Cancellous Bone Multiscale Morphology-Elasticity Relationship

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A B S T R A C T

The cancellous bone effective properties relations are analysed on multiscale across two aspects; properties of representative volume element on micro scale and statistical measure of trabecular trajectory orientation on mesoscale. Anisotropy of the microstructure is described across fabric tensor measure with trajectory orientation tensor as bridging scale connection. The scatter measured data (elastic modulus, trajectory orientation, apparent density) from compression test are fitted by stochastic interpolation procedure. The engineering constants of the elasticity tensor are estimated by last square fitt procedure in multidimensional space by Nelder-Mead simplex. The multiaxial failure surface in strain space is constructed and interpolated by modified super-ellipsoid.

***Key words**: cancellous bone, effective properties, microstructure*

Introduction

For many years, researchers have been trying to quantify the effects of disease and drug treatment on the strength of bone. Changes in the three dimensional (3D) architecture of trabecular bone play an important role in determining the mechanical competence of bone[1]. Understanding the age-related microstructure changes in trabecular bone and their consequence on mechanical properties may be essential in bone fracture and osteoporosis prevention. Cancellous bone is a biphasic structure consisting of a continuous three-dimensional network of interconnected rods and plates and a pore space filled by a viscous fluid phase. There are strong indications that this fluid flow is responsible for the mechano-transduction from external mechanical loads to the cells responsible for bone apposition or removal. When bone is mechanically loaded, bone fluid flow induces shear stresses on bone cells involved in bone's mechanosensory system[2]. From the engineering point of view, the bone is a functionally graded structure with complex microstructure optimized for withstanding external loads. The bone continually adapts to its mechanical environment and for cancellous bone these adaptation results in varying trabecular architecture[3]. It was shown that adaptation to mechanical deformation energy leads to an architecture, which is an optimal configuration with respect to maximal stiffness and minimal mass. The aim of this work is to develop a relationship between morphology multiscale descriptors and mechanical macroscopic properties. Also we suggest a three dimensional yield surface in strain space by carefully analyzing experimental measurements.

Morphology-properties relationship

Cancellous bone microstructure is characterized by morphometric measures such as bone volume fraction, trabecular spacing, fabric tensors, and trajectory orientation to mention a few among many others. Bone mechanical response depend on some morphometric descriptors on macroscale, too[4]. Cancellous bone is hierarchically structured to provide maximum performance with a minimum of materials. Several trabecular bone microstructure models have been developed such as irregular 3D Voronoi cellular solids, 3D array of tetrakaidecahedra cells, strut-like random structure, fractal-like network[5]. Today, the relationship between local microstructure and global macroscopic properties of the bone is an important task in medical engineering[6]. Some approaches have been recently proposed in order to derive overall behavior heterogeneous materials[5]. There are two procedures relating to local and global behavior. The first case mate-

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rial can be described as spatially periodic using homogenization theory for periodic media[7]. In the second instance, the global behavior may be approached from the knowledge of certain statistic of the distribution of the local descriptors, which characterize the micro behavior. There is no unified method to bridge micro and macro scales. Cancellous bone on macroscale is inherently anisotropic suggesting the trabeculae to follow the major stress lines (Wolff's law). The rule, which determines the design of biological structures, is the constant stress axiom, meaning that biological load carriers always try to grow into a state of constant stress on a time average[8]. Many researches showed a significant correlation between trabecular orientation and principal stress direction[3]. The trabecular trajectories directions may be defined by the material unit vectors $\vec{a}$ (Figure 1). Therefore, we suppose that the trajectory is meso quantity which connects micro with macro scale. The orientation state of a group of trajectories can be described by a probability distribution function $\psi(\vec{a})$, which provides a general description of the orientation state. Orientation tensors are widely used to provide a more compact representation of the trajectory orientation state, defined as the dyadic product of vector $\vec{a}$ averaged over orientation space, with ψ, as the weighting function.

$$A_{ij} = \int\int a_i a_j y(f, J) \sin J \, d f \, dJ \qquad (1)$$

The trajectories direction $\vec{a}$ determines the preffered direction of the material. The relationship between the elasticity tensor C_{ijkl} and structural tensor A_{ij}, for transversely isotropic bone become as follow[9]:

$$C_{ijkl} = C_{ijkl}(I_1, I_2, I_3, I_4, I_5) \qquad (2)$$

where are $I_1, I_2 \ldots I_5$ invariants of the strain tensor ε_{ij} and trajectory orientation tensor A_{ij}. The integrity basis in this case are the three principal invariants of ε_{ij} and two aditional invariants.

$$\begin{aligned} I_1 &= tr\varepsilon_{ij} \\ I_2 &= \frac{1}{2}[(tr\varepsilon_{ij})^2 - tr\varepsilon_{ij}^2] \\ I_3 &= \det \varepsilon_{ij}^3 \\ I_4 &= A_{ij} : \varepsilon_{ij} \\ I_5 &= A_{ij} : \varepsilon_{ij}^2 \end{aligned} \qquad (3)$$

The invarijant I_4 is associated with deformation in the trajectory direction, while I_5 is associated with deformation perpendicular to the preferred direction. The orientation tensor is convenient to be replaced by orientation averaging parameters[10]

$$\begin{aligned} f_1 &= \langle \cos 2\phi \rangle \\ f_2 &= 2 \cdot \langle \cos^2 2\phi \rangle - 1 \\ f_3 &= \frac{3}{4}\langle \cos 2\vartheta \rangle + \frac{1}{4} \\ f_4 &= \frac{15}{2}\langle \cos^4 \vartheta \rangle - \frac{15}{2}\langle \cos^2 \vartheta \rangle + 1 \end{aligned} \qquad (4)$$

where bracket $\langle\ \rangle$ is orientation averaging operator. The elasticity tensor C_{ijkl} on macro level on trajectory defined by angles (ϕ, ϑ) has the following form

$$C_{ijkl} = \mathrm{C_{ijkl}}\,(c_{ijkl}, f_1, f_2, f_3, f_4) \qquad (5)$$

where c_{ijkl} elasticity tensor of the periodic microstructural unit on trajectory. The tissue material of the cancellous bone is assumed to be isotropic and anisotropy comes from the geometry only, and architectural anisotropy on micro level are quantified by second-rank fabric tensor λ_{ij}. The elasticity tensor c_{ijkl} depend on density ρ and on microscale descriptors, such as fabric tensor λ_{ij}[11]

$$c_{ijkl} = c_{ijkl}\,(\rho, \lambda_{kl}) \qquad (6)$$

Now the elasticity tensor C_{ijkl} on macro level can be expresed in separable multiscale form

$$C_{ijkl} = \hat{C}_{ijkl}\,(f_1, f_2, f_3, f_4) \oplus c_{ijkl}\,(\rho, \lambda_{ij}) \qquad (7)$$

The inverse of c_{ijkl} is the compliance tensor, which can be expressed using engineering coefficients[11]. For the cancellous bone on local micro level Cowin suggest, that Young's E_i and shear module G_i, with Poisson's ratio's ν_{ij} are proportional to the density ρ and fabric tensor λ_{ij} as follows

$$\begin{aligned} \frac{1}{E_i} &= D_1 + 2D_6 + (D_2 + 2D_7)\cdot\Theta + 2\cdot(D_3 + 2D_8)\cdot\lambda_{ii} + (2D_4 + D_5 + 4D_9)\cdot\lambda_{ii}^2 \\ \frac{1}{G_{ij}} &= 4\cdot[D_6 + D_7\cdot\Theta + D_8\cdot(\lambda_{ii} + \lambda_{jj}) + D_9\cdot(\lambda_{ii}^2 + \lambda_{jj}^2) \\ -\frac{n_{ij}}{E_{ij}} &= D_1 + D_2\cdot\Theta + D_3\cdot(\lambda_{ii} + \lambda_{jj}) + D_4\cdot(\lambda_{ii}^2 + \lambda_{jj}^2) \\ \Theta &= \lambda_{11}\lambda_{22} + \lambda_{11}\lambda_{33} + \lambda_{22}\lambda_{33}, \quad \mathrm{i, j} = 1, 2, 3 \end{aligned} \qquad (8)$$

The constants D_i depend on density ρ and on descriptors at nanoscale (trabeculae lamelae). Another important quantity is the trajectory curvature tensor. Property variations on the mesoscale can be introduced through use high–order continuum theories, such as micropolar theory, couple stress theory[12]. The elastic modulus and yield strain can be used as a good property predictor for all sites and loading modes.

Materials and Methods

For the purpose of the study, a novel compression device with optical system was constructed to measure stress, strain and trabecular trajectory orientation in bone specimens[13]. The series of 10-mm cubes of cancellous bone specimens from human femur were prepared using a fine diamond saw. The microstructure unit follows trabecular trajectories according Wolff's law, and principal axes are determined by Euler angles ϕ and ϑ.

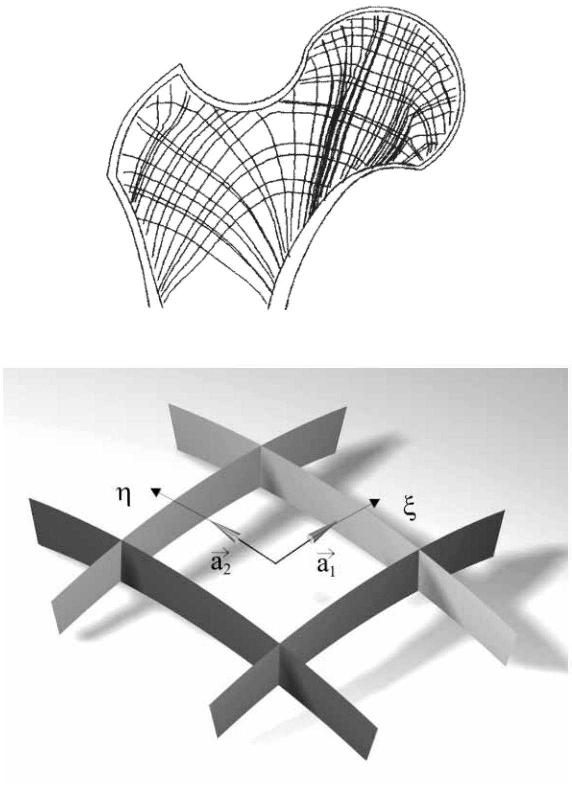

Fig. 1. Trabecular pattern in the proximal femur.

The slope on stress-strain curve defines Young's modulus in loading direction (Figure 2). Supposing that principal elastic axes coincide with trabecular trajectory orientations, loading direction in space is defined by the spherical coordinates ϕ and ϑ. The specimens are prepared and the trajectory lies in specimen plane ($\vartheta = 0$). For every compression tests were measured, elastic module E in loading direction, trajectory orientations ϕ and apparent density ρ. The complex load hystory and bone geometry need a sofisticated opto-mechanical measuring equipment[14]. The influence of the end effects and boundary conditions (i.e. friction effects) are carefully considered in the experimental procedure.

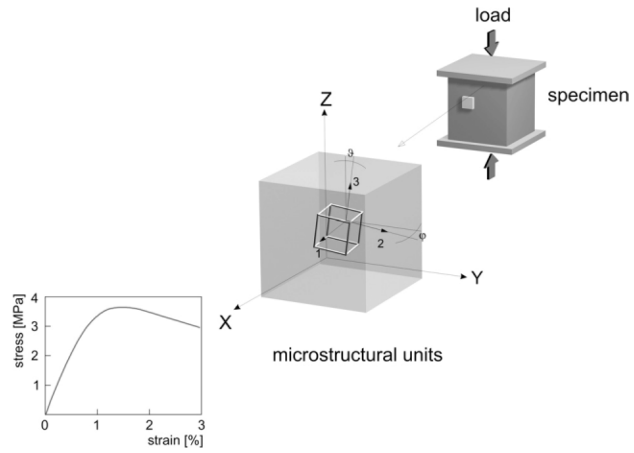

Fig. 2. The bone compression test.

Parameter's estimation

Spatial interpolation is used to construct relationship $E = \Re(\rho, \phi)$ from irregularly scatter data. Among many interpolation procedures kriging is chosen as the most possible. Scatter and irregularly distributed measurements are mapped on a regular grid by kriging procedure. A straightforward way to estimate the value of the modulus E at an unknown location (ρ_0, ϕ_0) (a point of the grid) is to make a linear combination of the of weights at known neighboring locations (ρ_i, ϕ_i), i = 1, M.

$$E(\rho_0, \phi_0) = \sum_{i=1}^{M} m_i \cdot E(\rho_i, \phi_i) \tag{9}$$

M is number measured neighboring points. The problem is to compute the weights μ_i in order to minimize the estimation error[15]. Kriging uses a semivariogram, a measure of spatial correlation between two points, so the weights change according to the spatial arrangement of points. In Figure 3 graphically presented relationship between Young modulus, trabeculae orientation ϕ and structural density ρ is constructed by kriging.

In order to establish cancellous bone structure-function properties relationship we need to determine unknown parameters in structure-properties relationships**.** On the other side, the Young's module in any direction defined by spherical angles ϕ and ϑ is possible calculate knowing the principal elastic constants by transformation formula

$$E(\phi, \vartheta) = \left[\frac{\cos^4 J}{E_1} + \frac{(\sin J \cos f)^4}{E_2} + \frac{(\sin J \cos f)^4}{E_3} + \left(\frac{1}{G_{12}} - 2\frac{n_{12}}{E_1}\right) \sin^2\vartheta \cos^2\phi \cos^2\vartheta + \left(\frac{1}{G_{23}} - 2\frac{n_{23}}{E_2}\right) \cos^2\phi \sin^4\vartheta \sin^2\phi + \left(\frac{1}{G_{31}} - 2\frac{n_{31}}{E_3}\right) \cos^2\vartheta \sin^2\vartheta \sin^2\phi \right]^{-1} \tag{10}$$

where E_i, G_{ij} i, j = 1, 2, 3 are longitudinal and shear module, ν_{ij} are Poisson ratio's according principal axes. The power-law approximation for engineering constant G_i or E_i are chosen, with *a, b, c* and *n* as constants

$$G_i = a + b \cdot \rho^n + c \cdot \left\langle \cos^2 f \right\rangle \tag{11}$$

Curve fitting across experimental point by expressions (10) for modulus, with use of formula (11) gives the possibility to determine modules and Poisson ratio's, better to say, the unknown material constants *a, b, c* and *n* for each module set. The main idea of parameter estimation is the space transformation from (E, ρ, ϕ) to

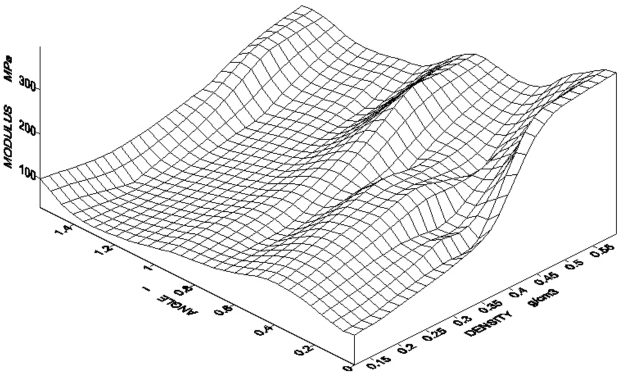

Fig. 3. Modulus dependence on density and orientation-experimental data.

(E_{ij}, ρ, $\langle\cos^2 f\rangle$) as shematic ilustrated by Figure 4. The sum over all experimental points, the square of the difference between theoretical expression for module (10) and experimental value module must be minimal.

$$\psi = \min_{n,a,b,c_i} \sum_{i=1}^{N} [E_{theoretical}(r, \langle\cos^2 f\rangle, a, b, c, n) - E_{experimental}]^2 \quad (12)$$

The method of optimization chosen for this problem was the Nelder and Mead simplex algoritam[16]. The main idea of the algorithm is to replace the vertex of the current simplex that has the highest function value by a new and better point. Scatter and irregularly distributed measurements are mapped on a regular grid by kriging in order to give possibility establish simplex everywhere.

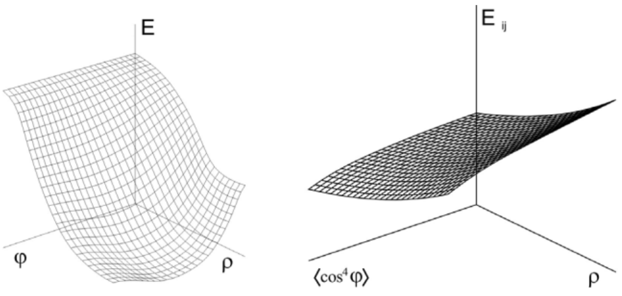

Fig. 4. Transformation of space.

Results and Discussion

In Figure 5, for given experimental data points are shown isoclines of constant modulus as function of density and trabeculae orientation determined by kriging. Some experimental points with strong property gradients are removed. Significant correlation of apparent density and different mechanical properties of cancellous bone have been demonstrated for large populations using power-law regressions The different power exponent suggests an influence other structural parameters such as trajectory orientation and fabric tensor.

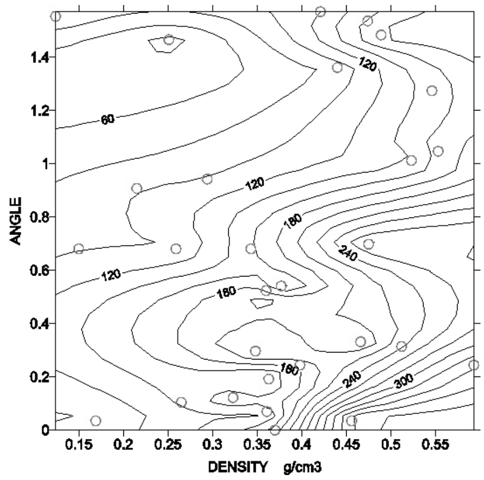

Fig. 5. Spatial interpolations by kriging.

Taking the plane perpendicular on trajectory as the plane of isotropy material becomes transversely isotropic. The five independent constants of elastic tensor (C_{11}, C_{33}, C_{12}, C_{13}, C_{44}) are determined by the above optimization procedure. The final results expressed in engineering constants are:

$$E_1 = 60 + 816 \cdot \rho^{3.08} - 26 \cdot \langle\cos^2 f\rangle \quad [MPa]$$
$$(E_2 = E_1)$$
$$E_3 = 100 + 1146 \cdot \rho^{2.23} - 35 \cdot \langle\cos^2 f\rangle \quad [MPa] \quad (13)$$
$$G_{23} = 30 + 180 \cdot \rho^{1.46} - 14 \langle\cos^4 f\rangle \quad [MPa]$$
$$\nu_{12} = 0.3$$
$$\nu_{13} = 0.25$$

The interpolation surface $E(\rho, \phi)$ is divided in patches for surface fitting by transformation formula (10). The results on Figure 6 ilustrated average trends on macro level for femur bone. This results based on nonlinear regression analysis can be improved material model for numerical remodeling bone processes.

During estimatio procedure Poisson's ratios are keept constant. Careffuly validation results it is find that Poisson's ratio depend on density too, what is shown by Figure 7. Measured normal strain data along each direction of samples are recalculated, and scatter data points are interpolated by closed curve. Yield envelopes in three biaxial normal strain planes are constructed. This envelopes are cross-section four parameter modified yield surface. The yield surface in strain space has the modified super-ellipsoid form[17] (see Figure 8)

$$F(\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}) = \left(\frac{e_{xx} + 0.2}{0.8}\right)^{2/0.45} + \left(\frac{e_{yy} + 0.2}{0.8}\right)^{2/0.45} + \left(\frac{e_{zz} + 0.2}{0.8}\right)^{2/0.45} + \left(1.45 \cdot \frac{e_{xx} + e_{yy} + e_{zz}}{0.8}\right)^{2/0.45} - 1 \quad (11)$$

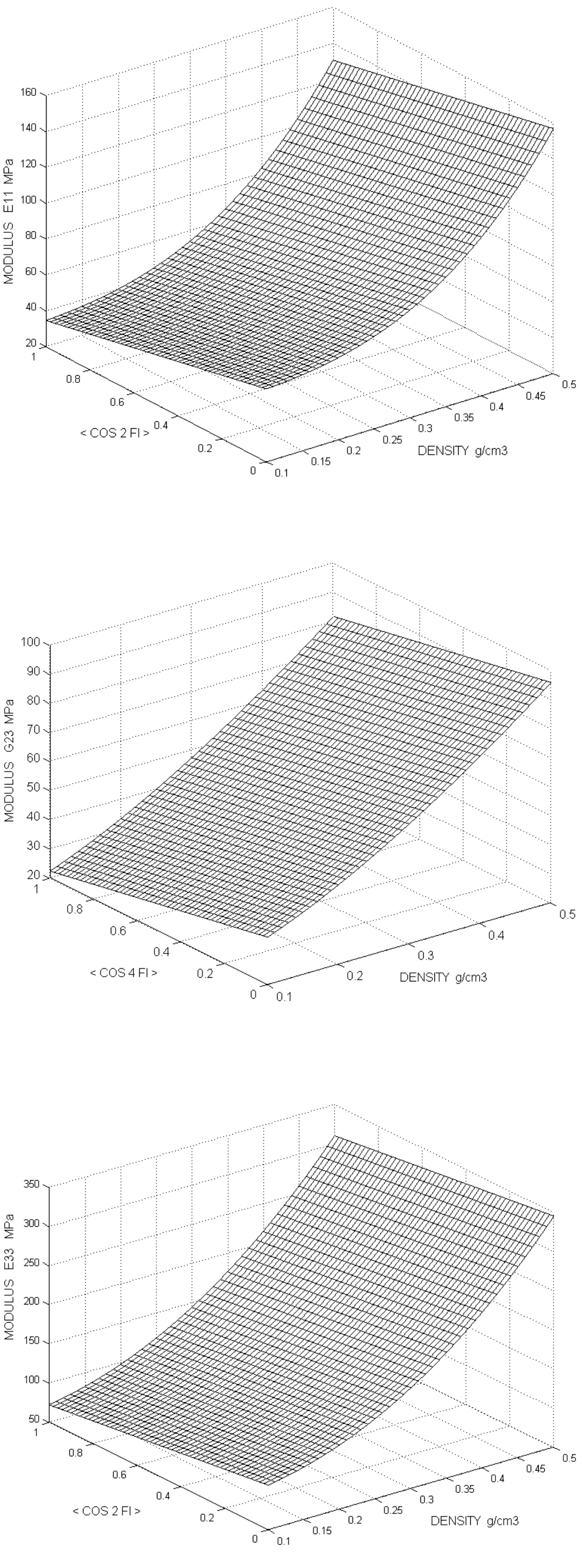

Fig. 6. Modulus dependence on density and trajectory orientation.

The 0.2 % offset lines used to determine yield strains along each loading axis. The compression octant is flattened in order to include tension-compression strength asymmetry.

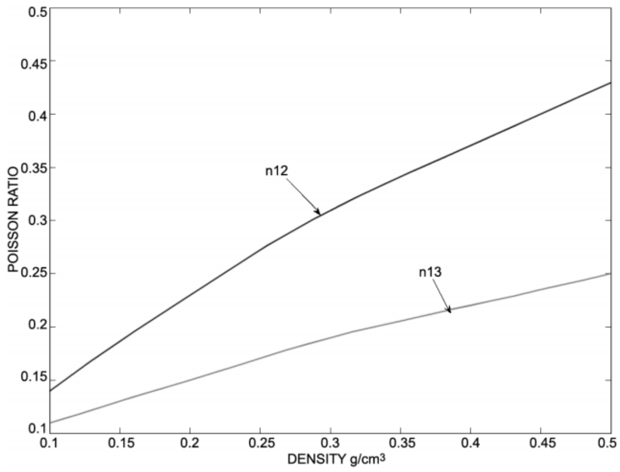

Fig. 7. The Poisson's ratio dependence on density.

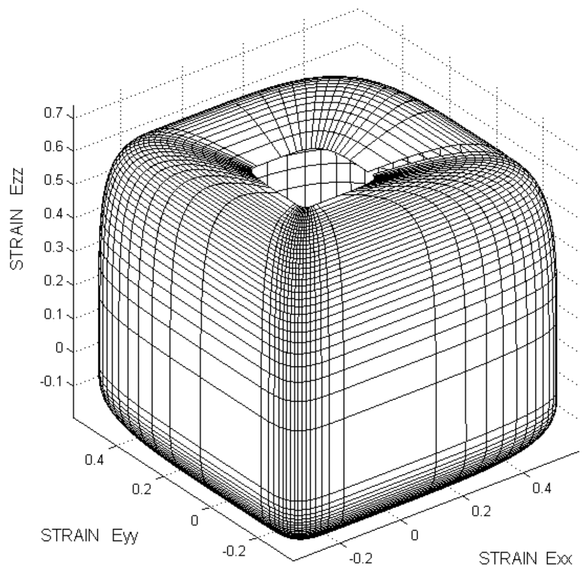

Fig. 8. The failure surface in strain space.

Conclusion

The cancellous bone effective properties on macroscopic level are described by microscopic properties descriptors for representative volume element with trajectory orientation tensor as measure on meso scale. The scatter experimental data are replaced by stochastic interpolation procedure. The engineering constants for elasticity tensor are determined by last square fit of experimental data on multistage. The multiaxial failure surface in strain space is constructed and interpolated by modified super-ellipsoid.

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RELACIJE MORFOLOGIJA-ELASTIČNOST ZA SPUŽVASTU KOST VIŠESTRUKE MATERIJALNE SKALE

SAŽETAK

Makroskopska svojstva spužvaste kosti na višestrukoj materijalnoj skali određena su svojstvima reprezentativnog volumnog elementa na mikroskali i tenzorom orjentacije trajektorija kao mjerom na mezoskali. Anizotropnost mikrostrukture opisana je strukturnim tenzorom i tenzorom orijentacije trajektorija kao povezmicom na višestrukoj materijaloj skali. Mjerni podaci (modul elastičnosti, kut trajektorije, gustoća kosti) testa tlačenja interpolirani su stohastičkom interpolacionom procedurom. Inženjerske konstante tenzora elastičnosti određene su kao minimum funkcionala greške koristeći Nelder-Mead simplex metodu. Ploha tečenja u prostoru tenzora deformacije je interpolirana modificiranim trodimenzijskim super-elipsoidom.