# DETERMINATION OF MECHANICAL PROPERTIES OF MATERIALS WITH COMPLEX INNER STRUCTURE USING MICROSTRUCTURAL MODELS

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***Abstract:*** *Among materials with complex inner structure are ranked cellular materials, typically represented by trabecular bone and polymer or metal foams. Geometrical similarity of their internal structure allows determination of material characteristics of trabecular bone using models originally developed for analysis of polymer and metal foams. In this paper, mechanical behavior of cellular materials is studied by modeling their internal structure and analysis using Finite Element Method (FEM). Alporas aluminium foam was selected as a reference material and the material characteristics were derived from tensile loading using numerical FEM analysis. Internal structure of the foam was modeled by two different methods - using voxel model created on the basis of a series of CT scans and by discretization using Gibson-Ashby's cellular model. Mechanical behavior analysis was performed in both elastic and plastic fields. The beam-only discretization is considered intentionally to investigate its suitability for modeling of closed cell foams and trabecular bone.*

**Keywords:** COMPLEX INNER STRUCTURE, METAL FOAMS, MODELING OF INTERNAL STRUCTURE, FINITE ELEMENT METHOD

## 1. Introduction

Typical representatives of materials with complex inner structure are cellular materials, in medicine represented by trabecular bones and in advanced engineering practice represented by polymeric or metal foams. Recent investigations show that inner structure of trabecular bone is notably geometrically similar to closed cell metal foams. Thus, microstructural models for determination of various mechanical characteristics of metal foams can be also used for prediction of mechanical properties of porous bones.

Recently, several different methods for determination of material characteristics have been developed as a result of efforts for cost reduction in cellular materials development and engineering use. This paper is aimed at the study of mechanical behavior of cellular materials by modeling their internal structure and analysis using finite element method. Such approach is of great significance due to the complexity and high cost of experimental measurements. Firstly, the internal structure was modeled using voxel FE model created on the basis of a series of CT scans. However, irregular character of the reference material lead to FE models with limited applicability, which was motivation for discretization of internal structure using Gibson-Ashby's equivalence. Results obtained from FE simulation are in the end compared to Gibson-Ashby's mathematical model.

## 2. Models created on the basis of CT scans

Modeling of internal structure from data derived from series of a CT scans is approach that facilitates modeling the internal structure in detail including all of its irregularities and defects. Simultaneously, material properties at the level of the individual cells can be assessed by nanoindentation with high reliability and reproducibility [1]; moreover Digital Volumetric Correlation (DVC) method can be used to identify the three-dimensional strain field in the loaded microstructure [2].

In this paper, data from a series of CT scans were used for creation of voxel FE model of the foam's microstructure. Firstly, the data were processed using Matlab as a preparation for image processing that was performed in segmentation application written in Python programming language. The segmentation application creates 3D binary image that is then directly converted to voxel FE model which is then loaded to ANSYS using its input file syntax. Every voxel is in the FE model represented by one linear hexahedral element with 24 degrees of freedom.

With respect to high resolution of used CT detector, size of the voxel model developed from $560 \times 560 \times 501$ pixel image data was more than 1.5 milion elements. Such model is extremely computationally demanding. Hence, location of contact between two adjacent cells was studied using a smaller model ($64 \times 64 \times 96$ pixels) subjected to tensile loading. However, obtained results were inconsistent due to extremely irregular internal structure of reference material (see Par. 3) and its defects that complicate image segmentation. Generated voxel model then contains elements that limit the model applicability. Furthermore, relatively big cell sizes make selection of smaller volume for successful segmentation difficult. These considerations were motivation for subsequent discretization of the internal structure using Gibson-Ashby's equivalence.

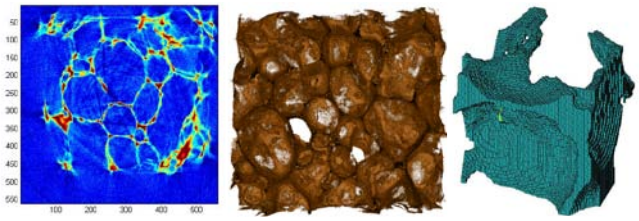

**Fig. 1:** Reconstructed micro-CT slice of the metal foam (left), surface model derived from CT data (middle), small part of the voxel FE model showing only two adjacent cells (right)

## 3. Geometrical and mechanical modeling

Instead of modeling the complex internal structure of metal foam directly, a unit cell approach is often used. Internal structure of cellular materials can be then represented by miscellaneous two- and three-dimensional models according to the various cellular forms. In 2D idealization, the regular, irregular and inverted hexagonal structures expressing isotropic and anisotropic behavior are most frequently used [3]. 3D models are typically represented by hollow sphere structures (HSS) [4], regular periodic microgeometries, which can be generated from space filling regular polyhedra such as cubes, rhombic dodecahedra and regular tetrakaidecahedra; composite structures containing different fractions are modeled using semi 3D slabs with circular, elliptic, rectangular and square closed cells [5]; SISS and 3P are model structures based on the structural similarity between porous bones

and metal foams [6]. However, many authors were also interested in mechanical characteristics of a single cell. The study of a regular network of tetrakaidecahedra of Kelvin then gives quasi-isotropic elastic properties [7], Gibson and Ashby considered the deformation of an elementary cell of cubic or hexagonal form.

Fundamentals of Gibson-Ashby's discretization are based on studies of beam deformation mechanisms considering that cell-wall bending is the principal mechanism of deformation of cellular materials. Deduction of macroscopic characteristics is thereby done by studying bending of a beam, which represents the foam strut. This model was originally developed for discretization of open cell foams. The arrangement of these elementary cells is such as the struts of the cells join those of the other cells in their centre. Thus, even if the parallelepipedic elementary cell does not correspond to physical reality, it has the advantage of becoming deformed according to same mechanisms of a real cell. In the last years, the random nature of the cell shape was also taken into account. In this study, the beam-only discretization with cubic cells is used intentionally to investigate its suitability for modeling of closed cell foams and trabecular bones.

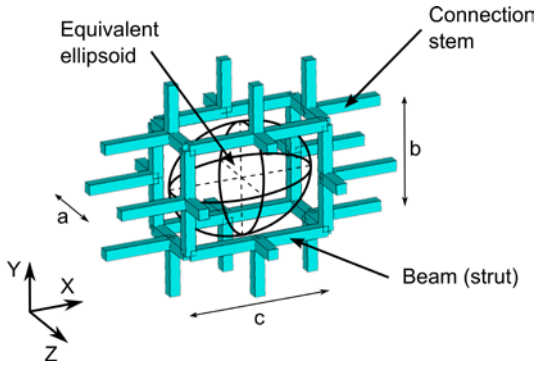


**Fig. 2:** Gibson-Ashby's cell with corresponding equivalent ellipsoid

The elementary cell is considered to have hexagonal or cubic form (which is used in this paper), and the whole structure is then modeled by periodical network of elementary cells [8]. Advantages of this approach are primarily reduction of computational demand factor and simple parameterization of cell shapes, dimensions and wall thicknesses. Disadvantages result from regularity of cell network – complicated modeling of defects and irregularities.

Overall material characteristics of the material were derived from tensile loading of the structure. The analysis was performed in ANSYS software in both elastic and plastic fields. Cell network was generated using linear hexahedral elements with 24 degrees of freedom.

Aluminium closed cell foam Alporas was selected as a reference material. Cell parameters were derived from real material characteristics [9]; behavior of geometrically isotropic and anisotropic elementary cells was studied according to typical production parameters, where spherical cells become polyhedron at porosities over 70 %. Alporas is manufactured using special unnormalized alloy containing 97 % of aluminium, 1.5 % of calcium and 1.5 % of titanium [10]. Because material properties of this alloy are not provided by the manufacturer, the material models use mechanical properties of 98 % aluminium as stated in [5]:

- $E = 69$ GPa
- $\mu = 0.33$
- yield strength $\sigma_y = 300$ MPa
- tangential modulus $E_t = 1.725$ GPa

With regard to irregularity of Alporas' internal structure, it is not possible (apart from statistical methods) to determine the representative cell. However, the cell sizes are distributed over the range from 1 mm to 13 mm with the mean cell size 4.8 mm [9], which is also used in this paper.

Two different material models were used in the FE study – linear elastic model and elasto-plastic material model with von Mises plasticity and bilinear isotropic hardening. Material characteristics in both elastic and plastic fields were derived from displacement controlled tensional loading. Investigated relations were particularly the evolution of overall elastic modulus according to different relative densities and in the plastic field the tensional stress-strain diagram.

## 4. Determination of structural characteristics

Structural characteristics for calculation of overall mechanical properties were derived using Maple mathematical software. Output parameters were particularly the density of discretized structure, relative density, volume fraction and porosity calculated as follows:

- $\rho_{\text{Foam}}$ - density of discretized structure:

$$\rho_{\text{Foam}} = \frac{\rho_{\text{Al}} \times V_{\text{Beams}}}{V_{\text{Solid}}}$$

where $\rho_{\text{Al}}$ is density of aluminium, $V_{\text{Beams}}$ is volume of beams in the model structure and $V_{\text{Solid}}$ is total volume of model structure.

- $\rho_{\text{relative}}$ – relative density:

$$\rho_{\text{relative}} = \frac{\rho_{\text{Foam}}}{\rho_{\text{Al}}}$$

- $V_{\text{f}}$ – volume fraction:

$$V_{\text{f}} = \frac{V_{\text{Beams}}}{V_{\text{Solid}}}$$

- $P$ – porosity:

$$P = \frac{1}{V_{\text{f}}}$$

## 5. Analysis using theoretical model

Results from FE analysis were compared to theoretical model developed by M. F. Gibson and L. J. Ashby in [8]. This model is valid in the elastic field only and is based upon relation:

$$\frac{E_{\text{foam}}}{E_{\text{Al}}} = \alpha \left(\frac{\rho_{\text{Foam}}}{\rho_{\text{Al}}}\right)^{\eta}$$

where $E_{\text{foam}}$ is elastic modulus of metal foam, $E_{\text{Al}}$ is elastic modulus of aluminium, $\frac{\rho_{\text{Foam}}}{\rho_{\text{Al}}}$ is relative density, $\alpha$ and $\eta$ are constants. Two different sets of constants obtained theoreticaly in [8] and experimentally in [11] were used:

- theoretical [8] – $\alpha = 0.6, \eta = 1.6$
- experimental [11] – $\alpha = 0.6, \eta = 1.6$

## 6. Results

Firstly the dimensions of representative volume element (RVE) were determined from a set of FE simulations with different number of cells. Evolution of elastic modulus vs. number of cells along each axis in the coordinate system was plotted. Fig. 3 shows that substantial error was acquired at low number of cells and with growing number of cells the elastic modulus was decreasing. Cell network consisting of 12 cells along each axis was identified as sufficient RVE with equivalent real specimen dimensions 57.6 mm × 57.6 mm × 57.6 mm.

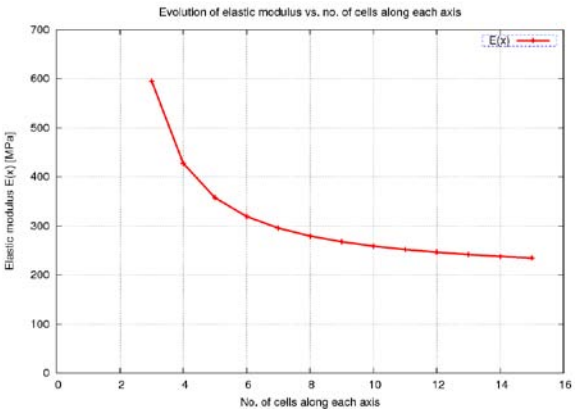


**Fig. 3:** RVE assessment

In the next step, parameters of the Gibson-Ashby's cell were assessed. Mechanical response of beam-like discretization highly depends on relative lengths of the connection stems. Analyses show that elastic modulus increase with shorter connection stems, in this paper $1/8$ length of the cell strut is considered as relevant value for the length of connection stems. Influence of cross-section shape was determined from comparison of rectangular and circular cross-section. Analysis of obtained relations indicate that the shape itself doesn't have any influence on results for relative densities lower than 0.12, for higher relative densities the circular shape model becomes stiffer.

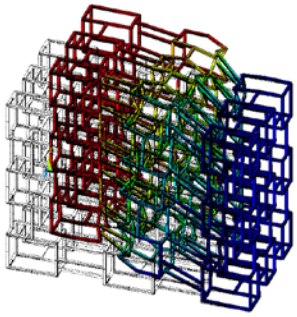

**Fig. 4:** Example of the cell network deformed under compressive loading

Essential part of the analysis was determination of relations between mechanical response and beam cross-sectional parameters. For the geometrically isotropic cell, published elastic modulus of Alporas foam was acquired with model relative density in 0.12 - 0.185 interval. Regarding Alporas porosity higher than 70 %, mechanical properties of geometrically anisotropic cells had to be also investigated. Dimensions of the most frequently occurring cell (4 mm×5 mm×6 mm) were used [12]. Declared elastic modulus of Alporas was acquired with model relative density in 0.08 – 0.13 interval, which is consistent with real mechanical characteristics.

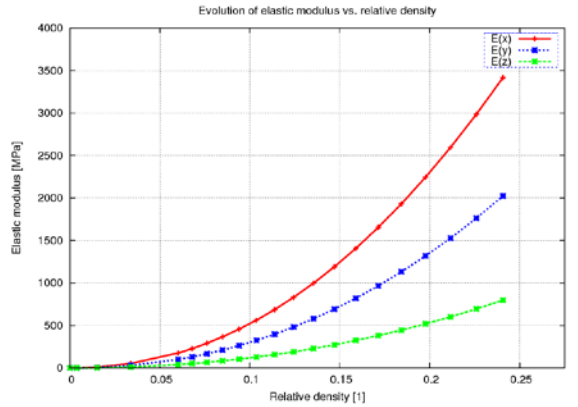


**Fig. 5:** Overall mechanical characteristics of geometrically anisotropic model

It was also important to investigate the difference between overall mechanical characteristics of geometrically isotropic and anisotropic cell. Fig. 6 compares evolution of elastic moduli ratio (quotient of elastic moduli of metal foam and aluminium respectively) vs. beam cross-sectional area (rectangular cross-section) for geometrically isotropic and anisotropic model.

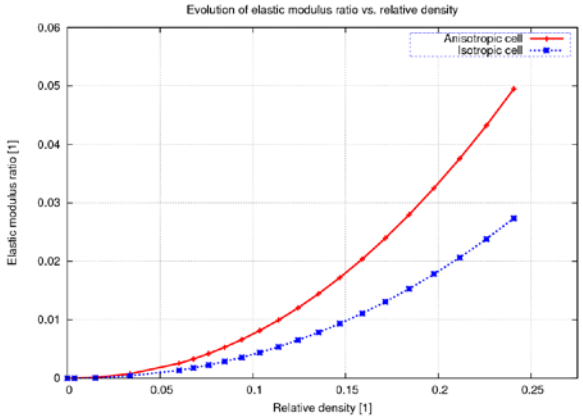


**Fig. 6:** Comparison between geometrically isotropic and anisotropic cell

Results from theoretical analysis are shown in Fig. 7. Elastic moduli ratio of theoretical model with experimentally assessed parameters quickly increases for increasing relative density. FE results are close to the model with theoretically assessed parameters and deviation decreases for relative density over 0.15.

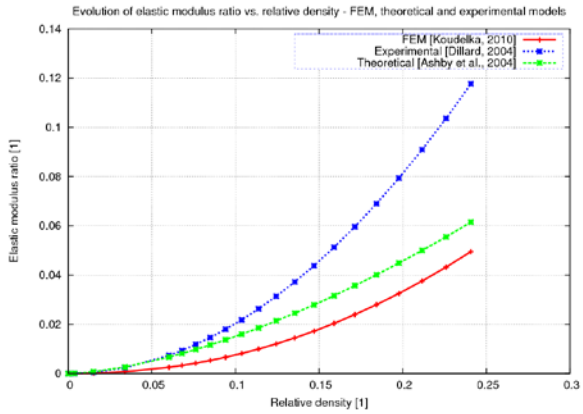


**Fig. 7:** Comparison between theoretical and FE results

Analysis in plastic field was concentrated at determination of tensional stress-strain diagram in $x$-direction. With respect to difficult convergence in geometrically nonlinear analysis, 10 % strain was selected as a maximum value. Results were studied for geometrically linear or nonlinear simulation, statically definite or indefinite boundary conditions and also for geometrically isotropic or anisotropic cell. Deformation behavior of geometrically anisotropic differs from isotropic model – strain perpendicular to direction of tensional loading causes lower overall stiffness of the model. Boundary conditions were subsequently adjusted using nodes (hereinafter called "directing nodes") that made movement only in direction of loading possible. This model was found suitable for representation of deformation behavior of Alporas under tensile loading.

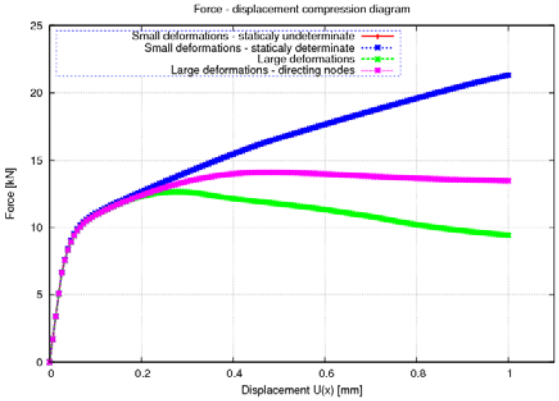


**Fig. 8:** Plastic field analysis – force- displacement diagram, geometrically anisotropic cell

Analysis shows that definiteness of boundary conditions have only negligible influence on overall mechanical characteristics with stress deviation lower than $10^{-3}$. Geometrically nonlinear simulation converged to real tensile behavior of Alporas with plateau of constant stress in extensive range of deformation even without direction nodes, as can be seen in Fig. 9.

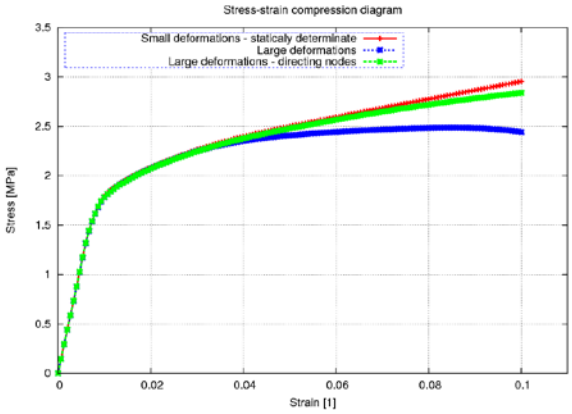


**Fig. 9:** Plastic field analysis - stress-strain diagram, geometrically isotropic cell

## 7. Conclusion

This study shows that considered discretization model can be used for numerical modeling of deformational behavior of closed cell aluminium foams and trabecular bones. Effects of beam parameters on total stiffness are highlighted and obtained results are in agreement with characteristics of real cellular materials. Increased length of connection stems decreases total stiffness, whereas increase in relative density increases total stiffness of the foam structure. Studies performed in plastic field are in agreement with plastic behavior of real specimens. Further investigations will be performed in the plastic field analysis. Presented results are derived from simulations with maximum 10 % strain value; no simulations were performed for deformations above 15 % due to convergence problems of the FE simulation. However, deformations above 60 % are required for simulation of material hardening mechanisms, where cell walls begin to collapse. Such models also have to be considered as self-contact problem because deformed cell walls begin to interfere with each other. Furthermore, statistical methods may be applied for determination of equivalent ellipsoid dimensions using optical identification.

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