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Macroscopic Modelling of Foams: an Order-Parameter Approach vs. a Micropolar Model

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The size-dependent mechanical properties of foam materials cannot be described by a classical continuum approach. Using extended continuum models such as the micropolar approach is one of the possibilities to model such mechanical behaviour. The presented order-parameter approach provides a way to describe size effects by means of an additional field variable which is not of kinematical nature as it is usually the case in the micropolar model. In the present contribution the micropolar approach is compared with the order-parameter approach in order to model the size-dependent behaviour. The investigated order-parameter model shows advantages over the micropolar approach, as it enables to cover both types of size effects: the stiffening as well as the weakening.

1 Introduction

With the growing acceptance and use of foam materials in engineering the need for appropriate models increases. The mechanical properties of foams are size-dependent and defined mainly by the underlying microscopic structure (Diebels and Steeb (2002); Tekoğlu and Onck (2008)). This size-dependent mechanical behaviour cannot be covered by the classical Boltzmann continuum. The extended continuum approaches with additional field variables allow, however, the description of size effects. Replacing real experiments an artificial open-cell foam model is used to generate the reference data from full-resolution microscale models. The artificial foam model is set up based on a stochastically disturbed Weaire-Phelan structure. In this foam model each strut of the foam is discretized with beam elements. The reference data is extracted from the effective mechanical properties of the specimens in virtual simple shear and tensile tests performed on a microscopic structure. The tests on geometrically similar specimens show the size-dependent macroscopic mechanical behaviour characteristic for cellular media. The work of Lakes (1983) addresses the dependency of macroscopic material properties on the size of specimen.

In the present contribution the micropolar continuum is considered an example for an extended continuum. In the micropolar continuum approach the kinematic relations are extended by additional rotational degrees of freedom. This approach is suitable to reproduce the stiffening size effect under shear loading. The micropolar model is however unable to model the weakening size effect under uniaxial loading (Tekoğlu and Onck (2005)).

The order-parameter approach is investigated as an alternative to the micropolar approach. The presented order-parameter approach covers the stiffening effect in shear test as well as the weakening effect in tensile test. The order-parameter approach is applied by Steeb and Diebels (2004), and Johlitz (2008) to model the influence of the boundary layer in polymer bonding. Furthermore the comparison of the new order-parameter approach and micropolar approaches is presented. At this point the differences and similarities of both approaches are shown in detail.

The additional field variable is introduced with the order-parameter approach. This additional field can be related to the morphological properties of the foam such as cell connectivity characterising the microstructure. To assess the impact of model's internal parameters onto the model response, several parametric studies are carried out. The examples of two different types of size effects and the modelling performance of micropolar and order-parameter approaches are shown. The model parameters required to simulate the effective mechanical behaviour in shear and tensile tests are determined using the parameter identification routine based on the evolutionary computational framework. For this purpose the setup and strategy as described in the works of Diebels and Scharding (2011), Chatzouridou and Diebels (2005) are adapted.

2 An Order-Parameter Model

The order-parameter approach presented here is an alternative possibility to describe the size dependency of macroscopic mechanical properties of cellular materials. Two types of size effects are investigated in the presented work. The first is the stiffening effect. This effect is usually observed in specimens in a simple shear test. Here, multiple geometrically similar specimens with different sizes show an increasing effective shear modulus with decreasing size of the specimen. This size-dependent effect is initiated by the influence of a boundary layer (Diebels and Steeb (2002)).

The boundary layer shows modified stiffness values due to applied mechanical constraints. The size of this boundary layer is independent of the specimen's size and it is strongly linked to microstructural properties like cell size. The second type of size effect is the weakening effect. This effect is observed in geometrically similar specimens in compression and tensile tests. This effect can be motivated, if the constraints of foam cells within the specimen and on its boundaries are considered. The cells on the boundary have less neighbouring cells than the cells in the bulk sample. Therefore, these cells are less restricted in their movements. (Tekoğlu and Onck (2005)). The decreasing compressive strength is documented in works of Bastawros et al. (2000) and Andrews et al. (1999).

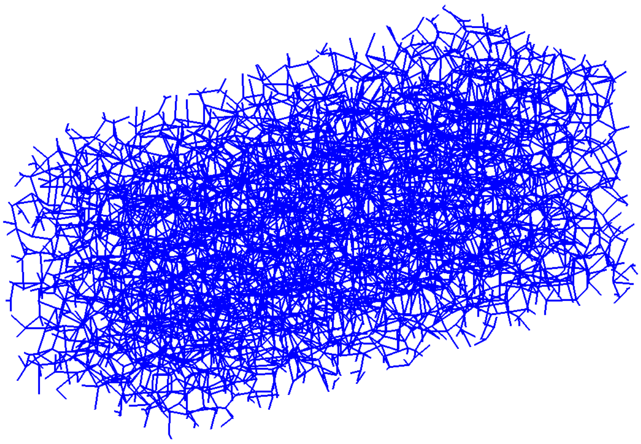


Figure 1: Stochastically disturbed foam specimen

In the presented order-parameter model an additional scalar valued order parameter is introduced. A similar approach is applied in works of Steeb and Diebels (2004) to describe the behaviour of polymeric thin films. Usually, the additional field is modelled using the Helmholtz differential equation. This equation is also used by Johlitz (2008), Diebels and Geringer (2012) to model the formation of an interphase layer in polymers close to a substrate.

We consider a problem posed on a domain Ω with a boundary denoted by $\partial\Omega$. The boundary consists of two regions Γ^N and Γ^D with $\Gamma^N \cup \Gamma^D = \emptyset$. The linear strain tensor is given in terms of the displacement vector $\mathbf{u}$ by

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\operatorname{grad}\mathbf{u} + \operatorname{grad}^T\mathbf{u})\,. \tag{1}$$

The equilibrium equation in static case is given as

$$\operatorname{div}\mathbf{T} + \rho\mathbf{b} = \mathbf{0}\,, \tag{2}$$

with the Cauchy stress $\mathbf{T}$. Subsequently the body forces $\rho\mathbf{b}$ will be neglected. The constitutive relation is given by the set of the following equations

$$\mathbf{T} = 2\mu(\xi)\boldsymbol{\varepsilon} + \lambda(\operatorname{tr}\boldsymbol{\varepsilon})\,\mathbf{I} \tag{3}$$

$$\mu(\xi) = (1-\xi)\mu_1 + \xi\mu_2\,. \tag{4}$$

The equation (3) describing the relationship between deformation and stress is a function of the additional field ξ. The stiffness distribution is controlled by a linear mixture rule (4) and the field ξ is described phenomenologically by the Helmholtz equation (7). The model parameters are the classical Lamé parameter λ and the additional parameters μ_1, μ_2. The boundary conditions have to be given for the displacement and the stress vector, respectively,

$$\mathbf{u} = \mathbf{g}_u \quad \text{on} \quad \Gamma_u^D \tag{5}$$

$$\mathbf{T} \cdot \mathbf{n} = \mathbf{h}_u \quad \text{on} \quad \Gamma_u^N \tag{6}$$

Finally the additional order-parameter field is determined by

$$\alpha\xi = \operatorname{div}\operatorname{grad}\xi\,, \tag{7}$$

with boundary conditions

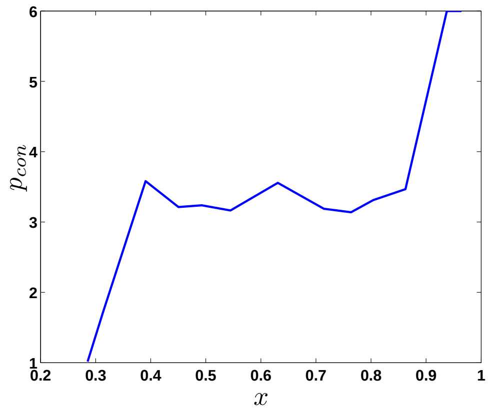
$$\xi = g_\xi \quad \text{on} \quad \Gamma_\xi^D \tag{8}$$

$$\frac{\partial\xi}{\partial\mathbf{n}} = h_\xi \quad \text{on} \quad \Gamma_\xi^N\,, \tag{9}$$

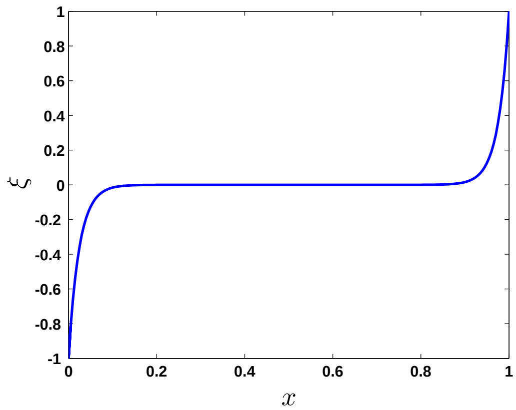
with $\mathbf{n}$ as an outward unit normal vector on the boundary $\partial\Omega$. The model parameter α determines the thickness of the resulting boundary layer.

The kinematic relation (1) used in the order-parameter approach is similar to the kinematic relation in the linear elasticity theory, considering the small deformation modes. Hence, the symmetric part of the strain tensor is used in equation (1).

In the present contribution artificial foam specimens are generated. These specimens are used in virtual experiments to determine the mechanical properties of generated foam material. The foam morphology of the tested specimens is based on the Weaire-Phelan structure (Weaire and Phelan (1994)). The foam structure is discretized using beam elements to provide a detailed resolution of the microstructure. To prevent the appearance of anisotropic behaviour of the regular Weaire-Phelan structure the generated specimens are stochastically disturbed (Figure 1).



(a) Average cell connectivity p_{con}



(b) Additional field ξ

Figure 2: Cell connectivity and the additional field ξ

The additionally introduced field ξ can be related to the morphological property of cellular media such as cell connectivity of open-cell foam material. To describe the connectivity of a unit cell we define a connectivity number p_{con}. This number implies the number of connections to cell's neighbours. Hence, the unit cells on free boundaries have one neighbour ($p_{con} = 1$) and cells within specimen have more connections to neighbouring cells ($p_{con} > 1$). With the given morphology of the Weaire-Phelan structure the maximum connectivity number is $p_{con} = 4$. The boundary conditions applied on a fully clamped specimen are given by an arbitrarily defined value $p_{con} = 6$. This arbitrary value is reproducing the connectivity conditions on the boundary with prescribed constraints, and should be different from connectivity values p_{con} on free boundaries and within the specimen.

The Figure 2(a) depicts the average distribution of cell connectivity over the specimen height for a free boundary at $x = 0$ and a fully clamped boundary at $x = 1$ (x : normalised thickness coordinate). The boundary conditions used for the order parameter model in Figure 2(b) are $\xi = -1$ for $x = 0$ and $\xi = 1$ for $x = 1$. By using the suitable boundary condition values of the order parameter field variable a distribution can be produced that is comparable to the distribution of the average cell connectivity. A closer comparison of connectivity distribution and additional field ξ indicates a strong similarity between both distributions (Figures 2(a) and 2(b)).

3 Comparison of an Order-Parameter and Micropolar Models

The size-dependent behaviour mentioned in Section 1 can be modelled by the extended continuum approach such as the micropolar model (Cosserat et al. (1909); Eringen (1965)). In this section the linear micropolar approach and the order-parameter approach are compared. In the micropolar model the additional rotational degrees of freedom $\bar{\boldsymbol{\varphi}}$ are complementing the translational degrees of freedom $\mathbf{u}$.

The additional deformation measures of a micropolar model are the Cosserat strain $\bar{\varepsilon}$ and the curvature tensor $\bar{\boldsymbol{\kappa}}$. The Cosserat strain tensor can be split into a symmetric and a skew-symmetric part with the permutation tensor $\overset{3}{\mathbf{E}}$

$$\bar{\varepsilon} = \bar{\varepsilon}_{sym} + \bar{\varepsilon}_{skw} = \operatorname{grad}\mathbf{u} + \overset{3}{\mathbf{E}} \cdot \bar{\boldsymbol{\varphi}}\,, \tag{10}$$

$$\bar{\varepsilon}_{sym} = \frac{1}{2}(\operatorname{grad}\mathbf{u} + \operatorname{grad}^T\mathbf{u})\,, \tag{11}$$

$$\bar{\varepsilon}_{skw} = \frac{1}{2}(\operatorname{grad}\mathbf{u} - \operatorname{grad}^T\mathbf{u}) + \overset{3}{\mathbf{E}} \cdot \bar{\boldsymbol{\varphi}}\,. \tag{12}$$

The curvature tensor is defined as the gradient of the micro rotations

$$\bar{\boldsymbol{\kappa}} = \operatorname{grad}\bar{\boldsymbol{\varphi}}. \tag{13}$$

The constitutive equations relate the non-symmetric stress tensor

$$\mathbf{T} = 2\mu\bar{\varepsilon}_{sym} + 2\mu_c\bar{\varepsilon}_{skw} + \lambda(\bar{\varepsilon} : \mathbf{I})\mathbf{I} \tag{14}$$

to the Cosserat strain $\bar{\varepsilon}$. The couple stress tensor (de Borst (1991))

$$\mathbf{M} = 2\mu_c(l_c)^2\bar{\boldsymbol{\kappa}} \tag{15}$$

is related to the curvature tensor $\bar{\boldsymbol{\kappa}}$. The material parameters μ and λ are the classical Lamé constants and the additional Cosserat parameters μ_c and l_c represent the additional stiffness and an internal length.

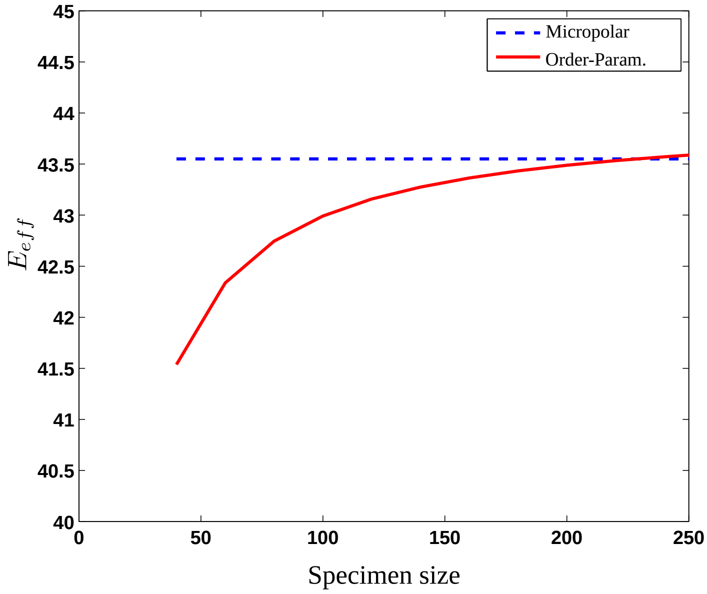


Figure 3: Weakening size effect in tensile test

The micropolar model represents a kinematically extended continuum approach by introducing the rotational degrees of freedom. With the extended material parameters μ_c and l_c the properties of the underlying microstructure are covered. The Lamé parameters μ and λ can be determined in simple shear and compression tests neglecting size effects. The extended material parameters can be identified using the evolutionary algorithms if size dependent results are used to setup an appropriate inverse problem.

The micropolar approach can be used to model the stiffening effects observed in simple shear experiments. The results of shear test simulations are discussed in Section 4. However, this approach is unable to describe the size-dependent behaviour observed in tensile and compression tests. This shortcoming is not present in the order-parameter model. The simulations of tensile tests on multiple but geometrically similar specimens demonstrate the weakening effect in small sized specimens. Figure 3 depicts the results of virtual tensile test experiments on microscopic models with detailed resolution of the underlying microstructure and the results of simulations carried out using the order-parameter approach and the micropolar model. The specimen geometry used for the virtual tensile test experiment is similar to the geometry used for the virtual shear test (Fig. 4). While the micropolar model does not show a size effect under tension, a typical weakening can be observed for the order-parameter approach.

Compared to the micropolar model the order-parameter model shows a lower numerical complexity since a total number of only four degrees of freedom (three classical translational plus one additional degree of freedom of order-parameter field) is used. In contrast to the micropolar approach, the order-parameter approach is using the classical Boltzmann continuum with translational degrees of freedom. The equilibrium equation and kinematics are identical with the corresponding relations in the theory of linear elasticity. The extension of the classical continuum model takes place at the level of the constitutive relations. Here, an additional field ξ is introduced describing the spatial distribution of stiffness. This is accomplished phenomenologically by means of the Helmholtz equation and a linear mixture rule. The parameters λ, μ_1, and μ_2 can be determined in a straight forward manner in simple experiments as described in Section 5. The parameter α is determined using the evolutionary computations routine.

4 Numerical Examples

The governing equations of the order-parameter approach presented here are the displacement-strain relation (1), the equilibrium equation (2) and the constitutive equations (3) - (7). Combining these equations results in a one-way coupled problem in the fields $\mathbf{u}$ and ξ. This problem can be solved numerically by means of the finite element method. The weak form of the order-parameter model can be formulated as follows:
Find $(\mathbf{u}, \xi) \in \mathbf{U} \times \mathbf{P}$, with $\mathbf{U}$ and $\mathbf{P}$ as the appropriate function spaces, such that for all $\delta\mathbf{u} \in \{\delta\mathbf{u} \in \mathbf{U} | \delta\mathbf{u} = \mathbf{0}$ on $\Gamma_u^{\mathrm{D}}\}$ and $\delta\xi \in \{\delta\xi \in \mathbf{P} | \delta\xi = 0$ on $\Gamma_\xi^{\mathrm{D}}\}$

$$a_u(\mathbf{u}, \xi; \delta\mathbf{u}) = l_u(\delta\mathbf{u}) \tag{16}$$

$$a_\xi(\xi; \delta\xi) = l_\xi(\delta\xi) \tag{17}$$

with

$$\mathbf{u} = \mathbf{g}_u \quad \text{on } \Gamma_u^{\mathrm{D}} \tag{18}$$

$$\xi = g_\xi \quad \text{on } \Gamma_\xi^{\mathrm{D}}\,, \tag{19}$$

where

$$a_u(\mathbf{u}, \xi; \delta\mathbf{u}) = \int_\Omega \mathrm{grad}\delta\mathbf{u} \colon \mathbf{T}(\mathbf{u}, \xi)\,\mathrm{d}\Omega \tag{20}$$

$$l_u(\delta\mathbf{u}) = (\mathbf{h}_u, \delta\mathbf{u})_{\Gamma_u^{\mathrm{N}}} + (\varrho\mathbf{b}, \delta\mathbf{u})_\Omega \tag{21}$$

$$a_\xi(\xi, \delta\xi) = \int_\Omega (\mathrm{grad}\delta\xi \cdot \mathrm{grad}\xi + \delta\xi\,\alpha\xi)\,\mathrm{d}\Omega \tag{22}$$

$$l_\xi(\delta\xi) = (h_\xi, \delta\xi)_{\Gamma_\xi^{\mathrm{N}}} \tag{23}$$

The numerical model of the order-parameter approach was implemented using the open-source FE-libraries provided by DEAL.II (Bangerth et al. (2007, 2012)).

In the following examples the macroscopic behaviour of the micromechanical reference specimens is modelled by the order-parameter approach. Furthermore the influence of the model parameters is demonstrated. A set of geometrically similar specimens with different sizes is tested. The boundary conditions correspond to the conditions of the displacement driven simple shear experiment as shown in Figure 4.

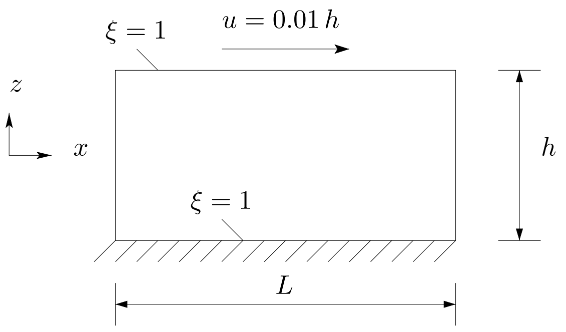


Figure 4: Shear test

It is clearly recognisable that the additional parameter α is controlling the distribution of field variable ξ. In the Figure 5 the field variable ξ is plotted over the height of specimen. For large values of α the boundary layer character of the solution can clearly be seen. The stiffness $\mu(\xi)$ is defined as the function of the variable ξ, which depends on the parameter α. Thus, the latter controls the distribution of the local stiffness of the specimen bulk.

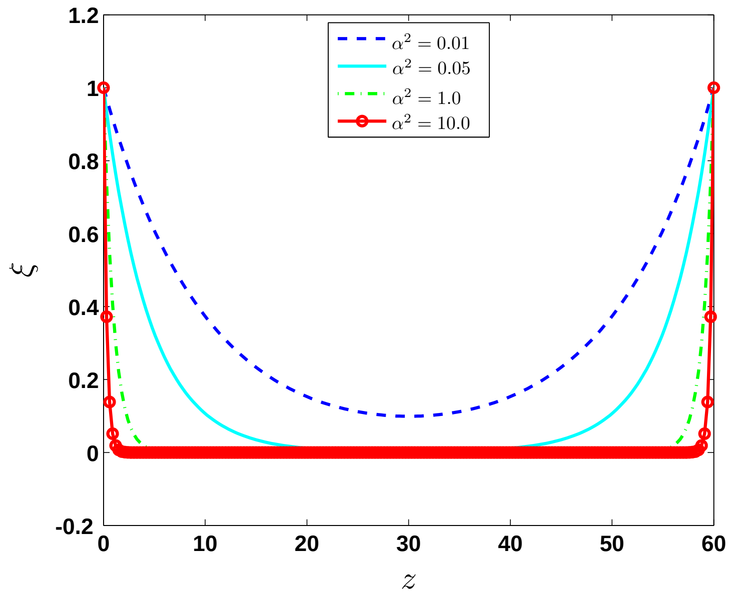


Figure 5: Parameter study for model parameter α $(0.01 \leq \alpha \leq 10)$

While μ_1 represents the local stiffness in the inner part of the specimen which is unaffected by the boundary, μ_2 represents the stiffness close to the boundary where the connectivity is changing.

The model parameter μ_2 is the quantitative measure of a specimen's local stiffness. Using the variation $\Delta\mu = (\mu_2 - \mu_1)$, the material stiffness on the boundaries can be modified. The effect of μ_2 on the displacement field $\mathbf{u}$ in y-direction is shown in Figure 6. The effective stiffness values on the boundaries are rising directly proportional to the value of μ_2.

Figure 7 shows the distribution of the field ξ over the specimen height for specimens of different size. The constant value of the boundary layer thickness in all of the considered specimens is clearly visible. The simulations of simple shear experiments using the order-parameter model with the appropriate set of model parameters are proving this model's property to describe size effects. In the presented case of the shear test the observed macroscopic mechanical behaviour can also be described using the micropolar continuum model (cf. Diebels and Steeb (2002), Diebels and Scharding (2011)).

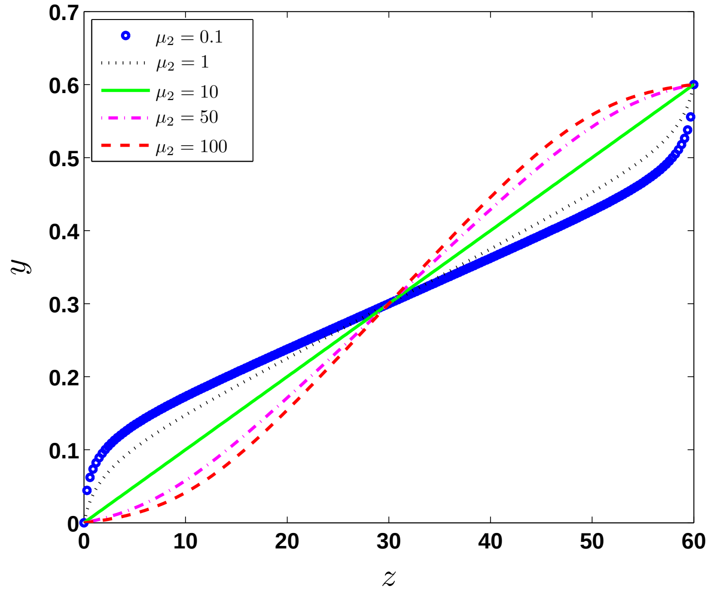


Figure 6: Parameter study for model parameter μ_2 ($0.1 \le \mu_2 \le 100,\ \mu_1 = 10$)

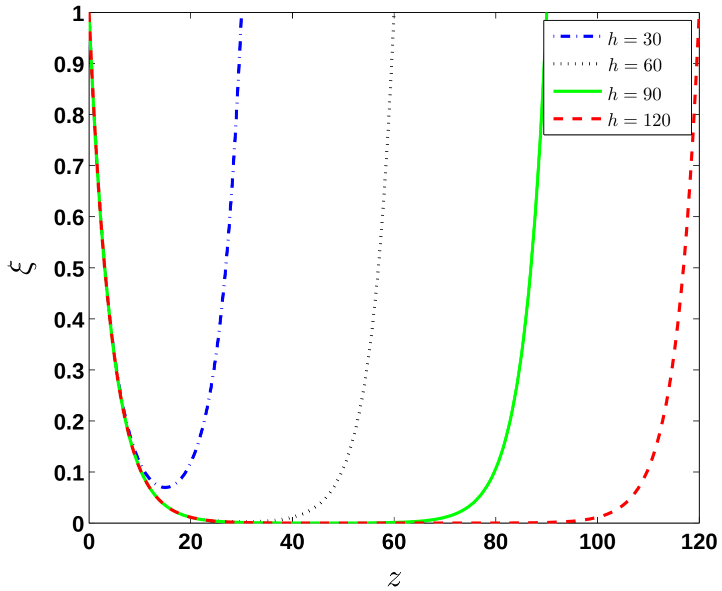


Figure 7: Distribution of field ξ for specimens of different size ($30 \le h \le 120$)

5 Identification of Parameters

With the set of appropriate model parameters the macroscopic mechanical behaviour of an open-cell foam can be modelled using the order-parameter approach. The reference data is extracted from an artificial foam structure discretized by beam elements of the Timoshenko type (Figure 8, 9). The specimens depicted in Figure 8 are used to reproduce the size effect observed in the shear test experiments. The virtual experiments on the microscopic models used in this work were completed using the commercial FE-solver RADIOSS® (Altair Engineering RADIOSS (2012)).

The determination of model parameters is treated as an inverse problem with a vector of model parameters

$$\omega = (\lambda, \mu_1, \mu_2, \alpha) \tag{24}$$

minimising the difference in the mechanical response of microscopic reference and macroscopic order-parameter models. This can be formulated as an optimisation problem. In the present contribution the Lamé parameter λ is determined *a priori* using the compression test without investigating size effects. The remaining parameters μ_1, μ_2 and α are identified using the parameter identification routine based on evolutionary computations. For this purpose the Genetic Algorithm Solver provided by MATLAB® (Mathworks MATLAB (2012)) is used.

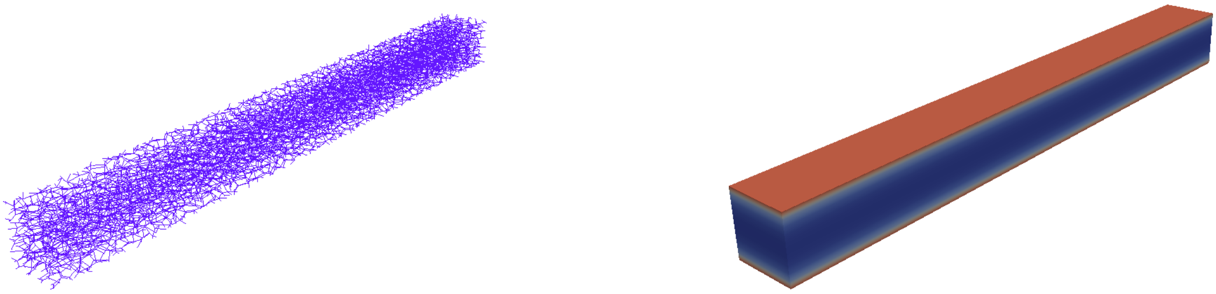


Figure 8: Microscopic and macroscopic models

Reasonable initial values for the parameter identification problem can be obtained by interpreting the parameter μ_1 as the effective stiffness of larger specimens with negligibly small influence of size-effects and the second parameter μ_2 as the effective stiffness of the smaller specimens with strong influence of the boundaries.

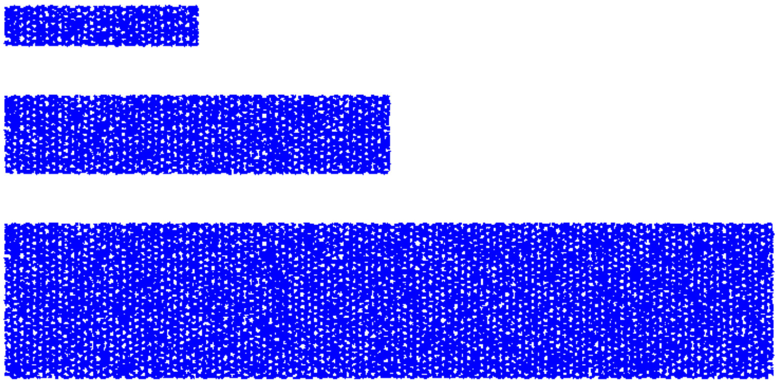


Figure 9: Geometrically similar specimens

In Figure 10 the effective shear modulus for reference, micropolar and order-parameter models is plotted against the specimen size. The reference micromechanical model shows a noticeable stiffening effect. For the larger sized specimens (more than 160mm of height) the stiffening effect becomes negligible (Fig. 10). Both micropolar and the order-parameter models appear to reproduce the size effect in shear test with comparable precision.

6 Conclusions

In the presented work, the order-parameter model is applied to describe the macroscopic mechanical behaviour of open-cell foams. The applied model is considered as an alternative to the micropolar approach which is also capable to reproduce the size-dependent mechanical behaviour of cellular materials. Both models are compared regarding the description of stiffening as well as weakening size effects at the macroscopic level. The numerical experiments verified the ability of the order-parameter approach to describe both types of size effects. Furthermore, the discussion of the effects of model parameters upon the modelling performance is provided. The closer comparison of the additional field ξ and the morphological property of micromechanical foam such as the connectivity of unit cells shows that these entities can be linked to each other. This connectivity information can therefore serve as the motivation for the additional field.

The validation of the presented approach regarding complex load cases and the identification of model parameters for uniaxial tension tests and related weakening effects are subject of future work.

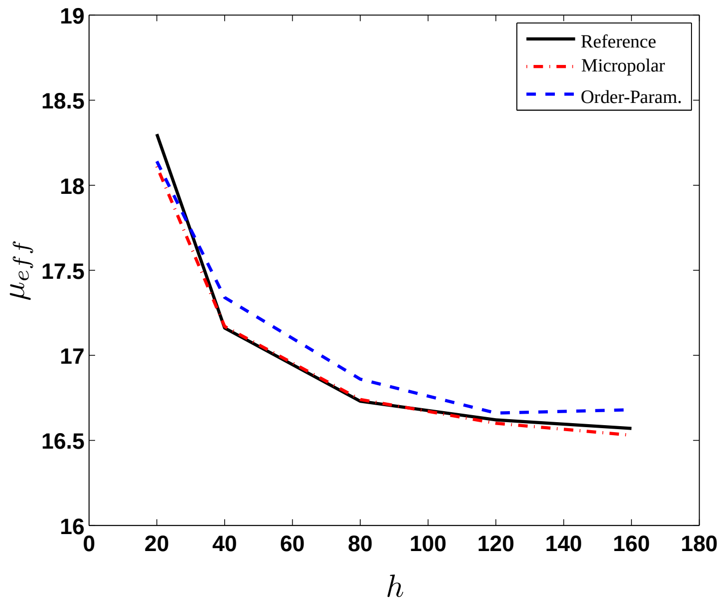


Figure 10: Size effect reproduced by micropolar and order-parameter models

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