DOI: 10.24352/UB.OVGU-2017-049

TECHNISCHE MECHANIK, 34, 1, (2014), 3 – 11
submitted: September 16, 2013

A Phase-Field Approach to Damage Modelling in Open-Cell Foams

A. Geringer, S. Diebels

Foams are complex and challenging materials. The damage process of the foam materials takes place on multiple scales changing several physical and structural properties of the material. In this study, the topology-based variable describing the connectivity state of a cell is introduced to formulate a non-variational phase-field model for the damage evolution in an open-cell foam. The material is considered consisting of the damaged and unimpaired phase with the proposed phase-field variable describing the separation of phases. The performance of the computational model is examined by means of the standard benchmarks such as tensile and simple shear test. The results show a qualitative correspondence with the two-dimensional artificial foam model used as a reference. Furthermore, the influence of the directional data extracted from the microstructure is investigated. The utilisation of the connectivity-based damage variable turns out to be a suitable choice for the simulation of the damage evolution in open-cell foam materials.

1 Introduction

The metallic foams are an advanced material which is becoming more and more attractive due to the unique combination of the mechanical properties such as high stiffness and low weight they offer. The increasing acknowledgement of the foams as an engineering material requires appropriate models for each aspect of this highly interesting material. The modelling of the damage effects is one of the challenges related to cellular materials.

Several material properties are affected as a consequence of the damage process. The modelling of these effects is carried out using an auxiliary continuous variable representing the damage state. The field of continuum damage mechanics was pioneered by Kachanov (1958) who introduced the effective stress concept, describing a virtual state of the material without damage. The further development of the theoretical framework has taken place a few decades later. Lemaitre (1985), Murakami and Ohno (1981) extended the framework by defining the damage modelling for ductile materials. The works by Krajcinovic et al. deal with the modelling of the effects of damage on brittle materials (Krajcinovic and Fonseka (1981), Krajcinovic and Srinivasan (1983)). The damage evolution in plasticity was formulated by Kattan and Voyiadjis (1990). The multiscale nature of the damage is addressed in the works considering the description of failure mechanisms using a framework of extended continuum theories (Steinmann (1995), Ebinger et al. (2004), Grammenoudis et al. (2009), Forest (2009), Rinaldi and Placidi (2013)).

The mechanical properties of foam materials are mainly defined by the material structure on the microscopic level. The characterisation of the cellular material microstructure can be made based on the porosity, mean cell diameter, dispersion of cell size, symmetry, the edge-connectivity, etc. (Gibson and Ashby (1999)). In the present contribution, the topological information obtained from the microstructure is used to define a damage evolution approach for an open-cell foam structure. Hereby the material is considered containing two distinct phases: the phase containing undamaged material and the phase with the material in damaged state. The damage variable is, therefore, used to describe the separation of these two phases together with the interface development.

The solution of interfacial problems is the subject of the phase-field modelling. The evolution of the interface position is characterised by the evolution of the continuous phase-field variable, which takes two different values depending on the phase domain. In the interface area, the value of the phase-field variable is changing gradually so that a diffuse interface is formed. The phase-field method allows for the description of the microstructure evolution in a wide range of applications such as solidification process (Artemev et al. (2001), Boettinger et al. (2002), Siquieri et al. (2007)), fracture mechanics (Miehe et al. (2010a), Miehe et al. (2010b)), nucleation kinetics (Emmerich and Siquieri (2006)) and many others. The contributions provided by Qin and Bhadeshia (2010), Steinbach (2009), Moelans et al. (2008) and Chen (2002) offer an overview of the recent developments and applications of phase-field method.

Open-cell foam structures can be modelled using beam elements on the microscale. The reference model used in the present contribution to incorporate the directional data from the microstructure is provided by the two-dimensional artificial lattice structure consisting of standard finite elements (Mangipudi and Onck (2011), Onck et al. (2001), Tekoğlu and Onck (2008), Reis and Ganghoffer (2010, 2012)). This level of microstructure discretization provides a detailed description of the foam material, resulting, however, in an inevitable large number of degrees of freedom and consequential computational limitations.

The utilisation of the phase-field approach in the context of damage mechanics as proposed in the current contribution offers the advantage of modelling the damage zone propagation in an open-cell foam without full discretization of the microstructure.

2 Phase-Field Model

In the damage modelling approach described here in following the isotropic and linear elastic material behaviour is assumed. The edge-connectivity characteristic for cellular materials, among numerous material properties, is affected by the damage process taking place on multiple scales.

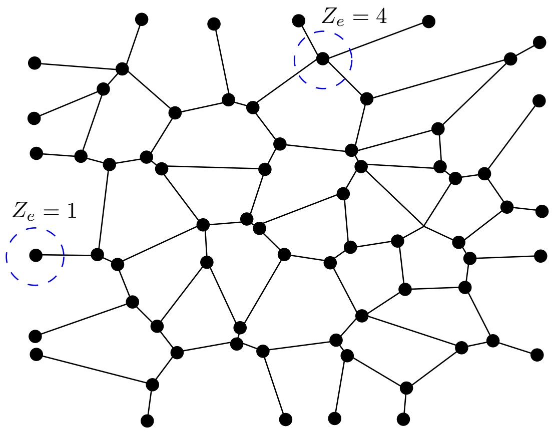


Figure 1: Edge-connectivity Z_e in an open-cell foam

For the sake of convenience, we consider a two-dimensional open-cell lattice structure shown in Figure (1). Each cell is connected with the neighbouring cells through struts. The number of the neighbour cells depends on the foam morphology. The edge-connectivity Z_e is one of the properties characterising cellular materials and is defined as the average number of edges linked to a vertex (Gibson and Ashby (1999)).

In the structure depicted in Figure (1) the edge-connectivity exhibits four connections within the bulk material and one connection on the specimen boundary, resulting in edge-conductivities of $Z_e = 4$ and $Z_e = 1$. Figure (2(a)) shows a three-dimensional example of a foam structure and a corresponding distribution of the average edge-connectivity (Figure 2(b)). Similar connectivity distribution is observed for each direction of the specimen.

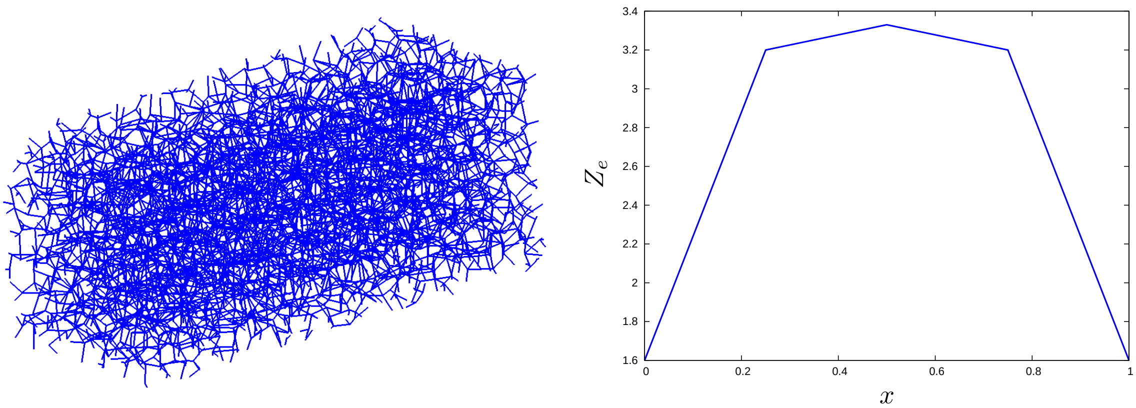
The microstructure-specific property of the edge-connectivity allows for the definition of a topology-based damage variable. Since the mechanical stability of an open-cell foam is directly linked to the number of connections between cells and the edge-connectivity is deteriorating with the ongoing damage process, the measure based on the edge-connectivity can be used to reproduce the damage state of the foam material.

In damage mechanics it is useful to utilise the continuity function defined as

$$\Psi = 1 - \xi \, . \tag{1}$$

We formulate the continuity relationship from Equation (1) as a function of edge-connectivity Z_e

$$\Psi = \frac{Z_e}{\|Z_e\|} \, . \tag{2}$$



(a) Artificial foam structure

(b) Edge-connectivity Z_e over normalised specimen length

Figure 2: Foam structure and the corresponding average edge-connectivity distribution

Regarding Equation (1) the topology-based damage variable reads as follows

$$\xi = 1 - \frac{Z_e}{\|Z_e\|} \, . \tag{3}$$

The damage variable takes the values $0 \leq \xi \leq 1$, with $\xi = 0$ for the material without damage (i. e. the cell has full number of connections) and $\xi = 1$ for fully damaged material (i. e. most of the connections to neighbouring cells are lost).

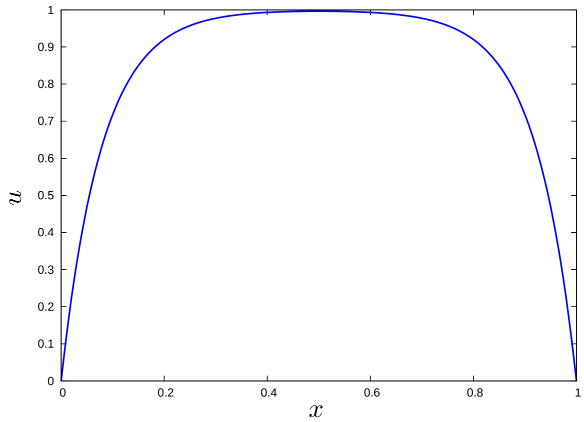


Figure 3: Approximation of the edge-connectivity using a differential equation

In the following we consider a domain Ω with a boundary denoted by $\partial\Omega$. The boundary consists of two non-overlapping regions Γ^D and Γ^N with $\Gamma^D \bigcup \Gamma^N$. The average connectivity distribution of a foam structure can be approximated using a phenomenological approach based on a partial differential equation of the Helmholtz type

$$-\mathrm{div}\,(\beta\,\mathrm{grad}\,u) + \alpha\,u - f = 0\,. \tag{4}$$

The structure of the Equation (4) exhibits the structure of the general balance equation (cf. Steeb and Diebels (2004)). This framework allows for a general thermodynamically consistent formulation of field equations. An example for a solution of Equation (4) is shown in Figure (3). The shape of the solution curve depicted in Figure (3) can be adjusted to reproduce the connectivity distribution curve by solving Equation 4 with a set of the appropriate parameters.

Combining the definition of the topology-based damage variable from Equation (2) and extending Equation (4) with the time derivative the evolution equation of the damage for an open-cell foam is governed

$$\frac{\partial \xi}{\partial t} = -\operatorname{div}\left(\beta \operatorname{grad} \xi\right) + \alpha(1-\xi)\,\xi - f\,, \tag{5}$$

with boundary conditions

$$\xi = g_\xi \quad \text{on} \quad \Gamma_\xi^D \tag{6}$$

$$\frac{\partial \xi}{\partial \mathbf{n}} = h_\xi \quad \text{on} \quad \Gamma_\xi^N\,, \tag{7}$$

with $\mathbf{n}$ as an outward unit normal vector on boundary $\partial\Omega$. In the following examples the Dirichlet boundary condition is chosen to describe the influence of free boundaries on the connectivity, i. e. to take into account the reduced connectivity close to free boundaries. In contrast the Neumann boundary condition is chosen in the sense of a symmetry condition. In this case $h_\xi = 0$ preserves the connectivity close to these boundaries. The second term on the right hand side of the Equation (5) represents the contribution to the damage field arising from the local interactions.

To complete the formulation of the proposed damage model the evolution Equation (5) is coupled with the deformation field which is the result of the solution of the linear elastic problem. The coupling is accomplished using the third term of Equation (5) which is, therefore, defined as a function of the strain energy W and the first principal strain

$$f = f(W, \varepsilon_1)\,, \tag{8}$$

with the strain energy defined as

$$W = \frac{1}{2}\,\tilde{\mathbf{T}} : \boldsymbol{\varepsilon}\,. \tag{9}$$

The damage affects the deformation field through the effective stress $\tilde{\mathbf{T}}$ which describes a virtual state of the material without damage

$$\tilde{\mathbf{T}} = \frac{\mathbf{T}}{(1-\xi)}\,. \tag{10}$$

The linear elastic problem coupled with the damage evolution is given by an equilibrium equation with neglected body forces in static case

$$\operatorname{div}\mathbf{T} = \mathbf{0}\,, \tag{11}$$

and the constitutive relation for the Cauchy stress tensor

$$\mathbf{T} = 2\mu\,\boldsymbol{\varepsilon} + \lambda\,(\operatorname{tr}\boldsymbol{\varepsilon})\,\mathbf{I}\,, \tag{12}$$

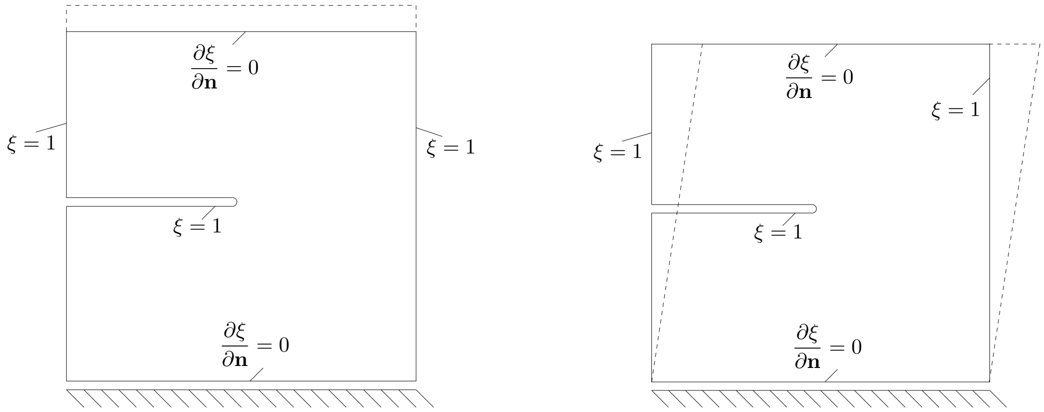
with μ and λ as the classical Lamé parameter. The linear strain tensor is provided in terms of the displacement vector $\mathbf{u}$ by

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\operatorname{grad}\mathbf{u} + \operatorname{grad}^T\mathbf{u})\,. \tag{13}$$

The boundary conditions of the linear elastic problem are given by the displacement and stress vectors on respective boundaries

$$\mathbf{u} = \mathbf{g}_u \quad \text{on} \quad \Gamma_u^D \tag{14}$$

$$\mathbf{T}\cdot\mathbf{n} = \mathbf{h}_u \quad \text{on} \quad \Gamma_u^N\,. \tag{15}$$



(a) Tensile test (b) Shear test

Figure 4: Single-edge notched specimen

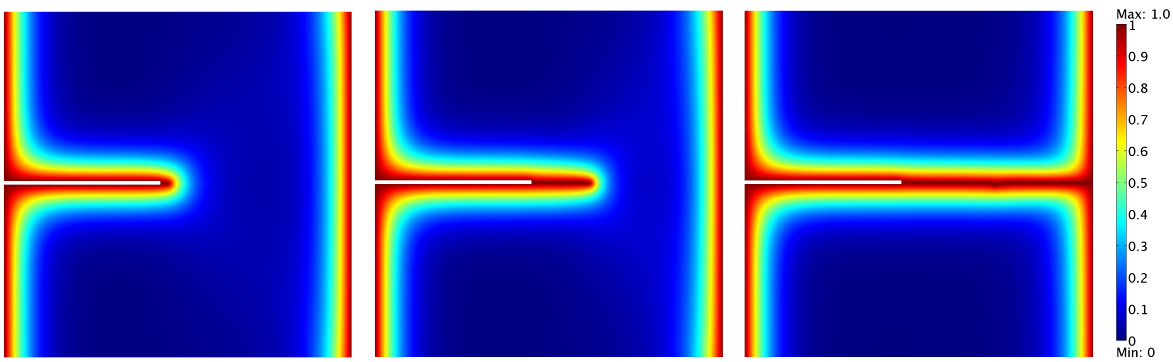
3 Results and Discussion

The governing equations of the damage model presented here are the evolution Equation (5), the displacement-strain relation (13), the equilibrium Equation (11), and the constitutive Equation (12). The combination of these equations leads to a two-way coupled problem in the fields $\mathbf{u}$ and ξ. The numerical solution of this problem is accomplished by means of the finite element method. The set of coupled equations is solved using COMSOL Multiphysics (2009) for a given boundary conditions.

In the following examples, the performance of the proposed damage modelling approach is demonstrated. For this purpose we consider two standard benchmark problems such as a tensile and a pure shear tests performed on a single-edge notched square specimen with equal-length sides of 100mm. The geometry of the specimen and the boundary conditions used for the tests are depicted in Figures (4(a)) and (4(b)). The computations in both examples are performed with monotonic driven displacements with a constant increment of $\Delta u = 0.02$ mm. The maximum prescribed displacement amounts to $u = 1$mm.

The value of $\xi = 1$ is given as the boundary condition for the free boundaries of the specimen since the cells on these boundaries exhibit the small edge-connectivity values resulting in values of $\xi \rightarrow 1$. The boundaries with constraints originating from the mechanical part of problem are marked as Neumann boundaries with $\frac{\partial \xi}{\partial \mathbf{n}} = 0$.

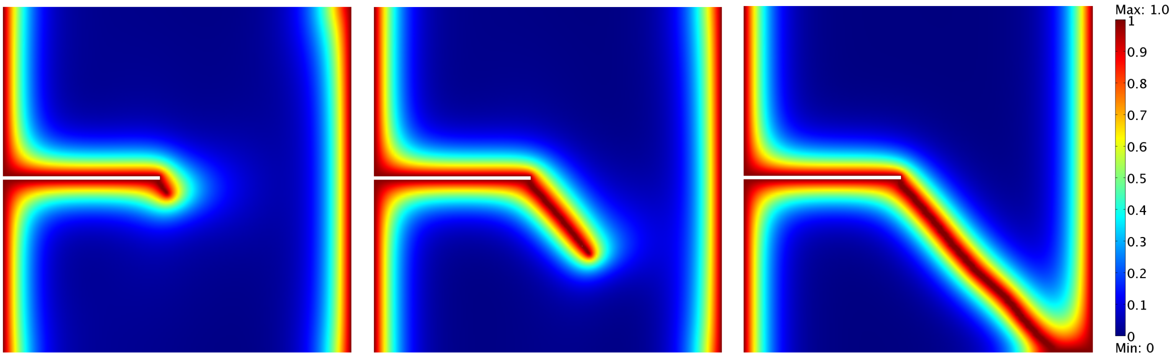
The computed propagation of the damage zone resulting from the tensile test is shown in Figures (5(a) - 5(c)). The red colour corresponds to the state of the total damage where only one connection to the neighbour cells is left and the blue colour displays the undamaged state of the structure where all of the connections to the neighbours are present. The tensile test leads to the propagation of the damage zone in horizontal direction.



(a) $u = 0.34$mm (b) $u = 0.38$mm (c) $u = 0.42$mm

Figure 5: Damage field distribution in a single-edge notched tensile test

The second example explores the evolution of the damage resulting from the shear test performed on a specimen displayed in Figure (4(b)). The resulting damage evolution is depicted in Figures (6(a) - 6(c)). The evolution of

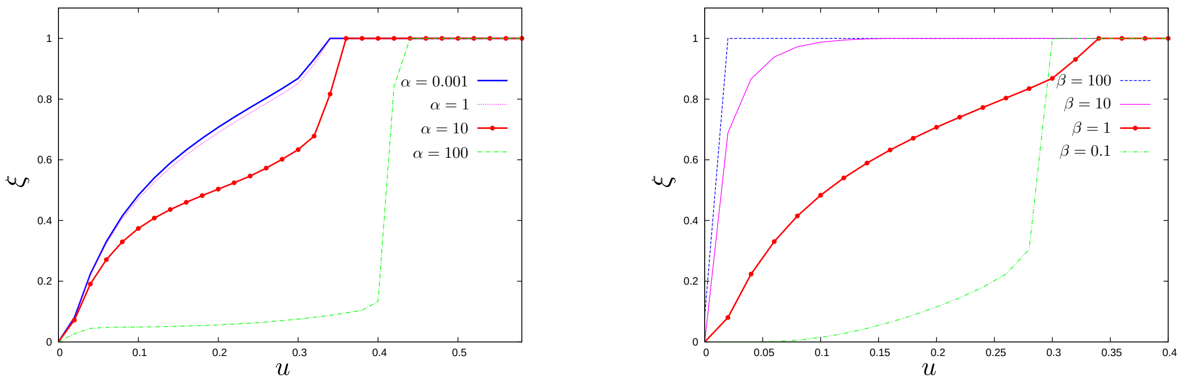


(a) $u = 0.72$mm (b) $u = 0.80$mm (c) $u = 0.92$mm

Figure 6: Damage field distribution in a single-edge notched shear test

the damage field is different from the one in a tensile test case. The damage zone takes the path from the notch down to the right bottom corner of the specimen.

The effect of the model parameters α and β on the damage variable evolution is evaluated in a standard tensile test performed with different parameter values. The values of the damage variable ξ are computed in a point close to the notch tip. From Figure (7(a)), one can clearly recognise that both parameters have significant influence upon the evolution of the damage zone. While the increasing values of the parameter β are speeding up the damage progression, performing the same with the values of the second parameter α forces the damage zone propagation to slow down.



(a) $0.001 \leq \alpha \leq 1000\,, \quad \beta = 1.0$ (b) $0.1 \leq \beta \leq 100\,, \quad \alpha = 0.001$

Figure 7: Parameter study

The influence of the microstructure on the damage zone evolution can be additionally increased by considering the local strut orientation of the foam cell. The orientation distribution function (ODF) is a generalisation of the directional data, representing the fraction of single elements with particular direction (Kanatani (1984)). The orientation distribution function $\rho(\mathbf{n})$

$$\rho = \rho(\mathbf{n}) = F_{ij}\, n_i\, n_j\,, \tag{16}$$

corresponding to the microstructure, is approximated using the fabric tensor of the second kind $\mathbf{F}$ and the fabric tensor of the first kind $\mathbf{N}$ (Kanatani (1984), Voyiadjis and Kattan (2006))

$$F_{ij} = \frac{15}{2}\left(N_{ij} - \frac{1}{5}\delta_{ij}\right)\,, \tag{17}$$

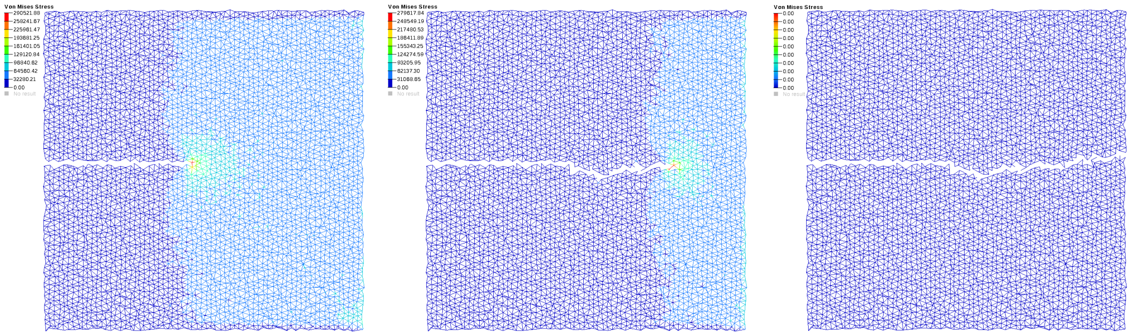
$$N_{ij} = \frac{1}{N}\sum_{k=1}^{N} n_i^{(k)} n_j^{(k)}\,, \tag{18}$$

with $\mathbf{n}$ as a unit vector indicating the strut orientation. The distribution function determined using the fabric tensor is then incorporated into the evolution equation

$$\frac{\partial \xi}{\partial t} = -\mathrm{div}\,(\beta\, \mathrm{grad}\, \xi) + \alpha(1-\xi)\,\xi - f(W, \varepsilon_1, \rho)\,, \tag{19}$$

with $f = W\varepsilon_1\,(1-\rho)$.

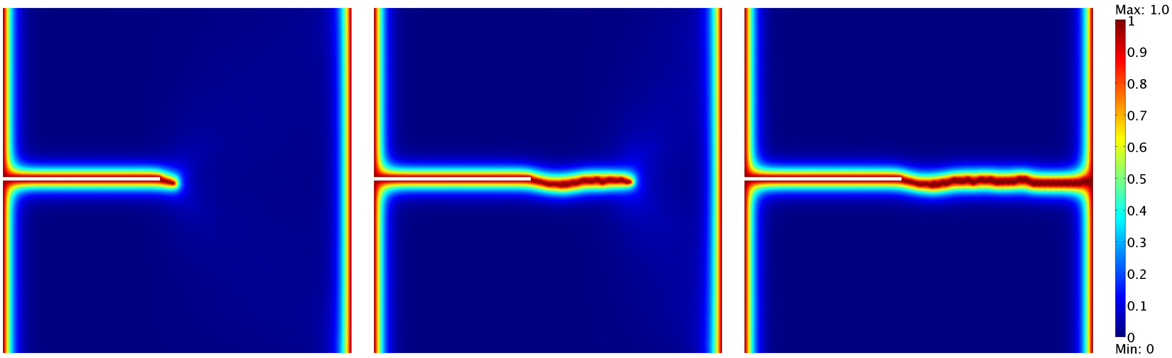
As an example, we consider a tensile test performed on a single-edge notched specimen constructed as a two-dimensional artificial foam structure. Each strut of the specimen is discretized using standard Timoshenko beam elements. The computations are performed using the FE-solver RADIOSS (Altair Engineering RADIOSS (2012)). During the tensile test computation the beam elements with the highest values of the von Mises stress are considered failed foam struts which are consequently deleted. Figures (8(a) - 8(c)) depict the crack propagation in the artificial foam structure.



(a) $t = 0.01$ (b) $t = 0.5$ (c) $t = 1$

Figure 8: Single-edge notched shear test performed on an artificial foam structure (normalised time values)

The directional data of the beams in the reference microstructure model is transferred to the phase-field model using the orientation distribution function $\rho(\mathbf{n})$, (Equation 16). Now, the tensile test is performed using modified phase-field formulation (Equation 19). The obtained damage zone distribution is shown in Figures (9(a) - 9(c)).



(a) $u = 0.38$mm (b) $u = 0.46$mm (c) $u = 0.50$mm

Figure 9: Damage field distribution resulting from the model incorporating directional data

The comparison of the damage zone distribution acquired with phase-field model incorporating the directional data and crack path from the reference model demonstrates a qualitative similarity of the results.

The presented phase-field formulation is constructed without a variational minimisation of a free energy functional providing the advantage of a high flexibility in the description of microstructure evolution in open-cell foams. The model can be further extended with regard to different constitutive models as well as finite strain theory. Apart from, the coupling of the damage phase-field with the deformations, other coupling mechanisms (chemical, temperature, etc.) can also be incorporated into the model formulation.

The phase-field formulation used in this study describes the evolution of connectivity which is linked directly to the damage state of an open-cell foam material. As a matter of fact, with the ongoing damage process the connectivity between the cells of a foam material is getting irrecoverably lost. Hence, the variable based on this topological property features the character of a non-conserved variable of the corresponding phase-field formulation. The inspection of the evolution Equation (5) and the Cahn-Hillard or Allen-Cahn equations often used in the phase-field formulations (Qin and Bhadeshia (2010), Moelans et al. (2008)) reveals these three equations as a reaction-diffusion equations, described in terms of an order-parameter and its gradients. This categorisation and also the non-conserving character of the connectivity-based phase-field variable emphasise the similarity of the proposed formulation with the equations used in variational phase-field formulations.

4 Conclusions

In the present contribution a non-variational phase-field approach is presented which allows for the description of the damage evolution in the open-cell foam materials. The topological property characterising the microstructure such as the edge-connectivity is used as the basis for the development of the proposed approach. The numerical results show that the connectivity-based variable drives the evolution of the damage phase field. The presented approach provides advantages in the description of the microstructural changes resulting from the damage process in open-cell structures. The possibility of incorporating the directional data of the microstructure by means of the orientation distribution function approximated with fabric tensors is examined. The performance of the proposed formulation and the effects of the model parameters on the overall behaviour of the model are shown by means of the respective numerical examples and parameter studies.

References

Artemev, A.; Jin, Y.; Khachaturyan, A.: Three-dimensional phase field model of proper martensitic transformation. *Acta Materialia*, 49, 7, (2001), 1165–1177.

Boettinger, W.; Warren, J.; Beckermann, C.; Karma, A.: Phase-field simulation of solidification. *Annual review of materials research*, 32, 1, (2002), 163–194.

Chen, L.-Q.: Phase-field models for microstructure evolution. *Annual Review of Materials Science*, 32, (2002), 113–140.

COMSOL Multiphysics: *Version 3.5a*. COMSOL AB, Stockholm, Sweden (2009).

Ebinger, T.; Steeb, H.; Diebels, S.: Higher order continuum models for cellular materials including damage. *PAMM*, 4, 1, (2004), 276–277.

Emmerich, H.; Siquieri, R.: Investigating heterogeneous nucleation in peritectic materials via the phase-field method. *Journal of Physics: Condensed Matter*, 18, 49, (2006), 11121.

Forest, S.: Micromorphic approach for gradient elasticity, viscoplasticity, and damage. *Journal of Engineering Mechanics*, 135, 3, (2009), 117–131.

Gibson, L.; Ashby, M.: *Cellular solids: structure and properties*. Cambridge university press (1999).

Grammenoudis, P.; Tsakmakis, C.; Hofer, D.: Micromorphic continuum. part ii: Finite deformation plasticity coupled with damage. *International Journal of Non-Linear Mechanics*, 44, 9, (2009), 957–974.

Kachanov, L.: On creep rupture time. *Izv. Acad. Nauk SSSR, Otd. Techn. Nauk*, 8, (1958), 26–31.

Kanatani, K.-I.: Distribution of directional data and fabric tensors. *International Journal of Engineering Science*, 22, 2, (1984), 149–164.

Kattan, P. I.; Voyiadjis, G. Z.: A coupled theory of damage mechanics and finite strain elasto-plasticityi. damage and elastic deformations. *International Journal of Engineering Science*, 28, 5, (1990), 421–435.

Krajcinovic, D.; Fonseka, G.: The continuous damage theory of brittle materials, part 1: general theory. *Journal of Applied Mechanics*, 48, (1981), 809.

Krajcinovic, D.; Srinivasan, M.: Dynamic fracture of concrete (1983).

Lemaitre, J.: Continuous damage mechanics model for ductile fracture. *Journal of Engineering Materials and Technology, Transactions of the ASME*, 107, 1, (1985), 83–89.

Mangipudi, K.; Onck, P.: Multiscale modelling of damage and failure in two-dimensional metallic foams. *Journal of the Mechanics and Physics of Solids*, 59, 7, (2011), 1437–1461.

Miehe, C.; Hofacker, M.; Welschinger, F.: A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Computer Methods in Applied Mechanics and Engineering*, 199, 45, (2010a), 2765–2778.

Miehe, C.; Welschinger, F.; Hofacker, M.: Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field fe implementations. *International journal for numerical methods in engineering*, 83, 10, (2010b), 1273–1311.

Moelans, N.; Blanpain, B.; Wollants, P.: An introduction to phase-field modeling of microstructure evolution. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, 32, 2, (2008), 268–294.

Murakami, S.; Ohno, N.: A continuum theory of creep and creep damage. In: *Creep in structures*, pages 422–444, Springer (1981).

Onck, P.; Andrews, E.; Gibson, L.: Size effects in ductile cellular solids. part i: modeling. *International Journal of Mechanical Sciences*, 43, 3, (2001), 681–699.

Qin, R.; Bhadeshia, H.: Phase field method. *Materials science and technology*, 26, 7, (2010), 803–811.

RADIOSS: *Version 11.0*. Altair Engineering Inc., Troy, Michigan (2012).

Reis, F. D.; Ganghoffer, J.: Discrete homogenization of architectured materials: Implementation of the method in a simulation tool for the systematic prediction of their effective elastic properties. *Technische Mechanik*, 30, (2010), 85–109.

Reis, F. D.; Ganghoffer, J.: Equivalent mechanical properties of auxetic lattices from discrete homogenization. *Computational Materials Science*, 51, 1, (2012), 314–321.

Rinaldi, A.; Placidi, L.: A microscale second gradient approximation of the damage parameter of quasi-brittle heterogeneous lattices. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*.

Siquieri, R.; Emmerich, H.; Jurgk, M.: Computation of solidification problems with hydrodynamic convection resolving energetic anisotropies at the microscale quantitatively. *European Physical Journal: Special Topics*, 149, 1, (2007), 27–41, cited By (since 1996)3.

Steeb, H.; Diebels, S.: Modeling thin films applying an extended continuum theory based on a scalar-valued order parameter.: Part i: isothermal case. *International Journal of Solids and Structures*, 41, 18, (2004), 5071–5085.

Steinbach, I.: Phase-field models in materials science. *Modelling and Simulation in Materials Science and Engineering*, 17, 7, (2009), 073001.

Steinmann, P.: Theory and numerics of ductile micropolar elastoplastic damage. *International journal for numerical methods in engineering*, 38, 4, (1995), 583–606.

Tekoğlu, C.; Onck, P.: Size effects in two-dimensional voronoi foams: a comparison between generalized continua and discrete models. *Journal of the Mechanics and Physics of Solids*, 56, 12, (2008), 3541–3564.

Voyiadjis, G. Z.; Kattan, P. I.: Damage mechanics with fabric tensors. *Mechanics of Advanced Materials and Structures*, 13, 4, (2006), 285–301.

Address: Prof. Dr.-Ing. Stefan Diebels, Dipl.-Ing. Alexander Geringer, Saarland University, Chair of Applied Mechanics, D-66123 Saarbrücken, Germany
E-mail: `s.diebels@mx.uni-saarland.de, a.geringer@mx.uni-saarland.de`