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Effective Dynamic Material Properties for Materials with Non-Convex Microstructures

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Abstract

Usually in homogenization, it is assumed that on the microscale inertia can be neglected. Here, contrary to these approaches, inertia effects are taken into account, leading to a frequency dependent microscopic behavior. Additionally to this effect, non-convex microstructures are treated. Under these micromechanical assumptions on the macroscopic scale a frequency dependent, i.e., viscoelastic and auxetic behavior is expected.
The numerical homogenization is performed using a Genetic Algorithm. The frequency dependent macroscopic material parameters are found for a frequency range from 0 up to 10^3 kHz. The system responses on micro- and macroscale show a good agreement for the considered frequency range.

1. Introduction

Nearly all common materials present a certain heterogeneous microstructure. The determination of macroscopic, effective properties of such microstructured materials is referred to as homogenization. The objective of the homogenization process is to find macroscopic properties of a homogeneous material which represents the behavior of the nonhomogeneous microstructure. The methodologies to evaluate the effective mechanical properties of heterogeneous materials have attracted attentions from many researchers. A comprehensive overview of different approaches is given in [1] or [2].

Many materials exhibit a cellular or foam-like structure in order to provide a certain amount of stiffness with minimal weight. Cork, for example, is a common cellular material having a closed-celled hexagonal (honeycomb) architecture. In addition to natural materials, man-made cellular structures are used in aerospace structures, composite plates, or other lightweight applications. Due to the increasing importance of these materials, several studies have been performed to evaluate their properties. The effective elastic properties of regular isotropic triangular grid structures as well as square cells have been analyzed by Gibson and Ashby [3] and Torquato et al. [4]. Analysis of more general grid structures were provided by Hohe [5] who uses an energetic concept for the homogenization process. A comprehensive state of the art publication on homogenization methodologies is given by Hohe and Becker [6].

For microstructures composed of beams, it has been postulated that non-convex shapes (with re-entrant corners) are responsible for a negative Poisson's ratio effect. Several authors have published papers concerning this effect which is also referred to as *auxetic* material behavior [7, 8].

Most publications on homogenization assume that the influence of inertia can be neglected on the microscopic level [1]. Only a few approaches have been published to study the effect of micromechanical inertia, e.g. [9,10].

In this paper, a dynamical homogenization approach is presented, where dynamical means that, contrary to other approaches, inertia effects on the microscale are not neglected. Hence, the micromechanic calculations are performed in frequency domain with harmonic excitations. Therefore, a frequency-dependent behavior is expected also on the macroscale. Accounting for this frequency-dependence, a viscoelastic constitutive law is applied on the macroscale. Since the viscoelastic constitutive law requires a number of parameters to be found, the homogenization is formulated as an optimization problem, i.e., 'Find macroscopic material parameters that describe the micromechanical behavior as good as possible'.

The paper is arranged in the following way. First, the calculation of the considered microstructure is elaborated. The constitutive equation to be used for the macroscopic scale is then presented in section 3. Section 4 deals with the Genetic Algorithm used for the optimization and, finally, an example is presented and discussed.

2. Calculation of the unit cell

Within this work, cellular solids are considered which consist of simple beams. Such structures are found quite often in the literature, because they can represent sandwich cores or simplified models of foam-like materials. It is assumed that the material is periodic, i.e., it consists of equally shaped cells. For sandwich cores, this assumption is well justified; real materials, of course, have an imperfect microstructure, where neighboring cells have a slightly different geometry. But, in order to calculate effective, homogeneous material properties, this model should be sufficiently accurate to represent the microstructure.

If the assumption of periodicity is made, it is very easy to find a representative volume element (RVE), because if the microstructure consists of identical units, the smallest unit contains all information and is therefore representative. If on the microscale the dynamic effects are neglected, i.e., a static model is used, effective properties can be calculated from this single unit cell. However, in a dynamic calculation in frequency domain one unit cell does not suffice to obtain representative results. The reason is that different modes of deformation (structural modes) may occur when using a different number of unit cells. This can be explained by considering the example given in Figure 1.

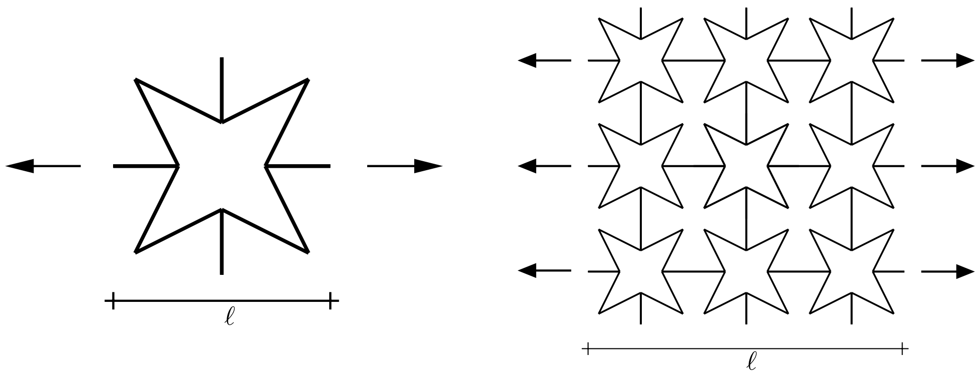

Figure 1: Example calculation of 1 and 3x3 unit cells

A unit cell is loaded with a force on the left and right hand side. The cell is calculated in frequency domain, i.e., the load is harmonic and thus, the resulting strain

$$\varepsilon = \frac{\Delta\ell}{\ell} \tag{1}$$

is also harmonic. Another calculation is done using 3x3 cells. Both strains are plotted over a frequency range of $0..10^6$ Hz in logarithmic scale in Figure 2.

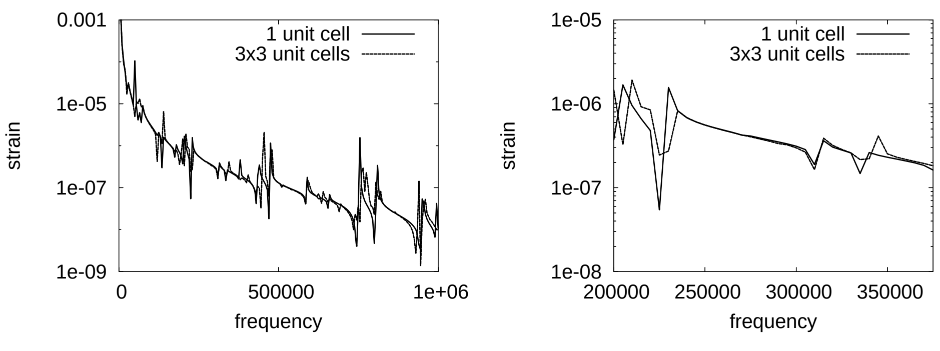

Figure 2: Strain of 1 and 3x3 unit cells

On the left hand side, the whole frequency range is plotted, whereas on the right hand side, only a small range is plotted. It can be seen that the results from both calculations are not identical. At approximately 3.4×10^5 Hz, an eigenfrequency is missing in the single unit cell calculation and at 2.3×10^5 Hz, the eigenfrequencies of both calculations are different. Therefore, it is necessary to calculate multiple unit cells to obtain characteristic microscale results. A simple and pragmatic approach is to calculate a specific number of unit cell and then average the results.

The frequency dependent response of the unit cell above as well as in the following is based on a frame model using the Timoshenko theory for the beams. This refined theory is used to take into account the shear deformation and the rotatory inertia which can not be neglected for higher frequencies [11]. Further, for the numerical model the Boundary Element Method for beams [12] is used because it solves the governing equations exactly, independent of the load, in contrast to a Finite Element model.

3. Macroscopic constitutive equation

Since inertia effects are taken into account on the microscale, the response of the unit cell is frequency-dependent. Thus, the effective properties on the macroscale must also feature a frequency-dependence. One of the easiest constitutive laws exhibiting a frequency-dependence is the linear viscoelasticity. The stress-strain equation of a linearly viscoelastic material can be expressed in the form [13]

$$\sum_{k=0}^{N} p_k \frac{d^k}{dt^k} \sigma_{ij} = \sum_{k=0}^{M} q_k \frac{d^k}{dt^k} \varepsilon_{ij} \,. \qquad (2)$$

In (2), M and N can have different values and must be adapted to the application, so their choice is somewhat arbitrary. Also, fractional derivatives may be used to better fit a larger frequency range [14].

In frequency domain, viscoelastic effects are described by complex moduli. Applying a Fourier-transformation on (2), the time dependence is replaced by a frequency dependence. In the present application, the constitutive equation

$$\sigma_{ij}(\omega) = \frac{E(\omega)}{(1+\nu(\omega))} \varepsilon_{ij}(\omega) + \frac{\nu(\omega)E(\omega)}{(1+\nu(\omega))(1-2\nu(\omega))} \delta_{ij}\varepsilon_{kk}(\omega) \qquad (3)$$

is chosen. For the Young's modulus, the viscoelastic model

$$E(\omega) = \overline{E}\, \frac{1+q_1(i\omega)^{\alpha_1} + q_2(i\omega)^{\alpha_2}}{1+p_1(i\omega)^{\alpha_1} + p_2(i\omega)^{\alpha_2}} \qquad (4)$$

with fractional derivatives and 7 parameters is used. The same model but with possible different parameters is used for the Poisson's ratio

$$v(\omega) = \bar{v}\,\frac{1+\tilde{q}_1(i\omega)^{\tilde{\alpha}_1}+\tilde{q}_2(i\omega)^{\tilde{\alpha}_2}}{1+\tilde{p}_1(i\omega)^{\tilde{\alpha}_1}+\tilde{p}_2(i\omega)^{\tilde{\alpha}_2}}\,. \qquad (5)$$

Again, the choice of these models is somewhat arbitrary. For the considered frequency range, they have shown to be sufficient. A number of trials with fewer parameters were not successful, as well as models with more parameters, yet without fractional derivatives. Note that in the above equations a special indication of the Fourier transform is skipped for the sake of brevity.

4. Homogenization using a Genetic Algorithm

The connection between the material behavior on the microscale and the macroscale is referred to as homogenization. The aim is to ’replace’ the heterogeneous microstructure by a homogeneous material which describes the material behavior at the macroscopic level correctly. Here, the homogenization is formulated as an optimization problem, i.e., ’Find material parameters on the macroscopic scale which describe the micromechanical behavior as good as possible’. Contrary to the static case where the homogenization is performed analytically, the consideration of dynamic effects on the microscale makes it necessary to use an optimization algorithm. There are too many unknown parameters in the macroscopic constitutive equation to perform an analytical homogenization.

As optimization procedure, a Genetic Algorithm is used, although the problem could as well be solved by other soft computing techniques, e.g., neural networks, or with conventional gradient-based procedures. As expected from the literature, tests have shown that the Genetic Algorithm is the robustest (but slowest) technique. Genetic Algorithms are stochastic search algorithms based on the mechanisms of nature selection and natural genetics. At the beginning of the algorithm, a population made up of a discrete number of individuals is generated. One individual corresponds to the solution of a problem, and consists of an array of gene values. Just as in nature, the individuals are optimized for their environment by successive modification over a number of iterations. In each iteration or generation, the algorithm evaluates, selects, and recombines the members of the population to produce the succeeding generation.

Evaluation of each individual which encodes a candidate solution is based on a fitness function. This function is used to select the relatively fitter individuals, i.e., the individuals with the best fitness value. The selected individuals form the parent generation, and they produce offspring by rules like mutation, crossover, or gene replacement (for details, see [15]). The algorithm stops after a specified number of generations or if a certain fitness value is obtained for the best individual.

In the present application, one gene corresponds to the value of a material parameter p_k or q_k and the whole set of parameters corresponds to one individual. As fitness function, the square difference between the microscopic and macroscopic system response is used. The differences are summed up over the considered frequency range. If a harmonic strain is applied on the unit cell, the minimization function reads

$$f = \sum_{\omega_{start}}^{\omega_{end}} (\sigma^{micro}(\omega) - \sigma^{macro}(\omega, p_k, q_k))^2 \to 0. \qquad (6)$$

In (6), the stress $\sigma^{micro}(w)$ must be calculated only once, whereas $\sigma^{macro}(w)$ is calculated for each new individual of the population via equation (3), using new gene values of p_k and q_k. In principle, the procedure can be inverted, i.e., stresses can be applied on the cell and the strain response on the macroscopic scale can be optimized. It should be mentioned that in the proposed algorithm a surface averaging is used to determine the effective data.

5. Numerical example

Effective properties for a wide frequency range are determined for both auxetic and non-auxetic microstructures in this section. The following two microstructures given in Figure 3 are used for the numerical study.

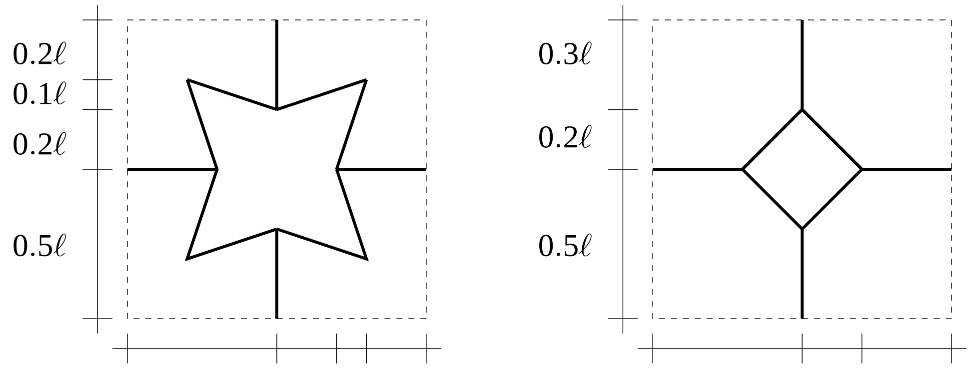

Figure 3: Auxetic and non-auxetic microstructures

Both cells consist of beams with a quadratic cross section of $0.1\ell \times 0.1\ell$. The microstructure material is PMMA with a slight damping. The material data were measured at the PTB (Physikalisch-Technische Bundesanstalt) in Braunschweig.

A frequency range from 0 up to $3 \cdot 10^3$ kHz is chosen. Due to the existence of higher eigenmodes for more than one unit cells (see section 2), multiple microstructures are included in the representative volume element, following recent approaches [10,16,17]. Calculations were done for 1,2x2,...,5x5 unit cells and the results were averaged. The load case for both cells is given in Figure 4. A displacement amplitude

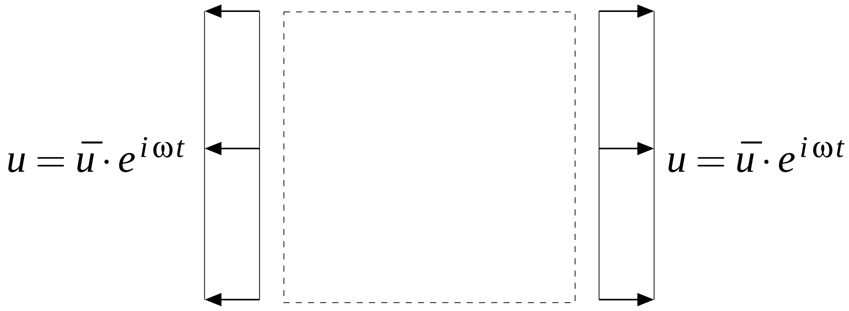

Figure 4: Load case

is applied on the left and right hand side of the cell.

As mentioned above a Genetic Algorithm is applied here to solve the optimization problem (6). The following parameters were used to determine the material parameters:

- A population size of 1000 individuals is chosen
- The starting population is created randomly
- New individuals are created via 2-point-crossover
- The mutation of an individual is done according to the standardized normal distribution, with a mutation probability equal to 10%
- 150 individuals are created newly in every generation, the remaining 850 are created as offspring of the previous generation
- The optimization is stopped after a maximum of 50000 iterations or if the best fitness value $f<10^{-5}$.

The results of the optimization are depicted in the following Figures. Figures 5 and 7 show the Young’s modulus and Poisson’s ratio for the auxetic microstructure, while in Figures 6 and 8 Young’s modulus and Poisson’s ratio for the non-auxetic microstructure are shown. In each diagram, the microscopic and macroscopic results are plotted versus the frequency.

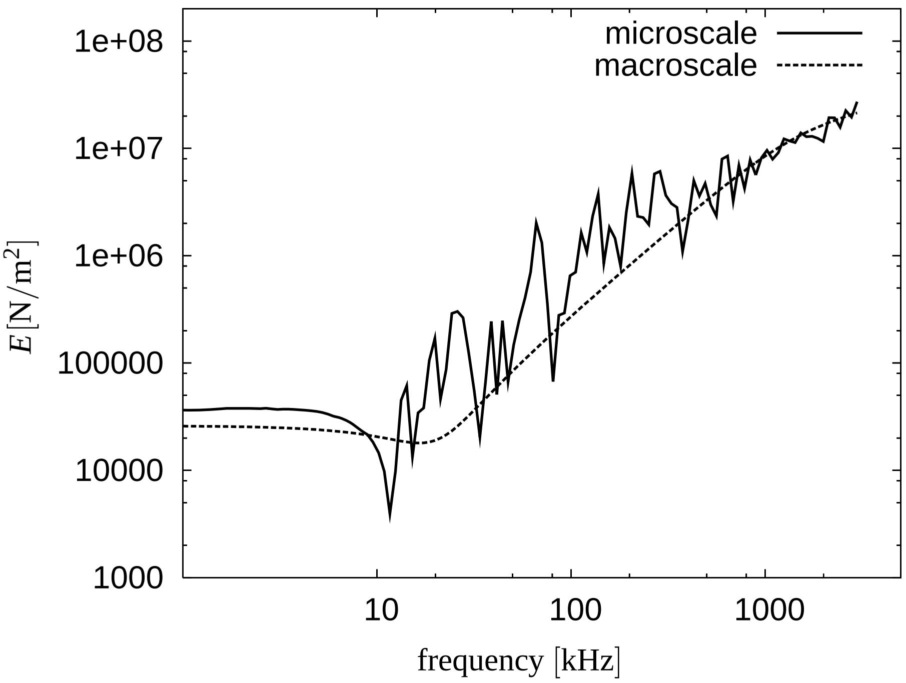

Figure 5: Young's modulus for auxetic microstructure

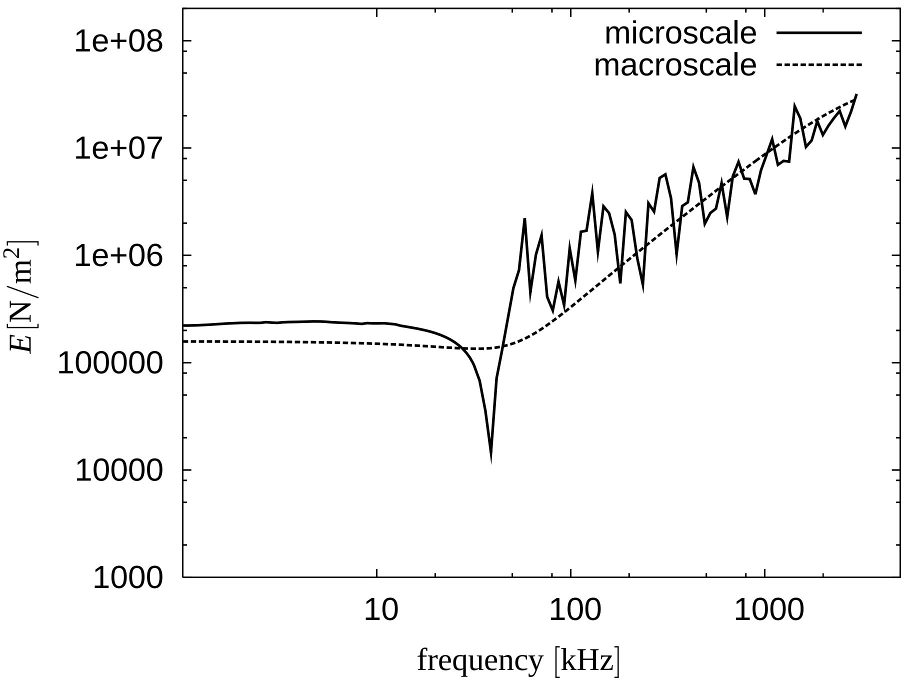

Figure 6: Young's modulus for non-auxetic microstructure

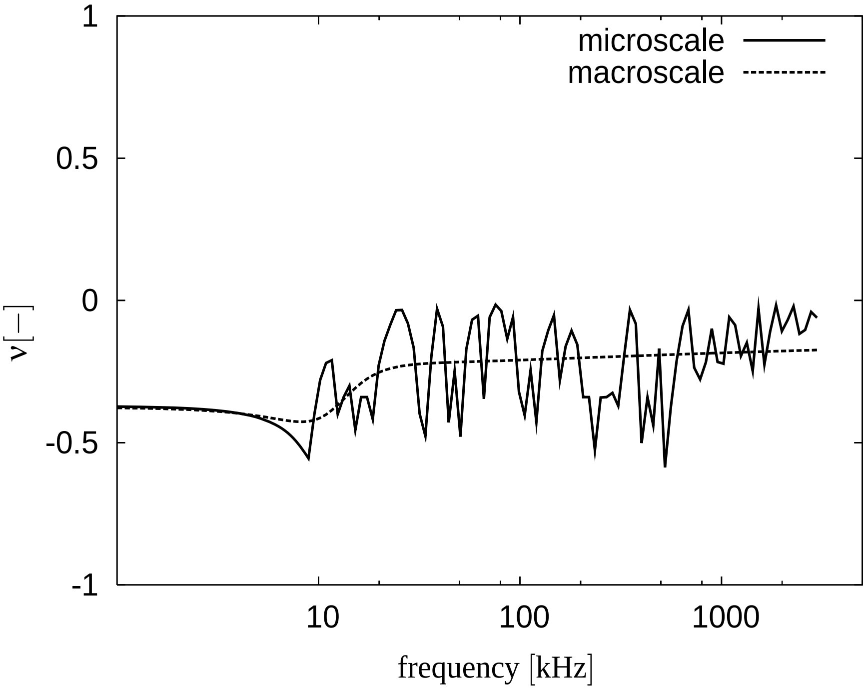

Figure 7: Poisson’s ratio for auxetic microstructure

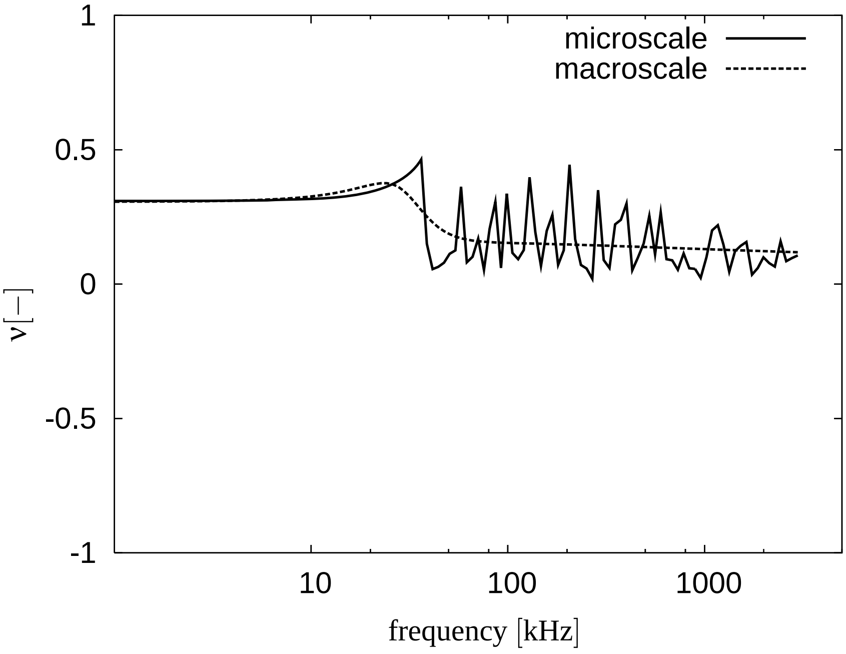

Figure 8: Poisson’s ratio for non-auxetic microstructure

As it can be seen, the optimization was not able to fit each single eigenfrequency of the microstructure results. However, the general tendency is preserved. In all four result plots, it can be seen that for small frequencies, the fitted parameters converge into the static solution. The obtained material parameters for ν and E are given in Table 1 for the auxetic microstructure and in Table 2 for the non-auxetic material.

Table 1: Obtained material parameters for auxetic material

Young's modulus				
k	$\bar{E}$	p_k	q_k	α_k
1	2.560×10^{4}	2.358×10^{-6}	1.842×10^{-8}	1.057×10^{0}
2		2.432×10^{-8}	1.448×10^{-12}	1.099×10^{0}
Poisson's ratio				
k	$\bar{\nu}$	$\tilde{p}_k$	$\tilde{q}_k$	$\tilde{\alpha}_k$
1	-0.376	4.995×10^{-8}	1.598×10^{-8}	1.497×10^{0}
2		1.534×10^{-8}	1.162×10^{-7}	1.335×10^{0}

Table 2: Obtained material parameters for non-auxetic material

Young's modulus				
k	$\bar{E}$	p_k	q_k	α_k
1	1.581×10^{5}	1.057×10^{-6}	2.666×10^{-8}	1.057×10^{0}
2		1.448×10^{-12}	1.856×10^{-8}	1.389×10^{0}
Poisson's ratio				
k	$\bar{\nu}$	$\tilde{p}_k$	$\tilde{q}_k$	$\tilde{\alpha}_k$
1	0.307	1.869×10^{-11}	1.407×10^{-8}	1.424×10^{0}
2		5.147×10^{-9}	8.443×10^{-10}	1.573×10^{0}

The slightly viscoelastic material on the microscopic scale had virtually no effect on the homogenization process. There were still eigenfrequencies on the microscale which make the search of the material parameters very difficult.

For the optimization, it can be observed that there is no difference whether an auxetic or non-auxetic microstructure is used as input data. This could have been expected à priori, because the same mathematical problem (with slightly different parameters) needs to be solved by the optimization procedure.

6. Conclusions

In this paper, a dynamical homogenization for a periodic, auxetic material consisting of simple beams was performed. Due to inertia effects on the microscale, the behavior of the unit cell is frequency dependent. Thus, a viscoelastic constitutive law had to be applied on the macroscale, requiring an optimization procedure for the homogenization process. The Genetic Algorithm used for the homogenization was able to find adequate material parameters on the macroscale. For the identified material parameters p_k and q_k, however, no plausibility check was yet made concerning thermodynamic restrictions. Therefore, further investigations have to be carried out assuring the correctness of the found values, i.e., setting thermodynamic constraints for the optimization problem.

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