GENERATING NON-PERIODIC MICROSTRUCTURES OF FIBER COMPOSITES

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Mathematical modeling of composite materials leads to the solving PDEs with strongly oscillating coefficients. The problem of large number of equations can be solved using homogenization, that replaces heterogeneous material by an 'equivalent' homogeneous one. This approach assumes periodic structure, which is not often true in reality. The first aim of the paper is to compare results obtained by solving the model problem describing the torsion of a bar applied to the random medium and the the periodic one, respectively. The second aim is to present four algorithms generating samples of random structures of a two-component fibre composite material similar to the real one.

Keywords: *non-periodic structures, homogenization, spatial processes, spatial randomness*

1. Introduction

Fiber composite materials consist of at least two different phases, particularly two-phase fiber composite material consists of the so called stiffening phase in the shape of fibers included into the second one, called matrix. By various distribution of inclusions we can develop materials with special properties and that is the reason, why they are intensively used in many branches of engineering e.g. automobiles, aircraft, space vehicles and many others. From a design point of view, and in strong contrast to metallic materials, we largely lack a rational philosophy based on mechanics, mathematics and physics for a prediction of a damage initiation, propagation and final failure of constructions made out of such material. Classical approaches which use a continuum description will ultimately fail in predicting long-term structural degradation of composites, because this process is deeply influenced by micromechanical events, caused by a random structure.

Solving of boundary-value problems modeling the behavior of composite materials is very demanding since we have to solve PDEs with highly oscillating coefficients, which leads to the solving too many equations.

Let us remind a mathematical method called homogenization for solving the problem. Adopting the assumption of periodic structure of the material, this method enables to compute its effective parameters from the knowledge of properties of the phases and their geometric distribution.

Real composite materials do not have periodic structure–the distribution of the fibres in the matrix is not periodic, see e.g. [1].

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We introduce four algorithms for generating samples with random structure i.e. random distribution of fibres of non-constant diameters. Many algorithms generating random structure are based on the so-called 'spatial point-processes', see e.g. [5], [13] or [11]. In our paper we introduce algorithms to work with non-constant diameter fibres.

The content of the paper is as follows. We start with a characterization of two-phase composite materials and describe periodic and random structures of composites. In Section 3 we set up the model problem. In Section 4 we show results of numerical simulations for a stress of both periodic and non-periodic material. A Section 5 deals with the comparisons of random and periodic samples.

A periodic unit cell (PUC) is introduced in Section 6. The developed algorithms will be presented in Section 7 and in the Section 8 we arrive to the conclusion.

2. Composite Material Considered

For our experiments we shall use a two-phase carbon–epoxy (C/E) composite material – epoxy matrix reinforced by very hard carbon fibres. We assume circle–shape fibres. According to [1] we choose a normal distribution of the fibre diameters with expected value of the diameter $6.78\,\mu$m, a standard deviation $0.38\,\mu$m and the volume fraction $56.5\,\%$. In our experiments we adopt these characteristics of the composite materials. Detailed analysis of real composite materials obtained from the microscope and CCD camera can be found in [1]. The corrected photograph of the real sample of this material we can see in the figure 1. The photograph is taken from [1].

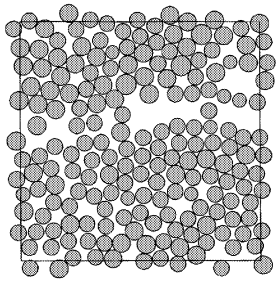


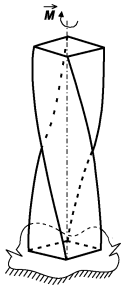
Fig.1: Real sample of the composite material taken from [1]

3. Model Problem

We shall make computer simulation for the following boundary value problem. We will assume that linear elasticity is sufficiently accurate for our purposes and that the material properties of the matrix and the fibres are accurately known. Of course this is not true in the reality, especially for the fibres. Nevertheless it is possible to assume that sensitivity (of the goals of our analysis) to this uncertainty is much smaller than to the uncertainty in the residual stresses of the composites. Let us consider a square-shaped domain and the elliptic partial differential equation

$$-\sum_{i=1}^{2} \frac{\partial}{\partial x_i}\left(a(x)\,\frac{\partial u}{\partial x_i}\right) = 2\,\alpha \quad \text{in} \quad \Omega\,,$$

$$u = 0 \quad \text{on} \quad \partial\Omega\,,$$



with non-constant periodic coefficient $a(x)$ with a small period ϵ. According to the generated samples, $a(x)$ will take value λ in the circles and value 1 in the complement.

This model problem can be interpreted as follows. Let us consider a bar made of a composite material reinforced with fibres. The square cross-section of the bar is the domain Ω shown in the previous section, the circles mean the fibres. The bar is fixed on one side and screw on the second side.

The described situation leads to the well known (see [10]) problem of linear elasticity called 'torsion of a bar'. The model has the form of the boundary value problem for elliptic partial differential equation, formulated above. The coefficient $a(x)$ takes the value of inverse value of shear-modulus of each phase. The solution $u(x)$ is the Prandtl's potential function. It gives the only non-zero skew components of the strain tensor σ_{ij} by the formulas

$$\sigma_{13} = \sigma_{31} = \frac{\partial u}{\partial x_2} \ , \qquad \sigma_{23} = \sigma_{32} = -\frac{\partial u}{\partial x_1} \ .$$

From the practical point of view we are not interested in values of Prandtl's function, but in its gradient magnitude which gives us information about the strain:

$$|\nabla u| = \sqrt{\left(\frac{\partial u}{\partial x_1}\right)^2 + \left(\frac{\partial u}{\partial x_2}\right)^2} \ .$$

In Figure 2 we show the periodic and random structures.

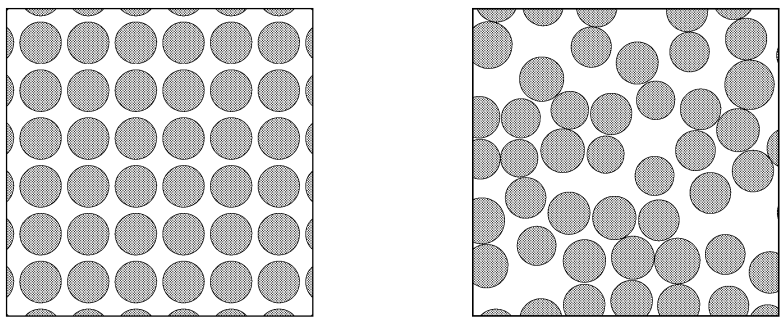


Fig.2: Periodic sample (left) and random sample (right)

The size of each sample is $50\,\mu\text{m} \times 50\,\mu\text{m}$. The density and the number of fibres in the case of periodic sample were chosen such that the volume fraction is the same as in the simulated samples. The value of volume fraction is 56.5 % and the number of fibres is 39.07. The diameter of fibres in the periodic sample is the expected value of random ones, i.e. $6.78\,\mu\text{m}$, see [1]. According to [B], [BL], [Fr1], [Fr2] we took for the demonstration the values of the coefficient $a(x)$ as follows:

$$a(x) = \begin{cases} 1 & \text{for a matrix} \ , \\ \frac{1}{114} & \text{for a fibre} \ . \end{cases}$$

We computed solutions for this boundary-value problem. For computations the finite element method with a finite triangle-shaped element was used. We looked for the solution in

the form of piecewise linear function i.e. first order polynom on each triangle. The triangulation was very fine (about 20000 elements) to obtain solution as accurate as possible.

4. Numerical Simulations

In this section we present solutions for both periodic and random media. We compute the homogenized solution for the periodic sample. Since the structures of computed samples are different, the pointwise comparison of gradients is meaningless. Therefore for each solution a diagram showing volume distribution of gradient magnitude was created.

In the following figures the solution and distribution of its gradient magnitude for the periodic sample is shown.

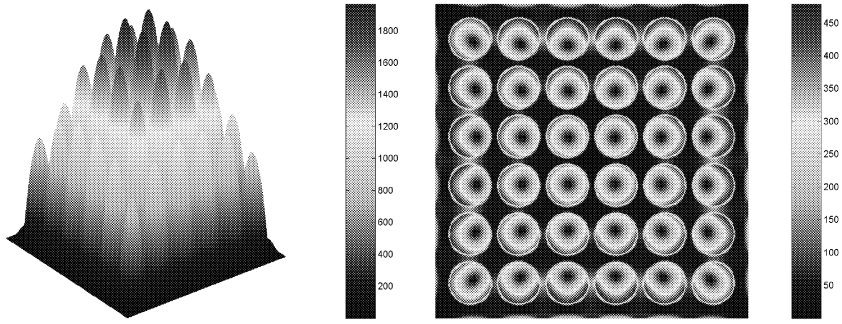


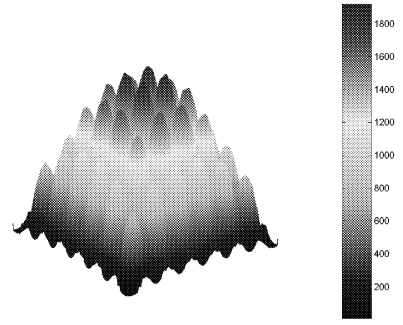
Fig.3: Prandtl's potential function (left) and gradient magnitude diagram (right) for the periodic sample

Let us mention that in the case of the periodic material all characteristics are symmetric, i.e. the solution, gradient magnitude and its distribution in the sample.

Now, we present the results obtain by homogenization theory for the periodic sample.

We start with the homogenized solution with the constant coefficient a_0, whose value was computed using homogenization theory, see e.g. [2], [3], [4]. Its value is $a_0 = 0.2402$. Let us remark that averages yield bad values: the arithmetic mean is 0.5044 and the harmonic one is 0.0174.

The homogenized solution has no local peaks which is due to the constant coefficient, while the solution to the periodic problem has peaks on the interface of the phases. Homogenization theory solves the problem by correctors, see [2], [3], [4], [6] or [7]. The homogenized solution with the second corrector approximates the periodic solution better, it approximates even the local peaks as can be seen on the neighbouring figure. Since the so called cut-off functions were not used, the approximation close to the boundary is not so good.



In the case of random media, due to lack of symmetry in the random structure both solution and its gradients are not symmetric. The behavior of the solution and gradient magnitude for the random media we can see in the next figure.

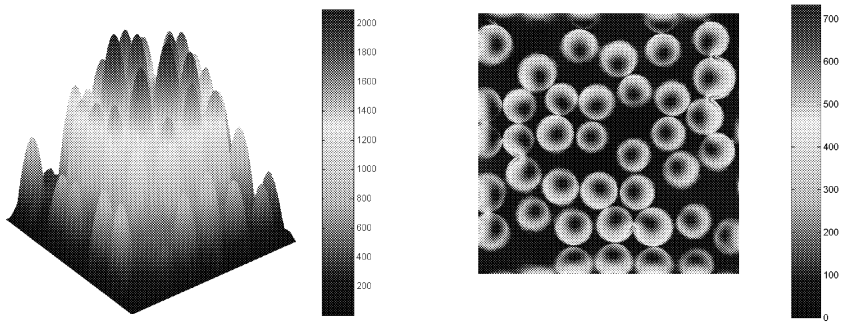


Fig.4: Prandtl's potential function (left) and gradient magnitude diagram (right) for the random sample

5. Comparisons of solutions

We compare solutions of a model problem for twenty random samples and for 'equivalent' period one.

5.1. Comparison of effective values—homogenized coefficients

For the periodic sample, the homogenization theory yields the homogenized coefficient a_0 which serves as an effective value. To compare it with the random samples we need to find its counterpart. For the random sample with non-periodic distribution the effective value will be computed as follows.

Since the homogenized problem depends linearly on the coefficient, the solution with a coefficient a_k is an a_k multiple of the solution with the coefficient 1. Thus by the least square method we can approximate the solution u_n of the simulated random sample by a multiple of solution u^* of the problem with constant coefficient 1.

$$-\Delta u^* = 2 \quad \text{in} \quad \Omega \,,$$
$$u^* = 0 \quad \text{on} \quad \partial\Omega \,.$$

More precisely for each random sample ($n = 1 \dots 20$) with solution u_n we minimize

$$\|u_n - u_{0n}\|^2 \to \min \ ,$$

where u_{0n} is the solution of the problem with constant coefficient a_n. Since $u_{0n} = a_n\, u^*$ replacing the norm by the sum of nodal differences, we obtain standard least square problem for value a_n.

The arithmetic average of all twenty values a_n for non-periodic samples is equal to 0.2123. For the periodic sample, we obtain value 0.2280. The homogenized coefficient a_0 computed by homogenization theory is 0.2402. Thus the average value 0.2123 is $88\,\%$ of the homogenized coefficient a_0 and for the periodic sample it is $95\,\%$. The difference between these two values is $7\,\%$ which can be taken as acceptable; for higher number of fibres the difference will be smaller.

5.2. Comparison of gradients

We have computed exact solutions for twenty random sample problems and to the 'equivalent' periodic one. Since every generated sample is of different structure, a pointwise comparison of gradients is meaningless.

Next figure shows behavior of a strain (gradient magnitude) in matrix and fibres. The dashed shadow curves denotes strain in the random material (the arithmetic average of twenty samples) and the black ones refer to the material with a periodic structure.

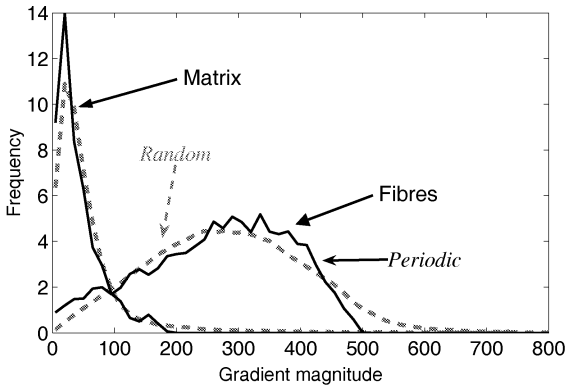


Fig.5: Curves of strain in periodic and random samples

The curves for random and periodic samples exhibits different behavior. Maximum value in the case of periodic sample is about 500, while in the case of random samples they are about 800. Fibres, which are nearest to the edge of the sample are much more stressed than the ones in the middle of the bar. The maxima are also influenced by a distance between neighboring fibres. Thus it is very important to keep minimum distance of neighboring fibres not close to zero, particularly to avoid contact of fibres in the material from the practical viewpoint.

From the preceding it follows, that omitting real, i.e. non-periodic structure of the material structure leads to the incorrect result. This fact was demonstrated in the previous example in the problem of the torsion of a bar. Therefore, studying and analyzing random structures has its right meaning.

6. Periodic Unit Cell

Due to the complexity of the microstructure, the analysis is usually left to rely on incomplete geometrical information about the composite microstructure. The problem is not successfully resolved even when considering a large sample of composite.

An essential ingredient of the present model applicable to both elastic and inelastic problems is a carefully selected material representative volume element (RVE) replacing

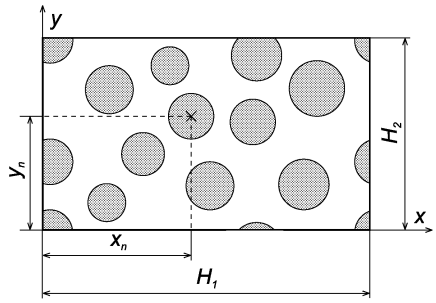


Fig.6: Geometry of the periodic unit cell

the real microstructure. Such a RVE is represented here by a periodic unit cell (PUC) consisting of a small number of particles–fibres, which statistically resembles the actual structure of a studied composite material. For an early study on this subject we refer the reader to [13] and references therein. Consider the periodic unit cell consisting of N particles. The geometry of such a unit cell is determined by the dimensions H_1 and H_2 and x and y coordinates of all particles. The principal problem is to select these values in such a way that material formed by this periodic unit cell is as much similar as to some given original microstructure as possible. In the following figures we can see examples of the PUCs. From the previous pictures it is clear that determination of a PUC, which is statistically equivalent to the original microstructure, is not trivial. The process of finding a PUC is described e.g. in [13] and is out of scope of this paper.

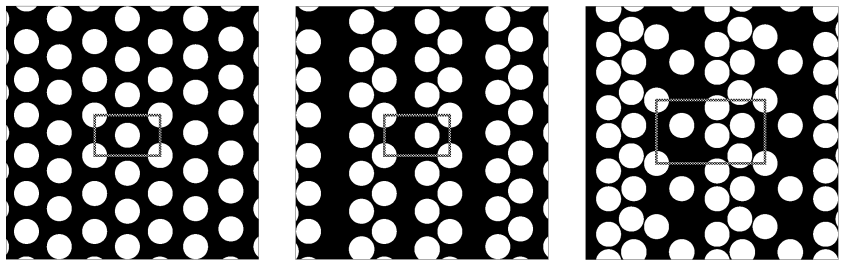


Fig.7: Periodic unit cells: Hexagonal lattice (left), 2-fiber PUC (middle) and 6-fiber PUC (right)

7. Random Structures

For our experiments we come from the data obtained from Czech Technical University in Prague, Klokner Institute, Department of Engineering Mechanics – those are bitmaps of a dimension 1144×1144, see figure 8. From the analysis of this data, we chose normal distribution of the fibre diameters with expected value of the diameter 71.87242 and standard deviation 4.57858 . The average amount of the fibres in selected rectangular area was 164.6 and the average volume fraction 48.69 %. In our experiments we adopt these characteristics of the composite material. Detailed analysis of real composite materials obtained from the microscope can be found in [8]. In the following figures we can see an example of the obtained data and corrected ones used to the experiments.

Having the set of bitmaps of the real composite media, it is desirable to have a tool for generating random structures that will be statistically similar to the real ones. The reason is to be able to extract from such simulated structures an adequate PUCs that will be used for the next computations.

The theory of spatial point processes is at present studied very deeply and intensively and it creates quite large branch of the statistics and probability theory. As an example let us mention the scope of its application: astronomy, engineering and building industry, textile industry, agriculture and geographics (geostatistics). In the literature are nowadays described many algorithms generating spatial point processes. Among point processes applicable to simulating random structure similar to the real one belong so called Hard-Core Models (i.e. Matérn's Model I, Matérn's Model II, Matern-Stoyan Model or Matern-Bartlett Model), see [5] for detailed description.

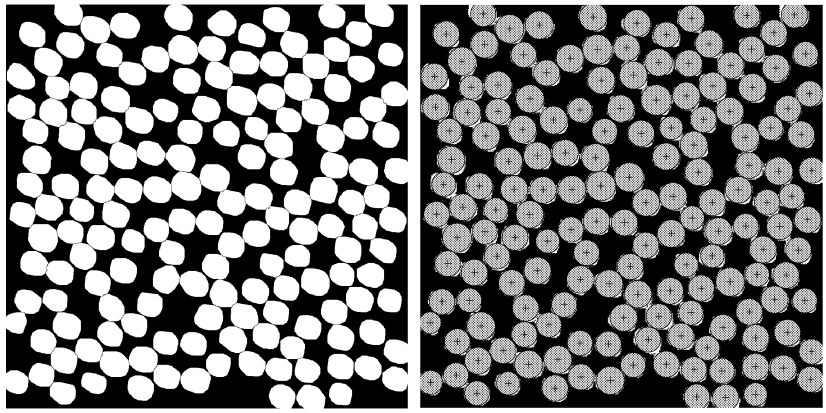


Fig.8: Real sample (left) and its correction for computation (right)

Now we describe four algorithms developed for the purpose of generating random structure similar to the real one and after that we compare this algorithms from the statistical viewpoint in the next paper.

7.1. Algorithm A1

The main idea of this algorithm is based on a stochastic process $S(t,\omega)$, whose separate trajectories have a character of a *'wavy-random sinusoid curve'*. In other words, they have different amplitudes and periods. The process is in the shape

$$S(t,\omega) = \sum_{n=0}^{K} \sin\left(\frac{(2n+1)\,\pi\,t}{2\,T}\right)\xi_n(\omega)\ ,$$

where $\{\xi_n\}_{n=1}^{\infty}$ is a sequence of mutually independent random variables having normal distribution with zero mean and unity variance, T is the length of the interval, over which we generate this process and K is the number of members we want to sum up (the higher K is, the more 'noisy' the trajectories are). This process is a modification of a Karhunen-Loève expansion of the Wiener process (Brownian motion), see [KPS] for additional information.

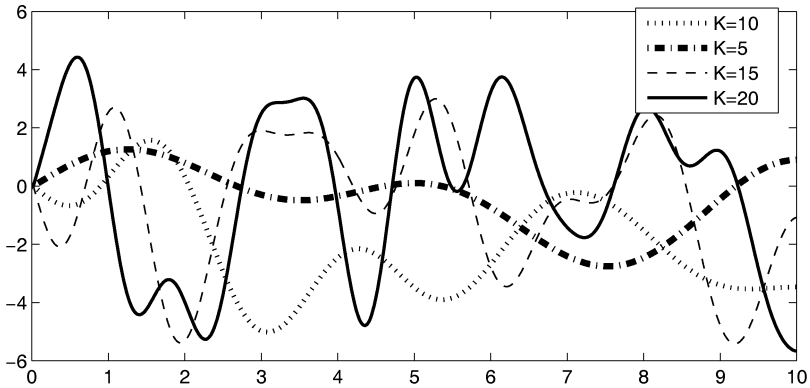


Fig.9: Trajectories of a stochastic process $S(t,\omega)$ for different K

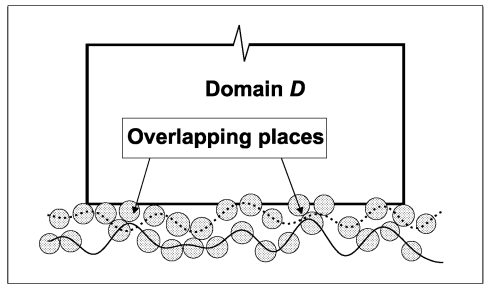


Fig.10: To the description of the algorithm

Let D be a domain, representing our sample, into which we want to place fibres with random diameters corresponding to the established distribution of the real samples.

A detailed procedure can be described in several steps. In the bottom of the following picture there is a solid curve which forms the centers of the fibres with random diameter. This solid curve was received by means of one realization of the stochastic process $S(t, \omega)$ with $K = 3800$. During putting the fibres on the line we also have to check overlapping of the fibres. After the solid line is filled we continue with a dashed one, which is generated in the same mean as the solid one, but is shifted up. Again, the fibres are placed to the line and checked with existing ones. In the case of overlapping(the arrows in the figure) they are shifted to the 'safe' distance. In this way we continue until the whole domain D is not filled up.

In the next figure there is finished a resulting structure of a two-phased fibre composite material according to the algorithm **A1**. By a different choice of a number K in the expansion of the stochastic process $S(t, \omega)$ we change an amplitude and period of a curve. This fact causes, that we are able to generate structures with various volume fraction and number of fibres in a sample. Of course, it is possible to set a minimum distance between two fibres. By means of this algorithm, fifteen samples were generated for the purpose to the next computations. It is important to note, that the centers of the generated fibres lies in the domain D. In other words it means that the fibres in the figure 10 are not included for further computations. This fact causes the so called *edge-effects*. Next we note, that this fact is fulfilled also in the next algorithms. To the theory of the so called *edge correctors* we refer to [1], [5] or [13].

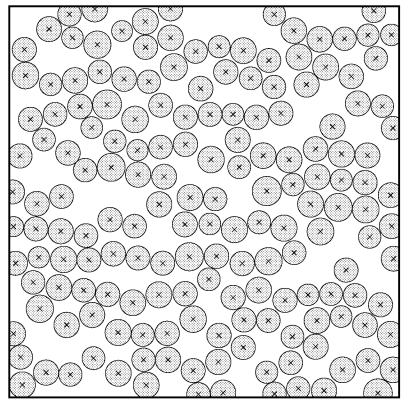


Fig.11: The final structure generated by the algorithm **A1**

7.2. Algorithm A2

The principle of this algorithm we can describe as follows: Firstly, we generate one fibre with random diameter and situate it approximately in the middle of the domain sample. Then we choose a random direction and a distance, where we put a new fibre. This procedure is repeated until the resulting volume fraction does not reach the requested one. During every step we are checking whether a new fibre does not cross the existing ones. In case of overlapping fibres, new position is generated. For the better illustration and result, see the following pictures.

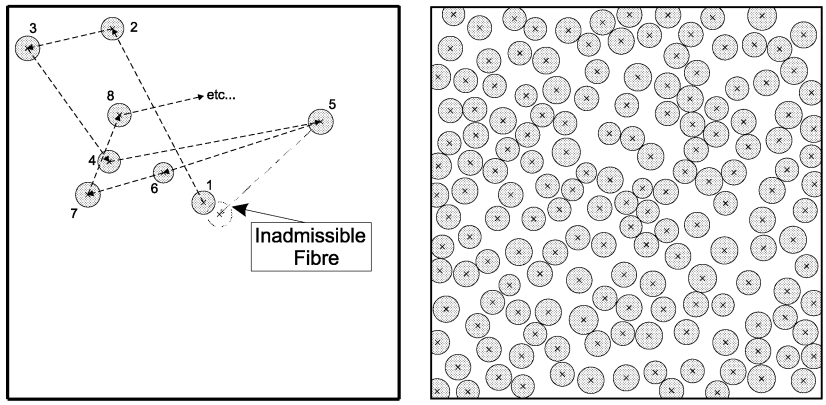


Fig.12: To the description of the algorithm **A2** *(left) and the final structure generated by the algorithm* **A2** *(right)*

7.3. Algorithm A3

It is based on the Brownian motion of the suspended particles in a liquid medium. The simulation starts with generating a sample with complete periodic structure, i.e. constant diameters of fibres and the same distance between them. The diameter must be chosen in such a way, that the resulting volume fraction has the same value as in the real samples. After such a structure is generated, the diameters of all fibres are changed according to the

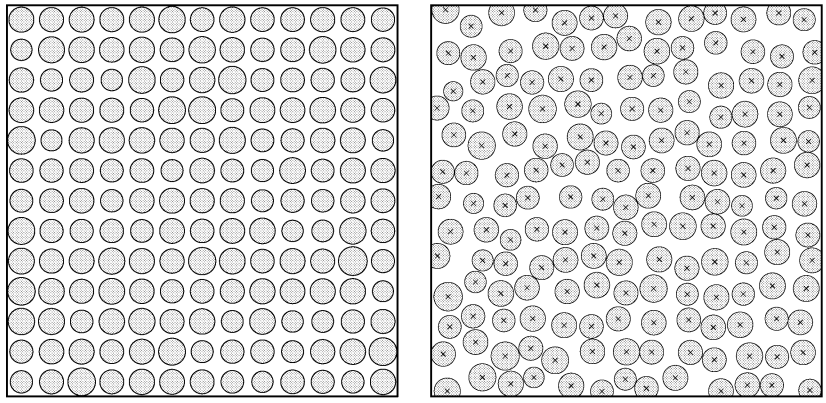


Fig.13: To the description of the algorithm **A3** *(left) and the final structure generated by the algorithm* **A3** *(right)*

distribution of real samples. In a next step each fibre is submitted to the Brownian motion. In other words, we choose a random direction and distance of shifting a fibre. Simultaneously we check for the crossing with neighboring fibres and the minimum distance between them. If it occurs, we change the direction and the distance and the process is repeated. This is repeated until everything is all right. It is important to note, that generated amplitude of vibrations are in tenths of fiber's diameter, so they are relative small. This fact corresponds to the real concept of the Brownian motion, but we do not consider the collisions of particles and transmitting their quantity of motion during collision of one particle into another one.

7.4. Algorithm A4

The principle of this algorithm is similar to the algorithm **A3**. The difference is in processing overlaying of fibers: if the deflection of the fibre will cause overlaying with neighboring fiber, the shifting is canceled – the fiber stays in its old position. It causes, that the final structure is not so random as in the case of algorithm **A3**, but the computing time is several times shorter. The only disadvantage of algorithms **A3** and **A4** is in a fact, that the amount of fibres is the same for all samples.

We have to note that in each of the previous algorithms, the diameters of the fibres are distributed according known probability distribution. The resulting distribution agrees with normal distribution $\mathrm{N}(71.87; 20.96)$.

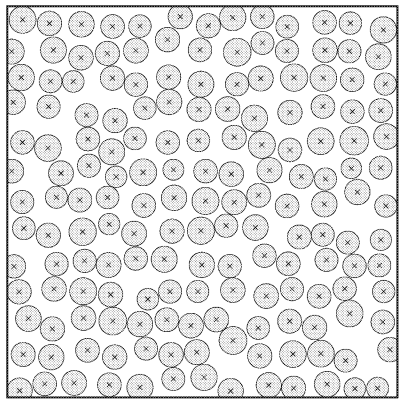


Fig.14: The final structure generated by the algorithm **A4**

8. Conclusion

The first aim of this contribution was to find out, whether we do an error, if we replace a random distribution of fibres with non-constant diameter in a two-phased composite material by a periodic distribution of fibres with constant diameter. This comparison carried out for the model problem in the form of the elliptic PDE $-\operatorname{div}(a\nabla u) = f$ with a random coefficient a and homogeneous Dirichlet boundary condition. The problem we can interpret as a torsion of a bar.

To do this we computed solutions with non-periodic distributions of fibres for twenty different samples. The resulting values of gradient depend on the positions, distance and diameters of fibres.

For comparison we computed the same problem for an 'equivalent' periodic sample using the homogenization theory. The differences of the 'effective values' (homogenized coefficients) for random and periodic case were not large and can be neglected. The influence of a random material to the homogenized coefficient a_0 is small. In the periodic case the homogenization results yield a good approximation, especially when the second corrector was used even the local peaks were approximated well.

But on the other hand, the results show that replacing random material by a periodic one cause big statistic deviations during approximation of strain-peaks. For gradient magnitude of solutions the corresponding diagrams shows significant differences, in random cases the maximum is much more higher. In practice it can cause dangerous severe destruction of the material. Thus for estimating local peaks we cannot neglect non-periodicity of the material. For the mathematical modeling taking material to be periodic brings significant errors. From the preceding it follows that it has the right meaning to deal with algorithms generating random structures similar to the real ones as most as possible.

According to this, four different algorithms **A1**–**A4** were developed. The algorithms were designed in such way in order to generate samples to be very similar to the real structures. The real samples (bitmaps) were obtained from the Czech Technical University in Prague, Klokner Institute. Then, fifteen samples are generated for each of the algorithm.

Finally, very interesting and challenging topic is the deeper analysis of the algorithms generating random structures as the real one. It is conditioned by having to disposal real samples, resp. bitmaps of them. It would be suitable to include to the algorithms such parameters, that will be able in some ranges influence the final structure to the reason of the best fitting of the real one.

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