

Article

Homogenization of Polymer Composite Materials Using Discrete Element Modeling

Andrey A. Zhuravlev, Karine K. Abgaryan, Alexander Yu. Morozov * and Dmitry L. Reviznikov

Federal Research Center “Computer Science and Control” of the Russian Academy of Sciences, Vavilov St. 44, 119333 Moscow, Russia; zhuravlyow.andrei@yandex.ru (A.A.Z.); kristal83@mail.ru (K.K.A.); reviznikov@gmail.com (D.L.R.)

* Correspondence: morozov@infway.ru

Abstract

A multiscale approach to calculating the effective elastic properties of a composite material with a fibrous filler and a polymer matrix is presented. Modeling at various scales is performed using a unified algorithmic scheme, solving Cauchy problems for systems of ordinary differential equations. At the atomic level, molecular dynamics modeling is used to calculate the elastic constant tensor of the polymer material. At the mesoscale, the author’s discrete element method is applied to calculate the effective elastic properties of the composite material. The method was tested on problems with regular fiber placement with symmetry, which have an analytical solution. The capabilities of the proposed approach are demonstrated using defect composite homogenization problems, where symmetry is broken. Fiber cracking and matrix–fiber debonding are considered.

Keywords: composites; multiscale modeling; homogenization; discrete element method; defects; Cauchy problem; ODE

1. Introduction

The paper is devoted to the development of methods for modeling layered polymer composite materials. The study is conducted within the framework of a general multiscale modeling scheme, which involves molecular dynamics modeling of the polymer matrix and fiber to determine their mechanical properties, homogenization of the composite material, and calculation of the stress–strain state of the homogenized composite sample under specified loads. In this modeling scheme, the calculation of the effective physical and mechanical properties of the composite material plays an important role. This allows us to consider a heterogeneous material as homogeneous and use advanced continuum modeling methods [1–3]. Traditionally, the homogenization problem (determining the effective characteristics of the material) is solved based on knowledge of the properties of the individual materials that make up the composite. Approximate analytical and semi-empirical formulas, asymptotic averaging methods [4–6], and stochastic methods [7] are used. With the development of computing power, it becomes possible to directly model the stress–strain state of a representative volume of the composite material in order to obtain effective characteristics. Here, it is possible to apply both continuous approaches, a prominent example of which is the finite element method, and discrete element methods. Discrete element methods are based on representing objects as a set of closely packed particles (elements) interacting with each other according to spe-

Received: 17 December 2025

Revised: 28 January 2026

Accepted: 1 February 2026

Published: 3 February 2026

Copyright: © 2026 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

cific laws. Typically, particle motion is described by a system of ordinary differential equations expressing the classical laws of mechanics. The application of the DEM is possible at various scales. At the atomic level, this is the molecular dynamics method. The system is represented as a set of interacting atoms (molecules), the interaction between which is specified by an appropriate potential. The potential parameters can be identified using *ab initio* (quantum mechanical) calculations. This approach is applied, in particular, to the modeling of polymeric materials [8,9]. For calculations at the mesoscopic and macroscopic levels, coarse-grained discrete element methods are used, a detailed review of which is presented in [10]. As in the molecular dynamics method, the definition of the laws of interaction between the elements plays a crucial role. Successful implementations of this approach are presented in [11–13]. A number of studies propose a combination of discrete element and continuous medium modeling [14,15]. Discrete element methods have found application in modeling polymers [16] and composite materials [17,18]. In [19], the authors proposed a discrete element method that allows for the adaptation of information about the material microstructure. The main feature of the proposed method is the combination of discrete elements and their associated atomic samples. Molecular dynamics simulation is performed for an atomic sample to determine the properties of the element. A natural assumption is used that the stress and strain tensors are equal for a discrete element and its atomic sample. This allows for the transfer of information between levels. In [19], the method was tested for materials with an embedded atom interatomic potential, and in [20], it was applied to the calculation of the properties of polycrystalline silicon with covalent bonds. In both cases, the modeling reproduced the elastic properties of the materials and the sound wave propagation velocities well. In [21], a similar approach to implementing microstructural information in macroscopic modeling was considered in the context of a combination of molecular dynamics modeling and the finite element method. Additionally, we note two works: in [22], a fractal model for predicting the mechanical properties of complex porous composites is considered, and, in [23], a strategy for generating representative volume elements with complex microstructure, such as fibers and spatially randomly distributed pores, is presented.

In our paper, multiscale modeling is used to solve the homogenization problem. In the first stage, based on the polymer and fiber formulas, their mechanical properties are determined using molecular dynamics modeling. For the polymer, the initial structure is formed using the SMILES format as a simple long chain of many atoms. This chain is replicated the required number of times to create a sufficiently representative element of the material. Next, the element is heated and compressed, which removes empty space and intertwines the polymer chains. The compression process ceases when further compaction of the material becomes difficult, after which the external stress is removed. The stiffness tensor of the polymer material is then calculated. The resulting specimen is deformed, and the mechanical properties of the deformed sample are determined using molecular dynamics modeling.

In the second stage, a representative specimen of the composite material is constructed, including the matrix and fiber. It is subjected to deformations to calculate the homogenized stiffness tensor. The aforementioned discrete element method is used [19,20]. Because the original method is difficult to use due to the high computational complexity of molecular dynamics modeling of an atomic sample for elements belonging to the polymer, the method was modified to work with pre-calculated tensors of the elastic constants of the polymer and fiber. Thus, modeling at various scales is carried out using a single algorithmic scheme—solving Cauchy problems for systems of ordinary differential equations.

2. Molecular Dynamic Modeling of Polymeric Material

Composite materials containing a polymer matrix require a special approach to modeling their physical properties. This is due to the need to use specific potentials, such as consistent-valence force field (CVFF) and polymer consistent force field (PCFF) [24], which can take into account the geometric structure of bonds between atoms in polymers. Calculating the energy of a system using such potentials requires several steps. First, each atom, in addition to its element and the set of chemical bonds with neighboring atoms, is assigned a specific subtype. This subtype is important because, for example, the interactions between carbon atoms in a benzene ring and in a linear chain differ significantly. Next, the effective charge is redistributed between the atoms. After this, the calculations themselves are performed. Within the PCFF potential, the potential energy of a system consists of several components: the interaction energy of pairs of bonded atoms, the energy determined by the plane angles formed by triplets of bonded atoms, the energy determined by the dihedral angles formed by quadruples of bonded atoms, and other energies that describe the geometry of interatomic bonds in molecules. Thus, the general expression for the total energy is as follows:

$$\begin{aligned}
 E = & \sum_b [K_2(b-b_0)^2 + K_3(b-b_0)^3 + K_4(b-b_0)^4] \\
 & + \sum_\theta [H_2(\theta-\theta_0)^2 + H_3(\theta-\theta_0)^3 + H_4(\theta-\theta_0)^4] \\
 & + \sum_\phi [V_1(1-\cos(\phi-\phi_1)) + V_2(1-\cos(2\phi-\phi_2)) + V_3(1-\cos(3\phi-\phi_3))] \\
 & + \sum_\chi K_\chi \chi^2 \\
 & + \sum_b \sum_{b'} F_{bb'}(b-b_0)(b'-b'_0) \\
 & + \sum_\theta \sum_{\theta'} F_{\theta\theta'}(\theta-\theta_0)(\theta'-\theta'_0) \\
 & + \sum_b \sum_\theta F_{b\theta}(b-b_0)(\theta-\theta_0) \\
 & + \sum_b \sum_\phi (b-b_0)[V_1\cos(\phi) + V_2\cos(2\phi) + V_3\cos(3\phi)] \\
 & + \sum_{b'} \sum_\phi (b'-b'_0)[V_1\cos(\phi) + V_2\cos(2\phi) + V_3\cos(3\phi)] \\
 & + \sum_\phi \sum_\theta \sum_{\theta'} K_{\phi\theta\theta'}(\theta-\theta_0)(\theta'-\theta'_0)\cos(\phi) \\
 & + \sum_{i>j} \frac{q_i q_j}{\epsilon r_{ij}} \\
 & + \sum_{i>j} \left[\frac{A_{ij}}{r_{ij}^9} - \frac{B_{ij}}{r_{ij}^6} \right],
 \end{aligned}$$

where K_i , H_i , V_i , and K_χ are parameters describing the energy change of the system due to bond length change, the change of angle between bonds, the change of angle between the bond and the plane formed by other atoms, and bond torsion, respectively; $F_{bb'}$, $F_{\theta\theta'}$, $F_{b\theta}$, and $K_{\phi\theta\theta'}$ are coupling parameters for bonds containing a common atom, angles containing a common bond, an angle and one of its bonds, and angles and their planes, respectively; q_i is the charge of the i -th atom; r_{ij} is the distance between the i -th

and j -th atoms; and all other parameters are determined in accordance with the material being modeled.

The motion of atoms is described by classical equations of dynamics:

$$\frac{dr_i}{dt} = v_i$$

$$\frac{dv_i}{dt} = \frac{1}{m_i} F_i$$

where $r_i = (x_i, y_i, z_i)^T$ is the position vector of the atom with the number i , $v_i = (v_i^x, v_i^y, v_i^z)^T$ is its velocity vector, m_i is its mass, and $F_i = (F_i^x, F_i^y, F_i^z)^T$ is the force acting on the atom, while

$$F_i = -\nabla_i E,$$

where E is the total energy of the system and ∇_i is the gradient along the position of the atom with number i .

The most common method for solving this system of ordinary differential equations (ODEs) is the Verlet velocity method. To perform the calculations, the monomer structure is specified in SMILES format, and the polymer structure is constructed based on the specified monomer and additional information about the nature of the monomer bonds. Thus, the initial polymer structure is formed as a simple long chain of monomers. This chain is replicated the required number of times to create a sufficiently representative element of the material. Next, heating and compression are applied using a molecular dynamics simulation, which removes empty space and intertwines the polymer chains.

In this study, the simulation was performed using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [25] molecular dynamics code. The number of atoms in the molecular dynamics sample was chosen to be approximately 20,000, in accordance with the analysis conducted in the article [26].

As an example, consider the following monomer structure: NC(=O)C1=CC=CC(=C1)C(=O)NCCCCCN.

First, a long chain of multiple monomers is generated and repeated in each direction. Next, to compact the resulting structure, a sequence of steps is performed, consisting of compressing the structure to the target density, heating, and then gradually relaxing the sample under decreasing external pressure and temperature.

Ultimately, the sample is brought to a temperature of 300 K and a pressure of 1 atm. Figure 1 shows the initially generated structure, consisting of separate chains of atoms.

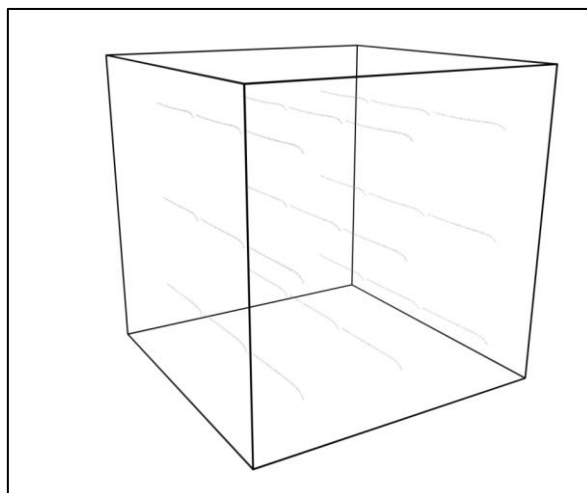


Figure 1. Initial structure.

Figure 2 shows chains of atoms close up from different angles.

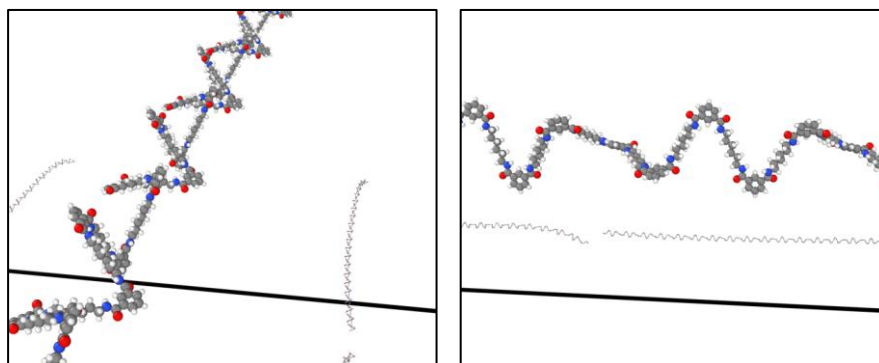


Figure 2. A chain of atoms in the initial structure.

Figure 3 shows how the original chains of atoms moved after the first action of increasing pressure and temperature.

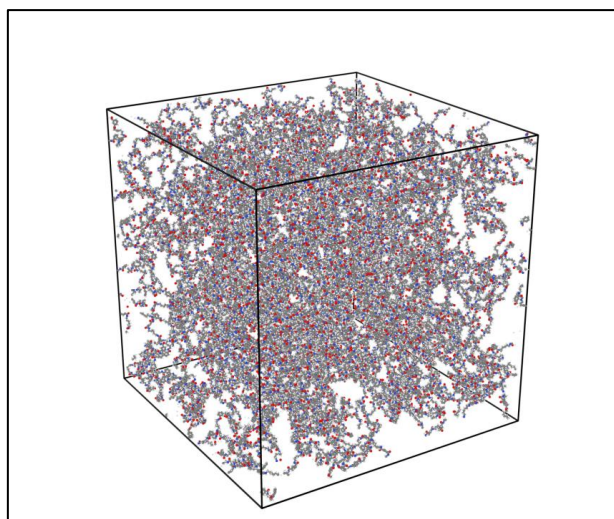


Figure 3. State of the specimen after the first action of changing the external temperature and pressure.

Figure 4 shows an enlarged part of the resulting structure. It is clear that the polymer chains are intertwined, although relatively large voids are still present.

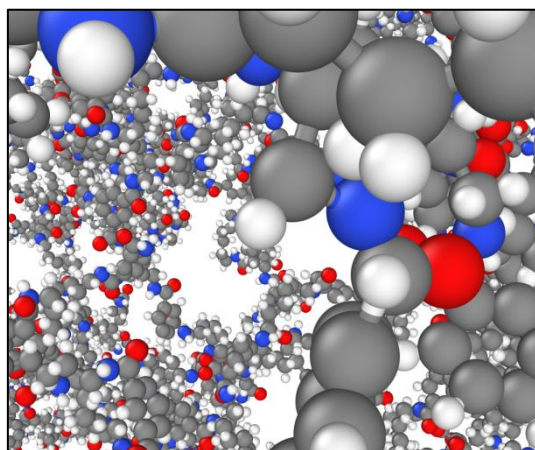


Figure 4. An enlarged portion of the specimen after the first change in external temperature and pressure (a different angle compared to Figure 3).

Repeating the cycle of increasing temperature and pressure leads to a gradual increase in packing density. Figures 5 and 6 show a specimen at the end of this procedure.

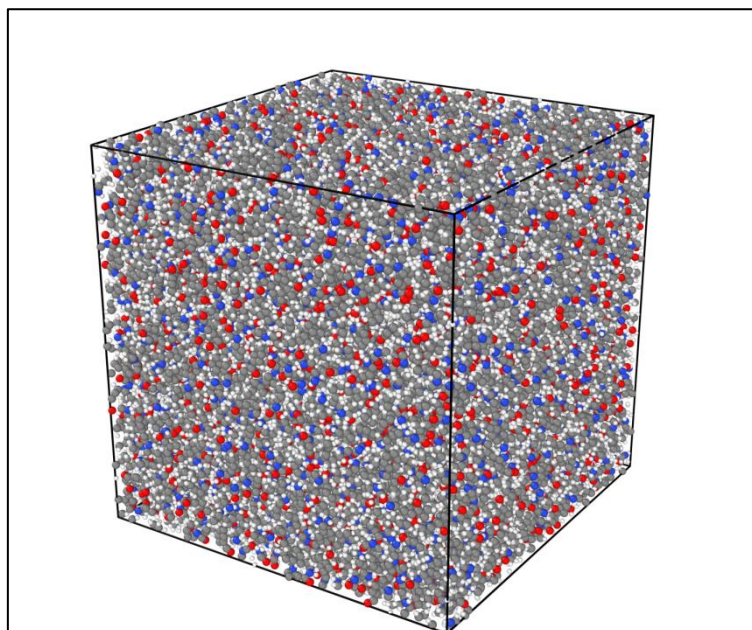


Figure 5. State of the specimen at the end of the compression procedure.

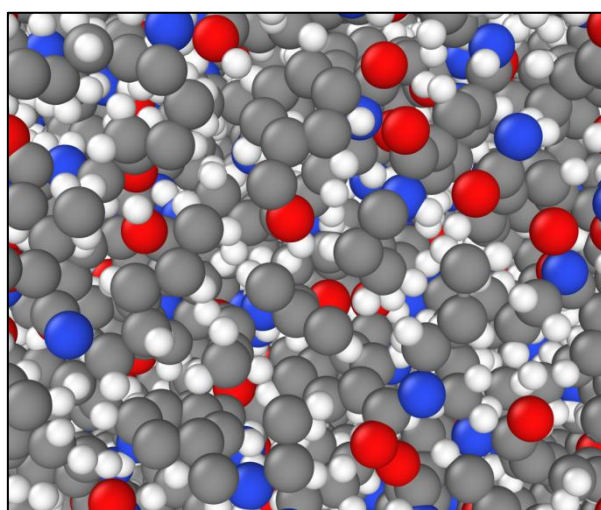


Figure 6. Enlarged portion of the specimen from Figure 5.

After completing all of the steps, the stiffness tensor of the polymer material is calculated. For this purpose, the resulting specimen is stretched, and time-averaged values are calculated using molecular dynamics simulation.

It should be noted that the sequence of steps used to obtain the material specimen is only one of several possible sequences. Depending on the initial state and the sequence of steps, the specimens will differ, and, accordingly, the stiffness tensor components will also differ. Two approaches are possible to account for this uncertainty. The first involves selecting average values of the tensor components over the realizations. The second method is based on an interval representation of the components. In this paper, averaging over realizations is used. Below is the stiffness tensor in Voigt notation, obtained by averaging over a set of constructed specimens (units in GPa):

$$\begin{pmatrix} 10.89 & 4.48 & 4.44 & -0.51 & -0.23 & -0.29 \\ 4.48 & 10.41 & 5.27 & -0.09 & 0.39 & -0.22 \\ 4.44 & 5.27 & 9.63 & 0.47 & -0.09 & -0.34 \\ -0.51 & -0.09 & 0.47 & 2.94 & 0.06 & -0.04 \\ -0.23 & 0.39 & -0.09 & 0.06 & 2.16 & -0.1 \\ -0.29 & -0.22 & -0.34 & -0.04 & -0.1 & 2.85 \end{pmatrix}$$

As expected, the resulting tensor is similar in structure to the tensor of an isotropic material, characterized by the presence of three distinct components, two of which are independent. Note that the scatter of values are approximately 10–15 percent of the mean. Extraction of mechanical properties from the resulting tensor can be performed, for example, using the least-squares method. The resulting Young's modulus and Poisson's ratio are 6.8 GPa and 0.33, respectively, and the shear modulus corresponding to these values is 2.56 GPa. In what follows, we will use the isotropic tensor obtained from these values. Note that the deviation of the polymer stiffness tensor components from isotropic components is significantly smaller than the difference between the elastic properties of the polymer and the fiber. Therefore, we use an effective isotropic stiffness tensor of the polymer, extracting its components from the original (weakly anisotropic) tensor using the least-squares method (i.e., averaging).

Similarly, the mechanical properties of a fiber can be obtained using molecular dynamics modeling. However, in this study, a model glass fiber with a given stiffness matrix was considered as a filler.

3. Calculation of the Stiffness Tensor of a Fiber Composite Material

The presence of oriented fibers in a polymer material makes the material transversely isotropic. Such a material is characterized by the presence of five independent stiffness tensor components. Because the stiffness tensor of a layered composite material with a regular fiber arrangement can be calculated analytically, this problem will be used to verify the model. To perform the calculation, a representative volume element is used—a cell containing a fiber and a polymer matrix with periodic boundary conditions. The mechanical properties are calculated for this element. In the case of a random composite material structure, homogenization is performed using the discrete element method [14,15]. According to this method, the specimen under study is represented by a set of tetrahedrons divided by material type (fiber and polymer), which determines the response to deformation. A representative volume element is created, and the structure of inclusions is specified. These inclusions can be embedded in the matrix either as individual random inclusions or as structural elements.

Discrete elements are tetrahedrons based on a common set of points, the movement of which determines the deformation of the body. The displacement of the nodes is described by standard dynamics equations, supplemented by viscosity term

$$\begin{cases} \dot{r}_i = v_i \\ \dot{v}_i = \frac{-\nabla_i U}{m_i} - \alpha v_i \end{cases}$$

where $r_i = (x_i, y_i, z_i)^T$ is the position vector of the vertex with the number i , $v_i = (v_i^x, v_i^y, v_i^z)^T$ is its velocity vector, m_i is its mass, $\nabla_i U = (\nabla_{ix} U, \nabla_{iy} U, \nabla_{iz} U)^T$ is the force acting on the vertex, and α is the damping parameter. The viscosity term is necessary to stabilize the solution; otherwise, the system will enter a state of undamped oscillation. It depends on the elastic properties of the materials and the dimensions of the discrete elements. The time integration step is selected automatically based on the required accuracy.

The total potential energy of a system is calculated as the sum of the potential energies stored in each element

$$U = \frac{1}{2} \sum_e C_{ijkl}^e \varepsilon_{ij}^e \varepsilon_{kl}^e$$

where C^e is the stiffness tensor and ε^e is the Lagrange strain tensor for the element e .

$$\varepsilon = \frac{1}{2}(C-E)$$

$$C = F^T F$$

$$F = DB^{-1}$$

$$D = (r_1 - r_0 | r_2 - r_0 | r_3 - r_0)$$

$$B = (r_1^* - r_0^* | r_2^* - r_0^* | r_3^* - r_0^*)$$

where r_i^* is the initial position of the vertex and r_i is its current position; here, the numbering of the vertices is indicated in the system of a separate element.

To calculate the force, the gradient of potential energy by the positions of all vertices of each element is evaluated.

$$\frac{dU^e}{dr_{p\alpha}} = C_{ijkl}^e \left(\frac{d\varepsilon_{ij}^e}{dr_{p\alpha}} \varepsilon_{kl}^e + \varepsilon_{ij}^e \frac{d\varepsilon_{kl}^e}{dr_{p\alpha}} \right)$$

$$\varepsilon_{ij} = \frac{1}{2}(C_{ij} - E_{ij})$$

$$C_{ij} = \sum_{\alpha} F_{\alpha i} F_{\alpha j}$$

$$F_{\alpha i} = D_{\alpha} B_{\alpha}^{-1} = (r_1 - r_0 | r_2 - r_0 | r_3 - r_0)_{\alpha} B_{\alpha}^{-1} = (r_{1\alpha} | r_{2\alpha} | r_{3\alpha}) B_{\alpha}^{-1} - r_{0\alpha} (1 \ 1 \ 1) B_{\alpha}^{-1}$$

$$\frac{dF_{\alpha i}}{dr_{0\alpha}} = -(1 \ 1 \ 1) B_{\alpha}^{-1}; \quad \frac{dF_{\alpha i}}{dr_{p\alpha}} = B_{(p-1)\alpha}^{-1}$$

$$\frac{dC_{ij}}{dr_{p\alpha}} = \frac{dF_{\alpha i}}{dr_{p\alpha}} F_{\alpha j} + F_{\alpha i} \frac{dF_{\alpha j}}{dr_{p\alpha}}$$

$$\frac{d\varepsilon_{ij}}{dr_{p\alpha}} = \frac{1}{2} \left(\frac{dF_{\alpha i}}{dr_{p\alpha}} F_{\alpha j} + F_{\alpha i} \frac{dF_{\alpha j}}{dr_{p\alpha}} \right)$$

It should be noted that the fundamental difference between the discrete element method and the finite element method traditionally used in homogenization problems is that the discrete element method represents the problem as a relatively simple dynamic system (a system of ordinary differential equations). Next, we discuss the results of the proposed approach by testing on problems of regular fiber placement, which have an analytical solution.

The analytical calculation is performed in the following sequence. First, using the known components of the polymer and fiber stiffness tensors, the components of the base stiffness tensor corresponding to a unidirectional layer of the composite material are found. In the case of regular placement, the properties of the composite material are determined by averaging the properties of the matrix and fiber according to their volume fractions. In the direction parallel to the fibers, the arithmetic mean of the properties of

the individual components is taken (the Voigt model), and, in the direction perpendicular to the fibers, the harmonic mean is taken (the Reuss model).

Note that this averaging is accurate for alternating flat layers of polymer and fibers, and, in our case, it will be used as an estimate.

Next, the fiber orientation relative to the tensile axis is taken into account. This is accomplished by rotating the stiffness tensor. Rotating the material's stiffness tensor by an arbitrary angle is specified as follows:

$$C_{i,j,k,l} = \sum_{p=1}^3 \sum_{q=1}^3 \sum_{r=1}^3 \sum_{s=1}^3 \omega_{i,p} \omega_{j,q} \omega_{k,r} \omega_{l,s} C_{p,q,r,s}^0, \quad i, j, k, l = 1, 2, 3,$$

where $C^0 \in R^{3 \times 3 \times 3 \times 3}$ is the base stiffness tensor and $\omega \in R^{3 \times 3}$ is the rotation matrix:

$$\omega = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\alpha_{yz}) & -\sin(\alpha_{yz}) \\ 0 & \sin(\alpha_{yz}) & \cos(\alpha_{yz}) \end{pmatrix} \times \begin{pmatrix} \cos(\alpha_{xz}) & 0 & -\sin(\alpha_{xz}) \\ 0 & 1 & 0 \\ \sin(\alpha_{xz}) & 0 & \cos(\alpha_{xz}) \end{pmatrix} \times \begin{pmatrix} \cos(\alpha_{xy}) & -\sin(\alpha_{xy}) & 0 \\ \sin(\alpha_{xy}) & \cos(\alpha_{xy}) & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$\alpha_{yz}, \alpha_{xz}, \alpha_{xy}$ —rotation angles in the corresponding planes.

Typically, composite material samples consist of a series of layers with varying fiber orientations. The following formula is used to arrange the layers:

$$C_{i,j,k,l} = \sum_w \frac{h_w}{H} C_{i,j,k,l}^w, \quad i, j, k, l = 1, 2, 3,$$

where H is the total thickness of the material, h_w is the thickness of the w -th layer, and C^w is the stiffness tensor of the w -th layer. Thus, a mapping is constructed from the linearized stiffness tensor of the material of one layer to the stiffness tensor of a composite material consisting of a set of differently oriented layers.

Let us examine the results of testing this approach using the polymer from Section 1 and the regular fiber placement.

The filler is fiberglass with a given stiffness matrix corresponding to a Young's modulus of 100 GPa and a Poisson's ratio of 0.25.

The modeled sample consisted of 8000 tetrahedra, 2224 of which were matrix elements and the remaining 5776 of which were fiber elements. The tetrahedra were constructed on 2205 nodes. The sample partitioning is shown in Figure 7.

The calculated basic stiffness tensor for a fiber volume fraction of 0.28 is as follows:

$$\begin{pmatrix} 36.93 & 6.47 & 6.47 & 0 & 0 & 0 \\ 6.47 & 15.18 & 6.37 & 0 & 0 & 0 \\ 6.47 & 6.37 & 15.18 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.76 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.31 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.31 \end{pmatrix}$$

The following mechanical properties were extracted from it: longitudinal and transverse Young's moduli are 33 and 12 GPa, Poisson's ratios are 0.37 and 0.3, and the shear modulus is 4.31 GPa. For comparison, the longitudinal and transverse Young's moduli obtained by averaging the properties of the fiber and polymer are 33 and 9.2 GPa, respectively. The modeling result coincided with the analytical result in the direction parallel to the fiber orientation and slightly exceeded it in the orthogonal direction. This is natural, as the analytical solution is valid for a set of parallel layers and serves as a lower bound for estimating the value. The results for parallel layers in comparison with analytical solutions are shown in Figure 8. The calculation results coincide with the analytical solutions.

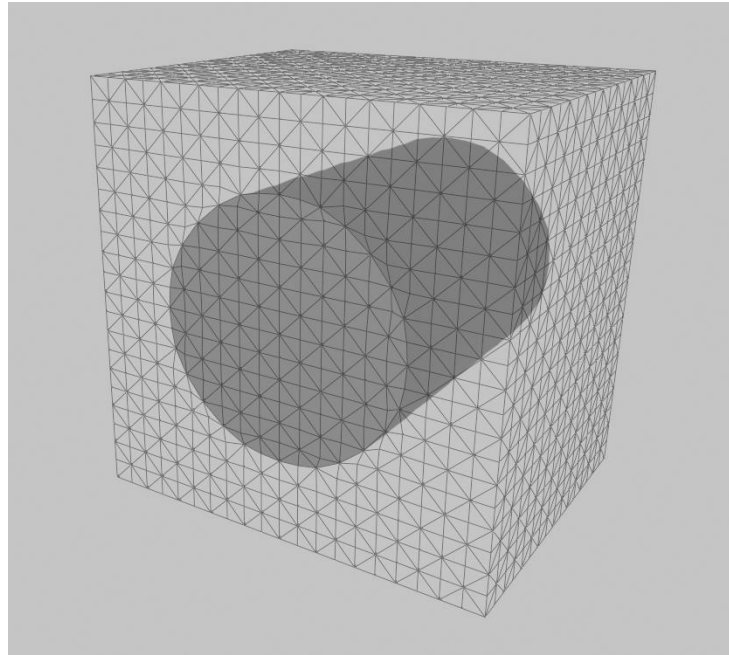


Figure 7. The simulated sample and its division into discrete elements.

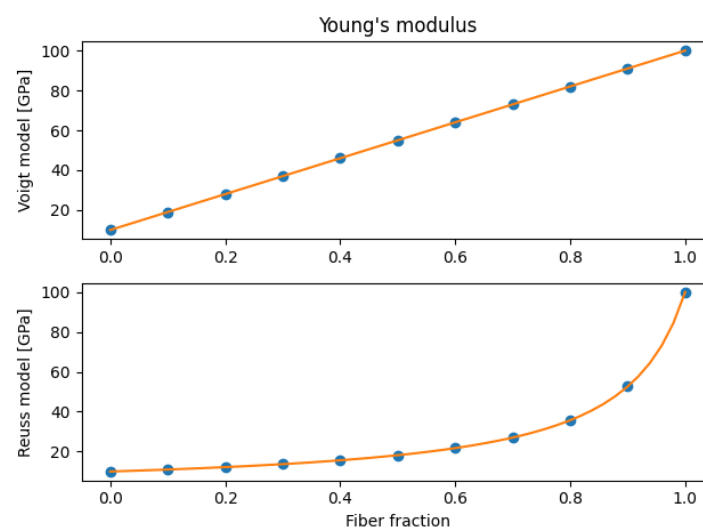


Figure 8. Comparison of numerical results with Voigt and Reuss models.

For the variant with long cylindrical fibers, the discrete element method gives good agreement of the elastic characteristics with the Mori Tanaka model [27], as shown in Figure 9. The difference in the Poisson's ratio in the transverse direction can be explained by the fact that the calculation was based on a periodic representative element with a single fiber (see Figure 7).

Next, we consider the homogenization results of a uniaxial material, taking into account the fiber orientation. In Figure 10, the markers represent the homogenization results of a uniaxial material. The top panel shows the fiber laying pattern, while the bottom panel shows the dependence of the elastic properties of the material on the laying angle. The first row shows Young's moduli in three directions, the second row shows Poisson's ratios, and the third row shows the shear moduli. Dimensional values are given in GPa, and x-axis values are in degrees. The solid curves show the analytical dependencies. It should be noted that the dependencies for the x- and y-axes are mirror images, as

the rotation occurs relative to the z-axis, and the x- and y-axes simply swap positions during the rotation. The calculated and analytical curves coincide.

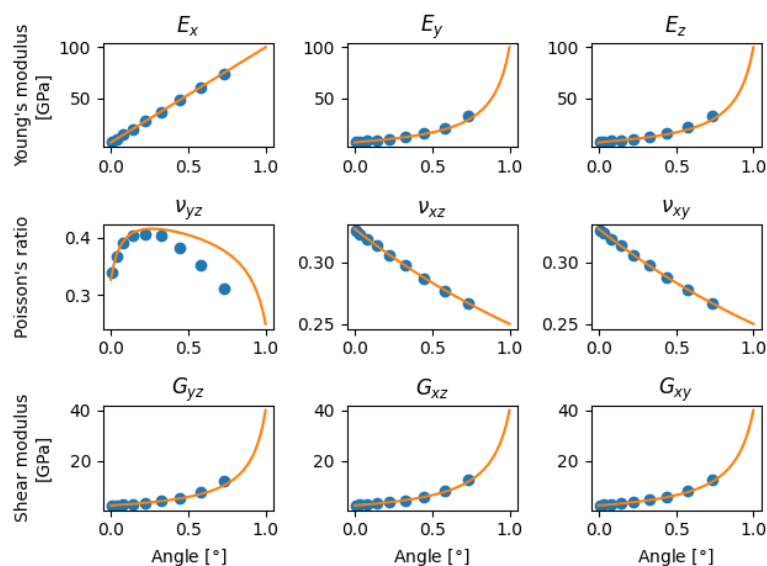


Figure 9. Comparison of numerical results with Mori Tanaka model.

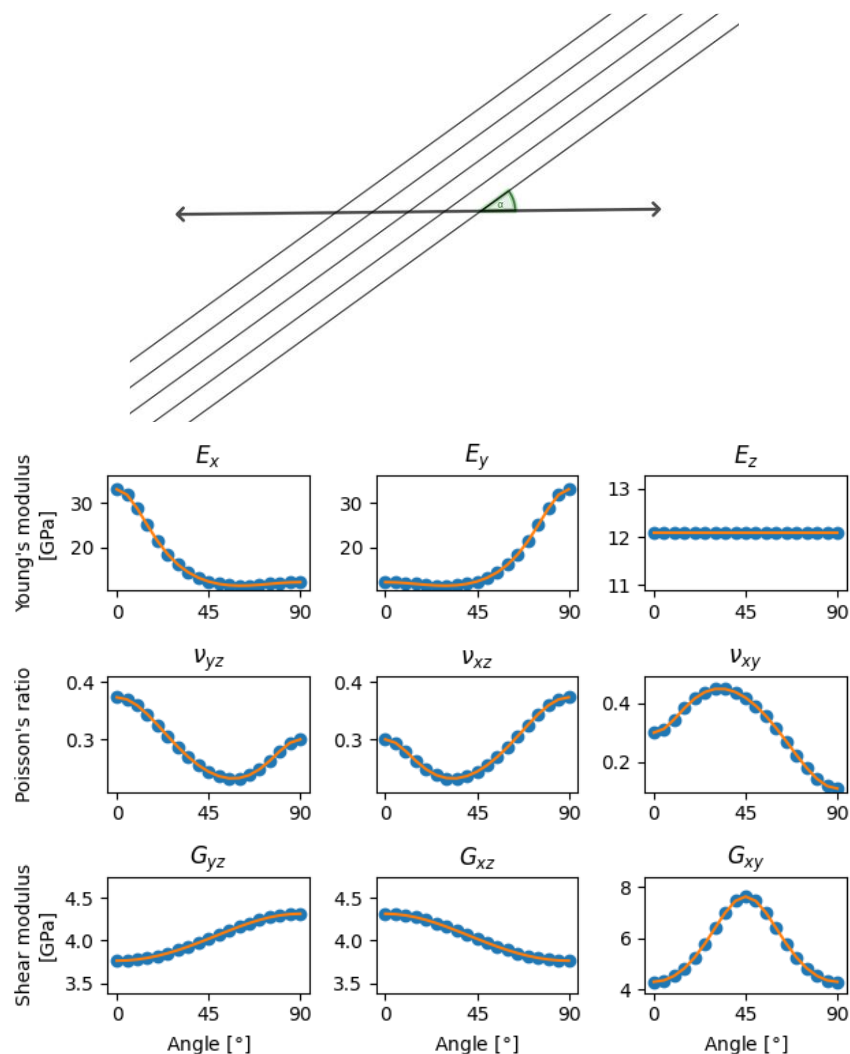


Figure 10. Homogenization of uniaxial composite material.

Figures 11 and 12 show similar patterns for a two-layer material and a multilayer material with random fiber orientation in the layers. Two layers of material are superimposed on each other at a certain angle, and the x-axis is chosen as the bisector of this angle. The x-axis in the graphs represents half of the angle between the fiber directions in degrees. The initial state corresponds to two layers with fiber oriented along the x-axis, while the final state corresponds to two layers with fiber oriented along the y-axis. It can be noted that the dependences for the x- and y-axes are mirror images, as similar graphs can be obtained by choosing an adjacent angle for the reference. In all cases, very good agreement between the calculated results and the analytical dependences is observed. For random laying (Figure 12), five layers were specified with laying directions of 0, 15, 18, 23, and 47 degrees relative to the x-axis. It is evident that the calculated results coincide with the analytical solutions.

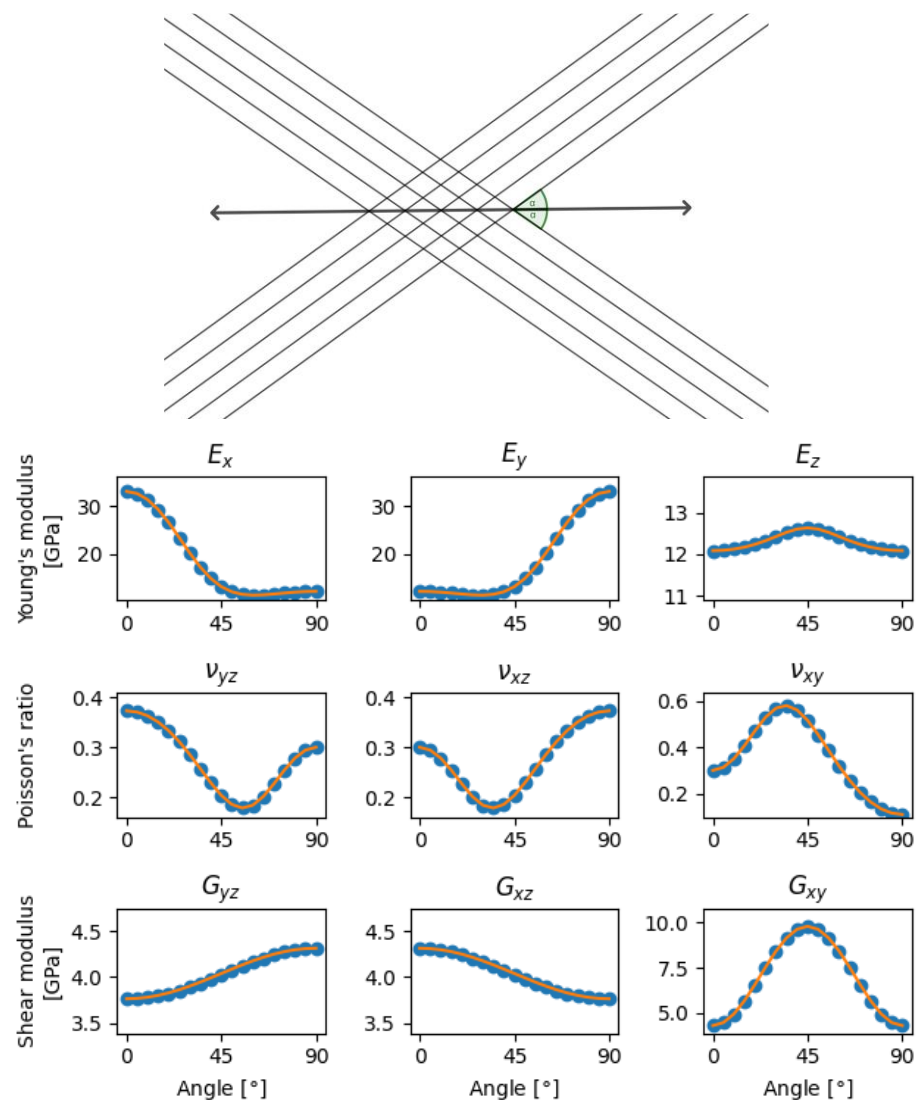


Figure 11. Homogenization of biaxial composite material.

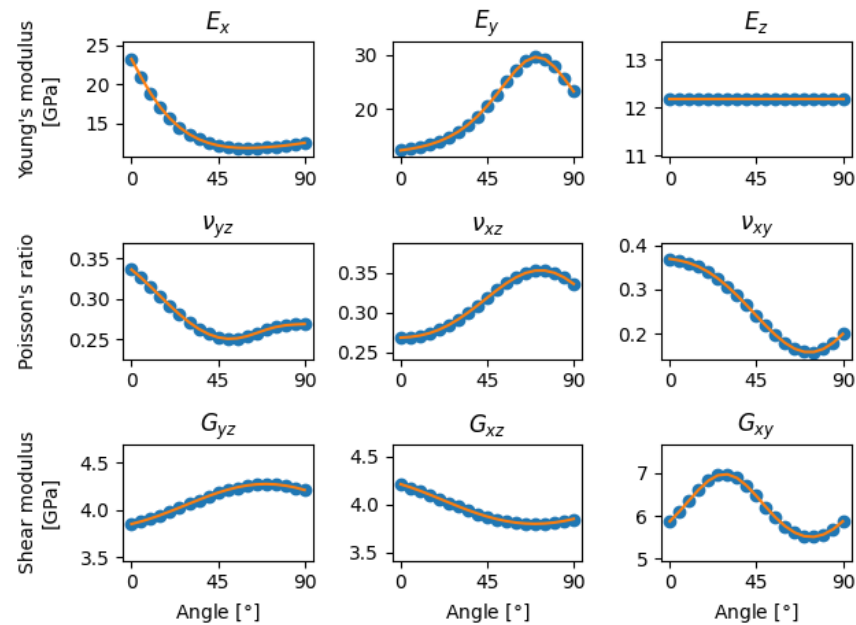


Figure 12. Homogenization of multilayer composite material with random fiber orientation.

Now, we consider more complex cases characterized by the presence of defects in the structure of the composite material. Obviously, obtaining an analytical solution for such cases is difficult.

Macroscopic defects in specimens are implemented by splitting every mesh vertex on the defect surface into two vertices initially located at the same position but logically belonging to different sides of the defect. Elements based on split vertices are rebased on new vertices depending on element location with respect to defect surface. Note that fiber fracture and interface debonding are taken into account through geometric separation. The interfacial traction–separation law, frictional contact, and progressive damage are not considered.

First, let us consider a single-layer composite material with transverse fiber cracking. Figures 13 (front view) and 14 (side view) illustrate variants under consideration (the cracks are shown in red). Different kinds of cracks are shown from the front view: 1—a quarter crack in fiber, 2—a half crack in fiber, and 3—a fractured fiber. Crack distribution in fiber by length for crack 2 is shown from a side view.

Figure 15 shows the results of homogenization of a single-layer material (Figure 7) with transverse fiber cracking. A uniaxial sample of infinite length is considered. Here, as before, three Young's moduli (top row), three Poisson's ratios (middle row), and three shear moduli (bottom row) are presented. The dependencies of these quantities on the dimensionless distance between cracks (related to the fiber radius) are shown for various fiber damage depths. Green corresponds to a crack depth of a quarter of the fiber diameter, orange to half the diameter, and blue to complete fiber rupture. It can be noted that cracks significantly affect the elastic properties only at very high concentrations, while at low concentrations (one crack per 10 fiber radii or more) the elastic properties remain virtually unchanged.

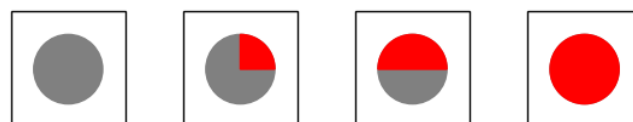


Figure 13. Crack shape in fiber (front view).

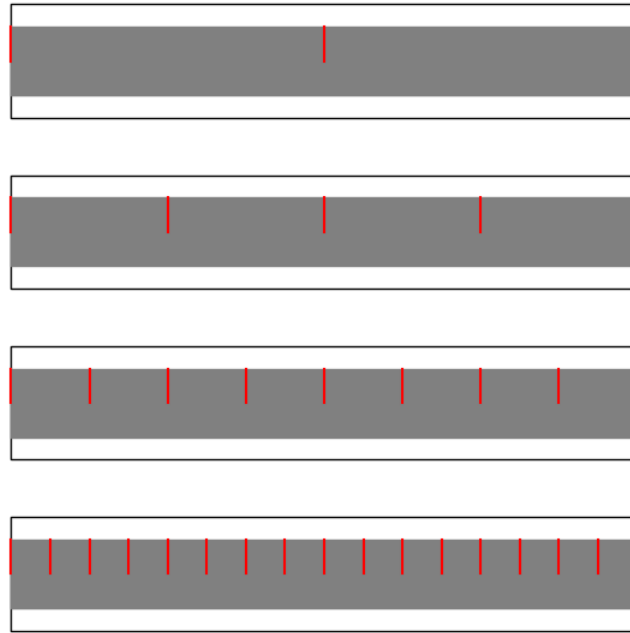


Figure 14. Crack distribution in fiber (side view).

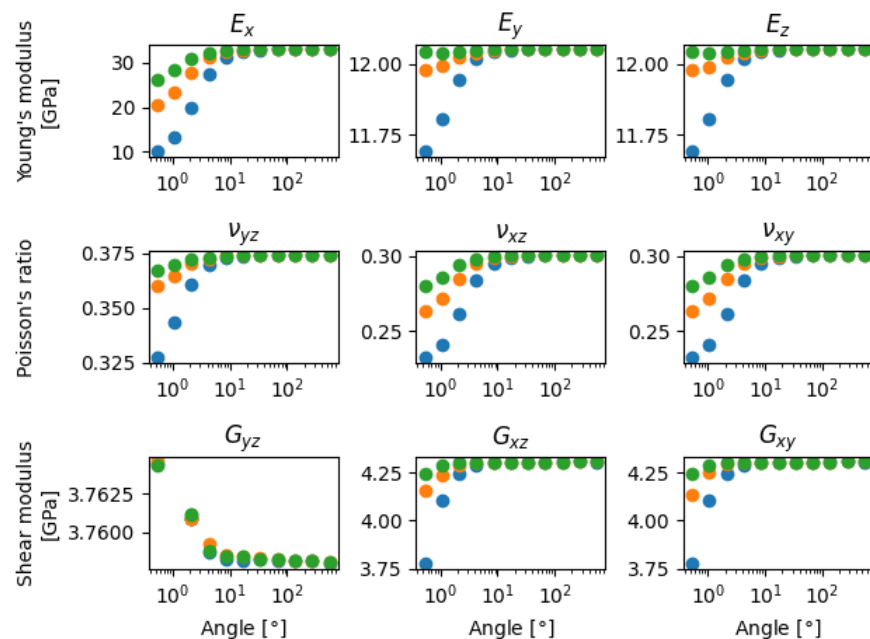


Figure 15. Homogenization of a single-layer composite material with transverse cracks of fibers.

Next, we consider a case with matrix–fiber debonding. Figure 16 illustrates this defect with different debonding angles (shown in red). The results are presented in Figure 17. The horizontal axis represents the angular size of the debonding in degrees. It can be seen that fiber detachment from the matrix significantly affects the elastic properties of materials in directions orthogonal to the fiber direction.

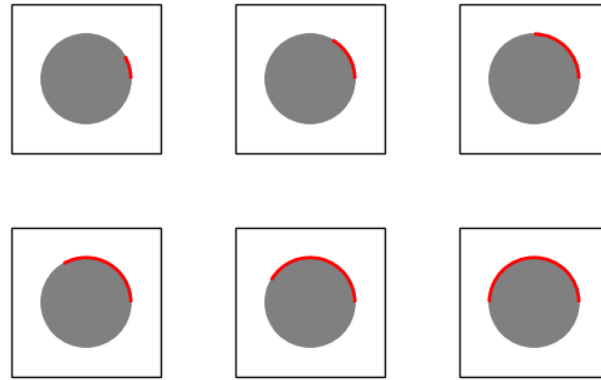


Figure 16. Matrix–fiber debonding shape.

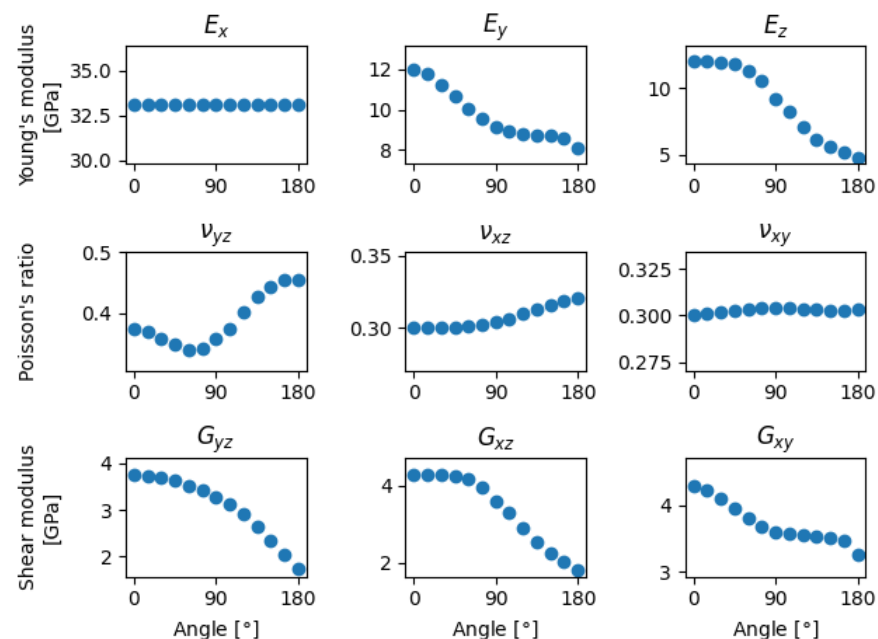


Figure 17. Homogenization of a single-layer composite material with matrix–fiber debonding.

4. Conclusions

A multiscale approach to calculating the effective elastic properties of a composite material with a fibrous filler and a polymer binder is presented. Modeling at various scales is performed using a single algorithmic scheme, solving Cauchy problems for systems of ordinary differential equations. At the atomic level, molecular dynamics modeling is used to calculate the elasticity tensor of the polymer material. At the mesoscale level, the authors' discrete element method is applied to calculate the effective elastic properties of the composite material. The method was tested on problems of regularly laid fibers with symmetry and an analytical solution. The capabilities of the proposed approach are demonstrated using defect composite homogenization problems, where symmetry is broken. Cases of fiber cracking and partial detachment of the fiber from the binder are considered. According to the modeled representations, cracks significantly affect the elastic properties of the composite only at relatively high concentrations, while, at low concentrations, the elastic properties change only slightly. The delamination of the fiber from the matrix significantly affects the elastic properties of the materials in directions orthogonal to the direction of the fiber. It should be noted that in the considered cases, the study was conducted within the framework of linear elastic characteristics; plastic deformation and material failure were not considered.

Author Contributions: Methodology, software, investigation, A.A.Z.; conceptualization, methodology, supervision, K.K.A.; methodology, software, A.Y.M.; methodology, investigation, validation, D.L.R. All authors have read and agreed to the published version of the manuscript.

Funding: The research was supported by the Ministry of Science and Higher Education of the Russian Federation, project No. 075-15-2024-544.

Data Availability Statement: Data are contained within the article.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Milton, G.W. *The Theory of Composites*; Cambridge University Press: Cambridge, UK, 2004; 719p.
2. Aboudi, J.; Arnold, S.M.; Bednarczyk, B.A. *Micromechanics of Composite Materials. A Generalized Multiscale Analysis Approach*; Butterworth-Heinemann: Oxford, UK; Elsevier: New York, NY, USA, 2013; p. 1011.
3. Vasiliev, V.V.; Morozov, E.V. *Advanced Mechanics of Composite Materials and Structural Elements*; Elsevier: New York, NY, USA, 2013; p. 816.
4. Panasenko, G. *Multi-Scale Modelling for Structures and Composites*; Springer: Dordrecht, The Netherlands, 2005; p. 407.
5. Dimitrienko, Y.; Sokolov, A. Numerical Modeling of Composites with Multiscale Microstructure. *Bull. Russ. Acad. Sci. Phys.* **2011**, *75*, 1457–1461.
6. Sokolov, A.P.; Schetinin, V.N. Computer-Aided Design of Composite Materials Using Reversible Multiscale Homogenization and Graph-Based Software Engineering. *Key Eng. Mater.* **2018**, *779*, 11–18. <https://doi.org/10.4028/www.scientific.net/KEM.779.11>.
7. Efendiev, Y.; Kronsbein, C.; Legoll, F. Multilevel Monte Carlo Approaches for Numerical Homogenization. *Multiscale Model. Simul.* **2015**, *13*, 1107–1135.
8. Schmid, F. Understanding and Modeling Polymers: The Challenge of Multiple Scales. *ACS Polym. Au* **2023**, *3*, 28–58. <https://doi.org/10.1021/acspolymersau.2c00049>.
9. Gartner, T.E.; Jayaraman, A. Modeling and Simulations of Polymers: A Roadmap. *Macromolecules* **2019**, *52*, 755–786.
10. Chen, Y.; Zimmerman, J.; Krivtsov, A.; McDowell, D.L.: Assessment of atomistic coarse graining methods. *Int. J. Eng. Sci.* **2011**, *49*, 1337–1349.
11. Izvekov, S.; Voth, G.A. A multiscale coarse-graining method for biomolecular systems. *J. Phys. Chem. B* **2005**, *109*, 2469–2473.
12. Larini, L.; Lu, L.; Voth, G.A. The multiscale coarse-graining method. VI: Implementation of three-body coarse-grained potentials. *J. Chem. Phys.* **2010**, *132*, 164107.
13. Xiong, L.; Chen, Y. Coarse-grained simulations of single-crystal silicon. *Model. Simul. Mater. Sci. Eng.* **2009**, *17*, 035002.
14. Munjiza, A. *The Combined Finite-Discrete Element Method*; John Wiley and Sons, Ltd.: London, UK, 2004; p. 350.
15. Argilaga, A.; Desrues, J.; Dal Pont, S.; Combe, G.; Caillerie, D. FEM×DEM multiscale modeling: Model performance enhancement from Newton strategy to element loop parallelization. *Int. J. Numer. Methods Eng.* **2018**, *114*, 47–65.
16. Kempfer, K.; Devémy, J.; Dequidt, A.; Couty, M.; Malfreyt, P. Development of Coarse-Grained Models for Polymers by Trajectory Matching. *ACS Omega* **2019**, *4*, 5955–5967.
17. Ferretti, E. DECM: A Discrete Element for Multiscale Modeling of Composite Materials Using the Cell Method. *Materials* **2020**, *13*, 880.
18. Ferretti, E. Multiscale Modeling of Composite Materials with DECM Approach: Shape Effect of Inclusions. *Int. J. Mech.* **2019**, *13*, 114–128.
19. Zhuravlev, A.A.; Abgaryan, K.K.; Reviznikov, D.L. Discrete element method adopting microstructure information. In *Advances in Theory and Practice of Computational Mechanics*; Smart Innovation, Systems and Technologies; Springer: Singapore, 2020; Volume 173. https://doi.org/10.1007/978-981-15-2600-8_17.
20. Zhuravlev, A.A.; Abgaryan, K.K.; Reviznikov, D.L. Multiscale discrete element modeling. *Symmetry* **2021**, *13*, 219. <https://doi.org/10.3390/sym13020219>.
21. Murashima, T.; Urata, S.; Li, S. Coupling finite element method with large scale atomic/molecular massively parallel simulator (LAMMPS) for hierarchical multiscale simulations. *Eur. Phys. J. B* **2019**, *92*, 211. <https://doi.org/10.1140/epjb/e2019-100105-9>.
22. Chao, X.; Tian, W.; Xu, F.; Shou, D. A fractal model of effective mechanical properties of porous composites. *Compos. Sci. Technol.* **2021**, *213*, 108957. <https://doi.org/10.1016/j.compscitech.2021.108957>.

23. Chao, X.; Qi, L.; Cheng, J.; Tian, W.; Zhang, S.; Li, H. Numerical evaluation of the effect of pores on effective elastic properties of carbon/carbon composites. *Compos. Struct.* **2018**, *196*, 108–116. <https://doi.org/10.1016/j.compstruct.2018.05.014>.
24. Sun, H.; Mumby, S.J.; Maple, J.R.; Hagler, A.T. An ab Initio CFF93 All-Atom Force Field for Polycarbonates. *J. Am. Chem. Soc.* **1994**, *116*, 2978–2987. <https://doi.org/10.1021/ja00086a030>.
25. Thompson, A.P.; Aktulga, H.M.; Berger, R.; Bolintineanu, D.S.; Brown, W.M.; Crozier, P.S.; Veld, P.J.I.; Kohlmeyer, A.; Moore, S.G.; Nguyen, T.D.; et al. LAMMPS—A flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Comput. Phys. Commun.* **2022**, *271*, 108171. <https://doi.org/10.1016/j.cpc.2021.108171>.
26. Kashmari, K.; Patil, S.U.; Kemppainen, J.; Shankara, G.; Odegard, G.M. Optimal Molecular Dynamics System Size for Increased Precision and Efficiency for Epoxy Materials. *J. Phys. Chem. B* **2024**, *128*, 4255–4265. <https://doi.org/10.1021/acs.jpcc.4c00845>.
27. Zhao, Y.H.; Weng, G.J. Effective Elastic Moduli of Ribbon-Reinforced Composites. *J. Appl. Mech.* **1990**, *57*, 158–167. <https://doi.org/10.1115/1.2888297>.

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.