SOFTWARE FOR AUTOMATIC GENERATION OF 3D MICROSTRUCTURAL MODELS OF FIBER REINFORCED COMPOSITES WITH DAMAGEABLE ELEMENTS

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ABSTRACT

Computational tools for 3D numerical analysis of the microstructure-strength and microstructure-damage resistance relationships of fiber reinforced composites are presented. The program code “Meso3DFiber“, which allows to automate the generation of 3D micromechanical finite element models of composites, was developed. The program, written in Compaq Visual Fortran, generates a command file for the commercial software MSC/PATRAN. The parameters of the model (volume content and amount of fibers, probabilistic/constant distributions of fiber radii, availability of interphase, etc.) are introduced interactively. In order to model interface damage and fiber cracking, damageable layers are introduced into the finite element model. Examples of the simulation of the fiber cracking and interface damage in polymer fiber reinforced composites are presented.

1. AUTOMATIC GENERATION OF 3D MICROMECHANICAL MODELS OF COMPOSITES

One of the ways to determine the optimal microstructures of materials is to carry out the "virtual testing" of different microstructures, using the micro- and mesomechanical models of the materials behaviour. The concept of optimal design of materials on the basis of the numerical testing of microstructures can be realized if large series of numerical experiments for different materials and microstructures can be carried out quickly, in a systematic way, automatically. This can be done, if labor costs of the numerical experiments, a significant part of which are the efforts of the generation of micromechanical models, are kept very low. To solve this problem, a series of programs was developed, which should automate the step of the generation of 3D microstructural models of materials. After a 3D microstructural model of a material with a complex microstructure is generated, the numerical testing of the microstructure is carried out with the use of commercial finite element software.

The microstructure-strength and microstructure-damage resistance relationships of composites can be analyzed numerically with the use of the unit cell approach. In particular, multiparticle unit cells make possible to analyze the overall response, nonlinear behavior and damage evolution in composites, taking into account both the interaction between phases, between elements of each phase (e.g., particles) as well as with evolving microcracks and cracks. Often, the following methods are used to incorporate complex microstructures of materials into discretized (finite element) models of materials:

- microgeometry based generation of finite element models of materials,
- pixel- or voxel-based model generation,
- multiphase finite elements (see Mishnaevsky Jr and Schmauder, 2001, Mishnaevsky Jr et al, 2003, 2004).

In the framework of the geometry-based approach, the (micro)geometrical model is first created, and then meshed with finite elements using the free meshing technique (Thompson et al, 1999) (cf. schema in Figure 1). After that, the mesh can be automatically improved (e.g., made finer at the interfaces). In order to simplify and automate the generation of 3D multiparticle unit cell models of composite materials, a program "Meso3D" was developed (see Mishnaevsky Jr., 2004). The program defines the geometry, mesh parameters and boundary conditions of different multiparticle unit cell models of materials, and then a multiparticle unit cell model of a representative volume of a composite material is created automatically. Both 2D and 3D versions of the program are available. The FE models of both artificial and simplified real microstructures (with particles approximated e.g. by the ellipsoids) can be generated with this method.

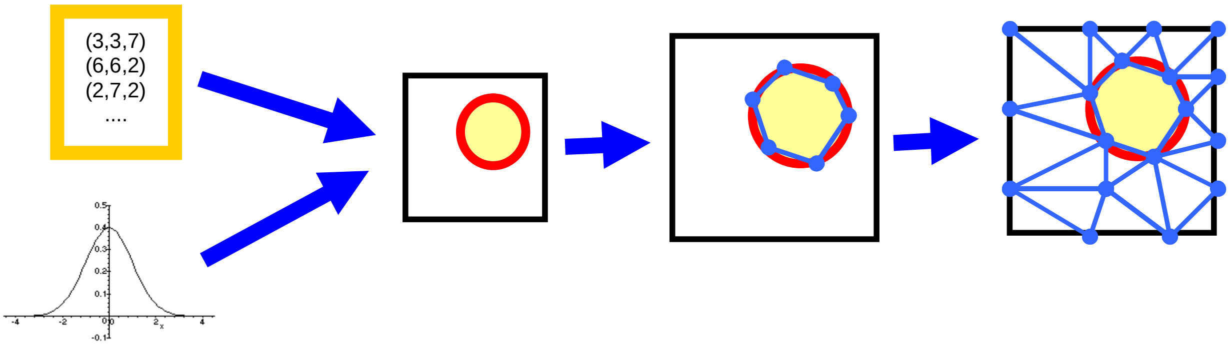

Figure 1. Schema of the generation of different artificial microstructures on the basis of pre-defined probability distribution of particle parameters.

However, the geometry-based approach, used in this program, is applicable only for relatively simple geometrical forms of microstructural elements in composites. In order to carry out the numerical analysis of arbitrarily complex 3D microstructures, an approaches based on the voxel array description of material microstructures, was realized in the framework of a new program "Voxel2FEM" (see Mishnaevsky Jr., 2005, 2007). The representative volume is presented as an Nx x Ny x Nz array of points (voxels), each of them can be either black (particle) or white (matrix) (for a two–phase material). (This approach can be generalized on multiphase materials simply as well.) The designed cells are meshed with brick elements, which are assigned to the phases automatically according to the voxel array data. Mishnaevsky Jr. (2007) compared the results of finite element simulations of mechanical behaviour of metal/ceramics composites carried out with the use of the geometry based and voxel array based models, and demonstrated that the differences are of the order of 5…6%.A disadvantage of the simple versions of the pixel or voxel based approaches to the model generation is that the smooth interfaces, available in real microstructures, are transformed into ragged interfaces in the pixel- and voxel-based models. However, this problem can be reduced to an acceptable level e.g. by adaptive remeshing.

The main idea of the multiphase element method is that the phase properties are assigned to individual integration points in the element independently on the phase properties assigned to other points in the element. Interfaces in the material can run through the finite elements in the mesh. Contrary to the microgeometry-based finite element mesh design, a FE-mesh in this case is independent of the phase structure of material, and one can use relatively simple FE-meshes in order to simulate the deformation in a complex microstructure. The disadvantage of the multiphase element method is that it does not allow taking into account fine interface effects. The multiphase finite elements, as well as some other methods (Voronoi finite element method, etc.) are discussed in more details in the review by Mishnaevsky Jr. and Schmauder (2001)..

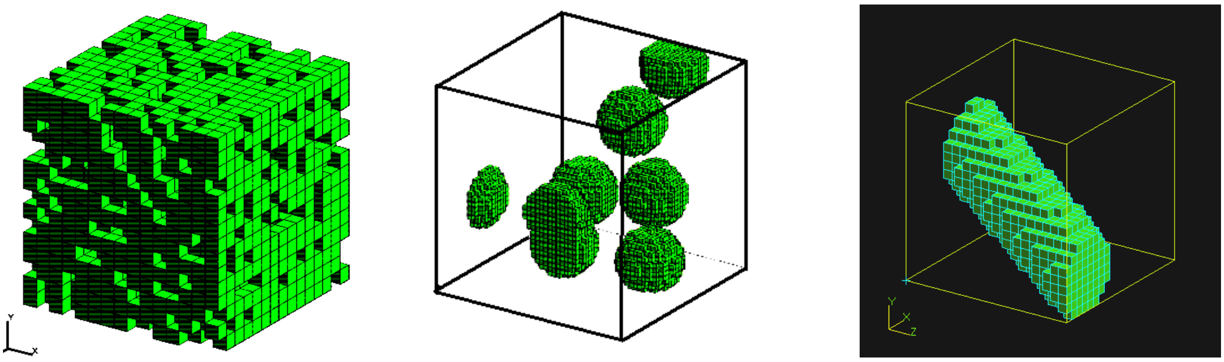

Figure 2. Examples of different generated microstructures: random 3D chessboard microstructure, a multiparticle unit cell, inclined fiber

3. COMPUTATIONAL TOOLS FOR THE MODELLING OF DAMAGE IN FIBER REINFORCED COMPOSITES

In order to simulate the strength and damage in fiber reinforced composites, a serie of special programs and subroutines were developed. A program code “Meso3DFiber“, which allows to automate the generation of 3D micromechanical finite element models of composites, was written in Compaq Visual Fortran. The program generates a command file for the commercial software MSC/PATRAN. The parameters of the model (volume content and amount of fibers, probabilistic/constant distributions of fiber radii, availability of interphase, etc.) are introduced interactively. The command file is played with PATRAN, and a 3D microstructural (unit cell) model of the composite with pre-defined parameters is generated. The finite element meshes are generated by sweeping the corresponding 2D meshes on the surface of the unit cell. The code allows to generate multifiber unit cells with random fiber arrangement, varied, random or constant fiber radii, as well as with some features allowing the damage modelling. Figure 3a shows an example of multifiber unit cells with 20 fibers generated with the use of the program “Meso3DFiber2.

Several damage modes are incorporated in the finite element model: fiber cracking, interface damage, matrix damage.

In order to model the ***fiber cracking***, we used the idea of introducing potential fracture planes (in form of damageable cohesive elements) in random sections of fibers, suggested by González and LLorca (2006). Following this idea, we introduced damageable layers in several sections of fibers. These layers have the same mechanical properties as the fibers (except that they are damageable). The locations of the damageable layers in the fibers were determined using random number generator with the uniform distribution. The random arrangement of the potential failure planes in this case reflects the statistical variability of the fiber properties. Figure 3b shows a multifiber unit cells with 20 fibers, with removed damageable layers.

A similar concept was used to simulate the ***interface damage***. Given that surfaces of fibers are usually rather rough, and the interface regions in many composites contain interphases (Huang and Petermann, 1996, Downing et al., 2000), the interface debonding was considered not as a two-dimensional opening of two contacting plane surfaces, but rather as a three-dimensional process in a thin layer. The interface was represented as a “third (interphase) material layer” between the homogeneous fiber and matrix materials. This idea was also employed by Tursun et al. (2006), who utilized the layer model to analyze damage processes in interfaces of Al/SiC particle reinforced composites. The thickness of the interface layer was taken 0.2 mm, but can be varied in further simulations. Figure 3 shows an example of a multifiber unit cell with 30 fibers of randomly varied radii, with and without the damageable layers. Figure 4 shows an example of a multifiber unit cell with 3 fibers with interphase layer (yellow).

In order to model the damage growth in the damageable layers (in fibers and in the interphase layers), the finite element weakening approach was employed (s. Mishnaevsky Jr, 2006, 2007). The idea of this approach is that the stiffness of finite elements is reduced if a stress or a damage parameter in the element or a nodal point exceeds some critical level. This approach has been realised in the ABAQUS subroutine User Defined Field. In this subroutine, the phase to which a given finite element in the model is assigned, is defined through the field variable of the element. Depending on the field variable, the subroutine checks whether the element failed or not, according to the properties of the matrix, interphase and fibers. Another field variable characterizes the state of the element (“intact” versus “damaged”). If the value of the damage parameter or the principal stress in the element exceeds the corresponding critical level, the second field variable of the element is changed, and the stiffness of the elements is reduced. The Young modulus of this element is set to a very low value (50 Pa, i.e., about 0.00001% of the initial value). The critical level of the maximum principal stress can be either a constant value, or a random value with a pre-defined probability distribution. The numbers of failed elements are printed out in a file, which can be used to visualize the calculated damage distribution.

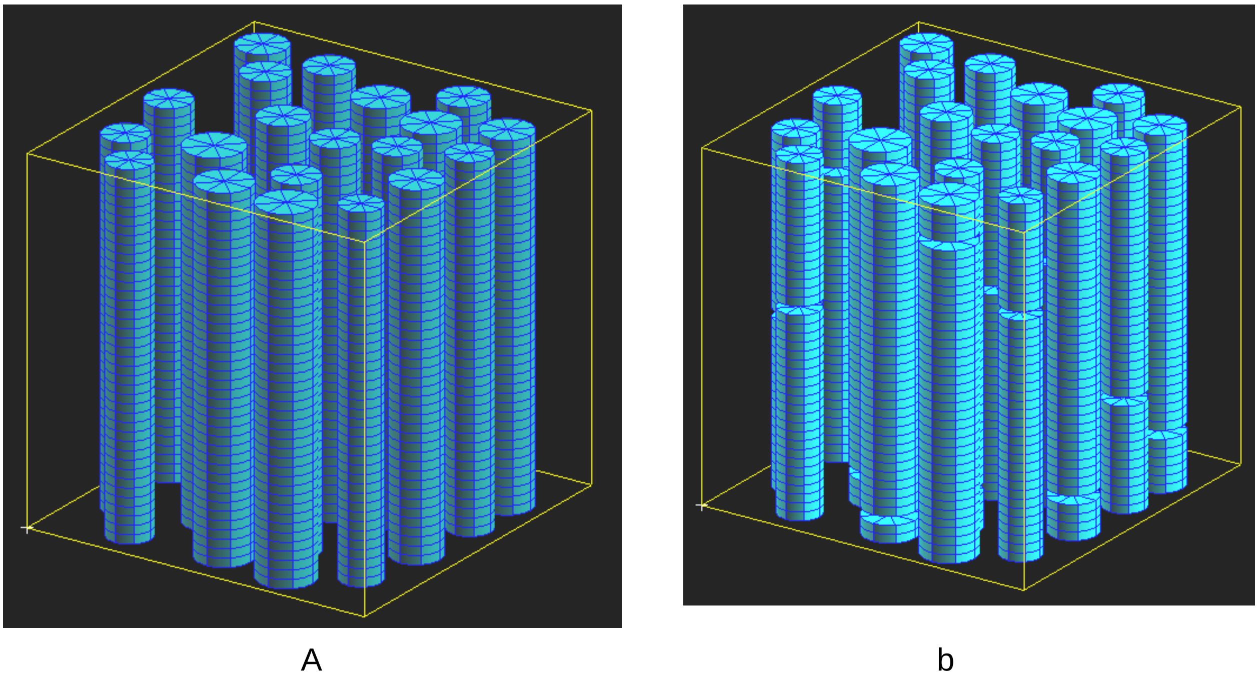

Figure 3. Examples of the 3D unit cell models: a unit cell with 30 fibers with randomly varied radii (a) and the cell with removed damageable layers (b).

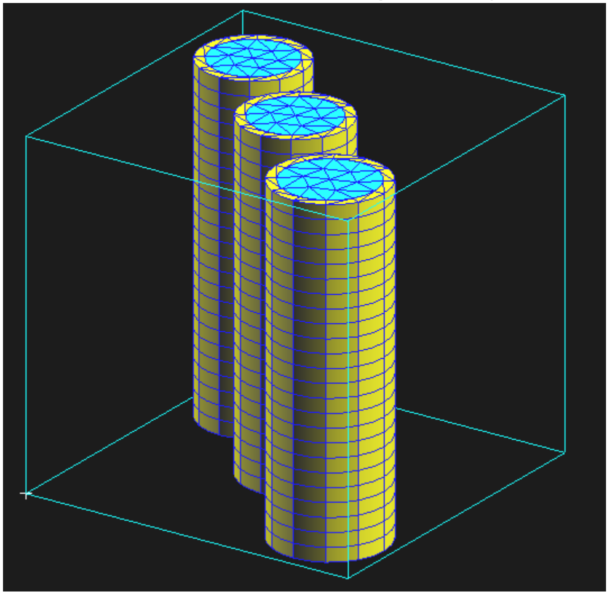

Figure 4. Example: a unit cell with 3 fibers and interphase (yellow) layers

4. EXAMPLES OF SIMULATION

The developed computational tools were employed to model the damage evolution in glass fiber reinforced fiber polymer (epoxy) reinforced composites. In so doing, the following properties of the composites were used. The glass fibers behaved as elastic isotropic solids, with Young modulus EP=72 GPa, and Poisson’s ratio 0. 0.26 (Agarwal and Broutman, 1990). The failure strength of glass fibers was assumed to be constant and equal to 3700 MPa (in our later simulations, the Weibull probability law distribution of fiber strengths with parameters σ0=1649 MPa and m=3.09 was assumed, see Feih, et al, 2005). The elastic properties of the epoxy matrix were as follows: Young modulus 3790 MPa, Poisson’s ratio 0.37, bulk modulus 5 GPa, instantaneous shear modulus 1.38 GPa . The viscoelastic properties were described by a single term Prony series, with the relaxation time 0.25 sec, and the modulus ratio g=0.125 (Gibson, 1976, Tevet-Deree, 2003, DeBotton and Tevet-Deree, 204). The failure condition of epoxy matrix was the maximum principal stress, 67 MPa.

First, the damage evolution in fiber was considered. A number of three-dimensional multifiber unit cells with 20 fibers and volume content of fibers 25 % have been generated automatically with the use of the program “Meso3DFiber” and the commercial code MSC/PATRAN. The fibers in the unit cells were placed randomly in X and Y directions. The dimensions of the unit cells were 10 x 10 x 10 mm. The cells were subject to a uniaxial tensile displacement loading, 1 mm, along the axis of fibers (Z axis). Figure 5 shows the Von Mises stress distribution in fibers before and after the fiber cracking.

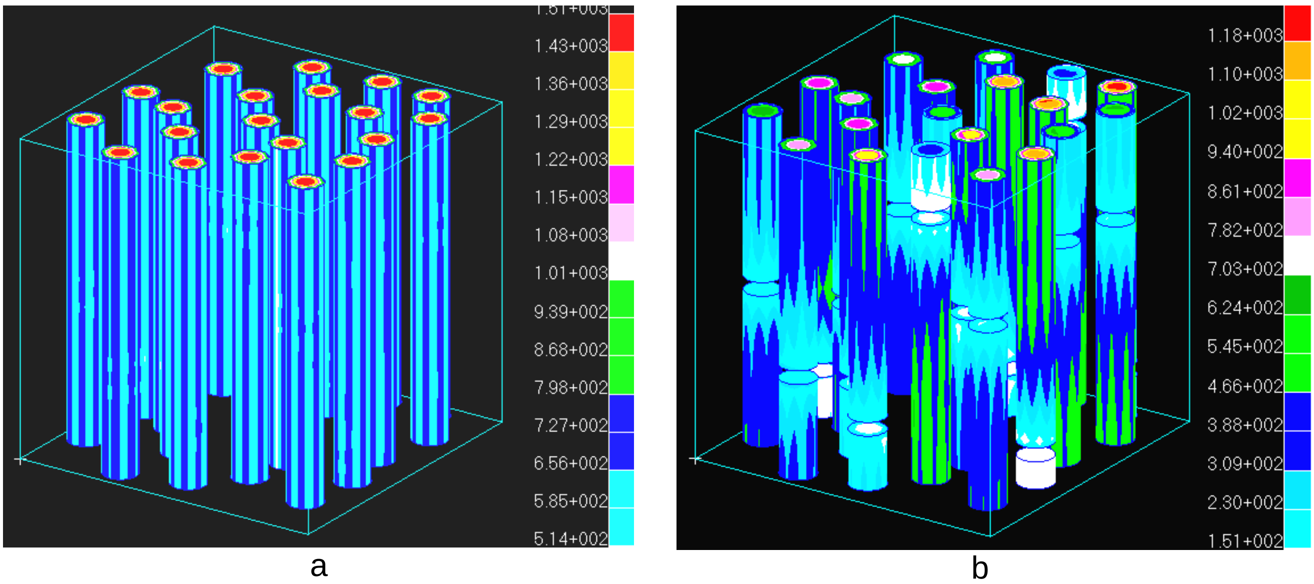

Figure 5. Von Mises stress distribution in fibers before and after the fiber cracking

Further, we sought to model the interface damage, caused by the fiber cracking. The interface layer was assumed to be a homogeneous isotropic material, with Young modulus 37.9 GPa (i.e., an averaged Young modulus of the fibers and matrix materials) and Poisson’s ratio of the matrix. The thickness of the layer was taken 0.2 mm. As a first approximation, we chose the maximum principal stress criterion for the interface damage (therefore, assuming rather brittle interface), and the critical stress 770 MPa (i.e., again, the mean value of the average strengths of fibers and the matrix). Figure 6 shows the evolution of von Mises stress distribution under loading: a) intact fiber and nondamaged interface (u=0.13mm), b) cracked fiber and stressed interface (u=0.15 mm), c) cracked fiber and damaged interface (u=0.16 mm)

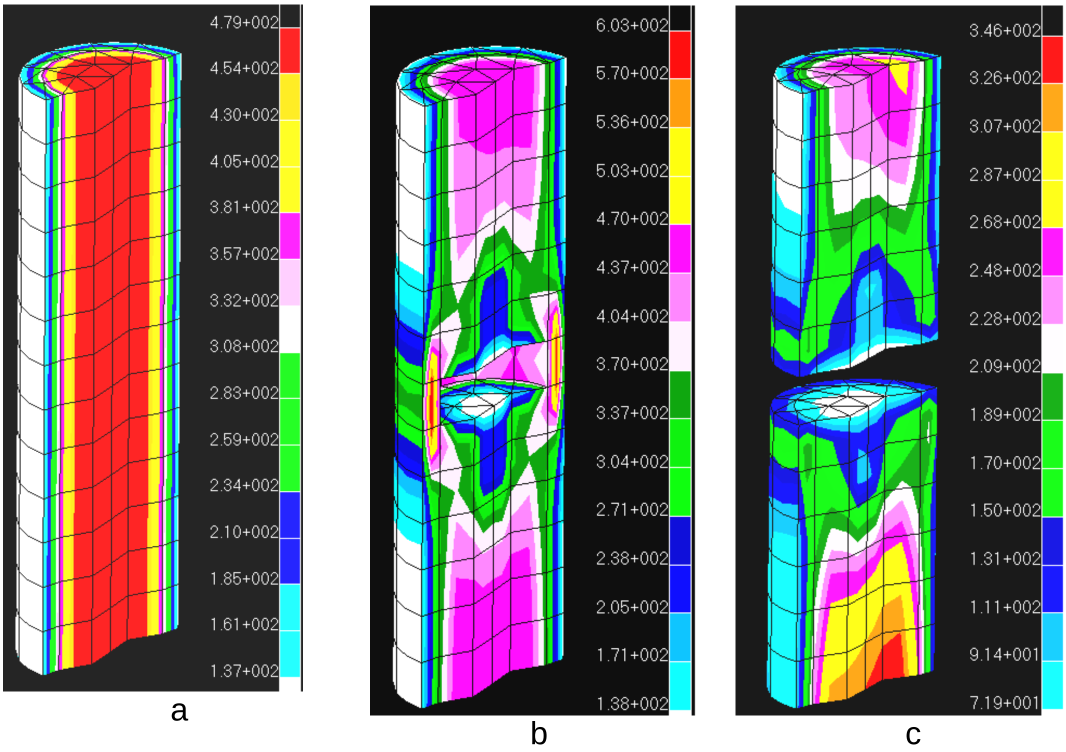

Figure 6. Evolution of Von Mises stress distribution: a) intact fiber and indamaged interface (u=0.13mm), b) cracked fiber and stressed interface (u=0.15 mm), c) cracked fiber and damaged interface (u=0.16 mm)

3. CONCLUSIONS

Computational tools for the micromechanical modelling of strength and damage in fiber reinforced composites are presented. A program code for the automatic generation of 3D multifiber unit cell models of composites with damageable fibers and interfaces has been developed. Examples of the 3D simulation of the fiber cracking and interface damage in polymer fiber reinforced composites, based on the developed programs, are presented.

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