Journal of
Mechanics of
Materials and Structures

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Volume 2, Nº 8

October 2007

mathematical sciences publishers

JOURNAL OF MECHANICS OF MATERIALS AND STRUCTURES
Vol. 2, No. 8, 2007

# EVALUATION OF EFFECTIVE MATERIAL PROPERTIES OF RANDOMLY DISTRIBUTED SHORT CYLINDRICAL FIBER COMPOSITES USING A NUMERICAL HOMOGENIZATION TECHNIQUE

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In this paper effective material properties of randomly distributed short fiber composites are calculated with a developed comprehensive tool for numerical homogenization. We focus on the influence of change in volume fraction and length/diameter aspect ratio of fibers. Two types of fiber alignments are considered: fiber orientations with arbitrary angles and parallel oriented fibers. The algorithm is based on a numerical homogenization technique using a unit cell model in connection with the finite element method. To generate the three-dimensional unit cell models with randomly distributed short cylindrical fibers, a modified random sequential adsorption algorithm is used, which we describe in detail. For verification of the algorithm and checking the influence of different parameters, unit cells with various fiber embeddings are created. Numerical results are also compared with those from analytical methods.

## 1. Introduction

Short fiber composites can be easily produced and have good mechanical properties. Since the mixture of short fibers and liquid resin can be manufactured by injection or compression molding, the production of parts with nearly arbitrary and very complicated shapes is possible. Composites consisting of spatially distributed short fibers have become popular in a wide variety of applications. Moreover, using spatial short fibers as reinforcing elements in a controlled manner can provide more balanced properties, which lead to an improved through-the-thickness stiffness/strength.

A classical problem in solid mechanics is the determination of effective elastic properties of a composite material made up of a statistically isotropic random distribution of isotropic and elastic short cylindrical fibers embedded in a continuous, isotropic and elastic matrix. Even though analytical and semianalytical models have been developed to homogenize fiber composites, they are often applicable only to specific cases. Numerical models seem to be a well-suited approach to describe the behavior of these materials, because there are no restrictions on the geometry, on material properties, on the number of phases (constituents) and on size. In order to obtain realistic predictions of a new material, micro-macro considerations are the appropriate approach. In this context the finite element method has been used to determine effective properties of the short fiber composites based on unit cell models.

*Keywords:* finite element method, unit cell, representative volume element, homogenization, short fibers, random sequential adsorption algorithm, effective material properties.

This work was supported by DFG Germany, Graduiertenkolleg 828 *Micro-Macro Interactions in Structured Media and Particle Systems.* This support is gratefully acknowledged.

A number of classical micromechanics theories have been developed. Using variational principles, Hashin [1962] and Hashin and Shtrikman [1963] established bounds on materials that could be considered as *mechanical mixtures of a number of different isotropic and homogeneous elastic phases* which are then treated as statistically isotropic and homogeneous. These two-point bounds were improved by three-point bounds [Milton 1982; Milton and Phan-Thien 1982], which incorporate information about the phase arrangement through the statistical correlation parameters. The dilute approximation can be used to model a dilute suspension of spherical elastic particles in continuous elastic phases. The interaction between particles is neglected. So the algorithm reduces to that of solving the problem of a spherical inclusion in an infinite matrix subjected to hydrostatic loading at infinity. Eshelby [1957; 1959] considered the problem of an ellipsoidal inclusion in an infinite isotropic matrix, assuming a well-defined matrix. That, however, is not always true in polycrystalline materials. A variety of properties can be exhibited, but there is no clearly defined matrix phase. In these cases the interactions between particles are more significant. The Mori–Tanaka method [Mori and Tanaka 1973] was designed to calculate the average internal stress in the matrix containing precipitates with eigenstrains. Benveniste [1987] reformulated it so that it could be applied to composite materials. He considered isotropic phases and ellipsoidal phases. Recently, Segurado and Llorca [2002] and Böhm et al. [2002] have assessed the effective coefficients of randomly distributed spherical particles using random sequential adsorption method and compared them with Hashin–Shtrikman bounds and other results from literature. Gusev et al. [2000] and Lusti et al. [2002] performed experiments of randomly distributed short cylindrical fiber composites and found good agreement with numerical results. However, due to the lack of literature which deals with randomly distributed short cylindrical fibers and the restriction to low volume fractions of fibers, we have been motivated to develop a numerical homogenization tool which extends the limits and provides the basis for investigation of composites with arbitrary inclusions. In our opinion micro-macro mechanical approaches offer new insights in the material behavior of such fiber composites, and may result in new procedures to develop realistic material models for design and optimization purposes.

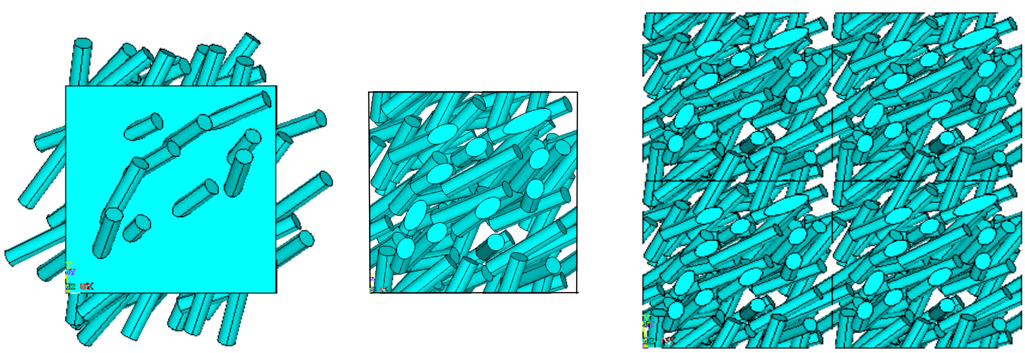
## 2. Numerical homogenization

**2.1.** ***Basic procedure.*** The mechanical and physical properties of the constituent materials are always regarded as a small-scale/micro structure. To predict the overall behavior of the structure on a macro level, the knowledge of effective material properties is necessary. One of the most powerful tools to estimate such effective properties is the homogenization method. The main idea is to find a globally homogeneous medium equivalent to the original composite, such that the strain energy stored in both systems is approximately the same. The common approach to model the macroscopic properties of fiber composites is to create a unit cell or a representative volume element (RVE) that captures the major features of the underlying microstructure.

The RVE can generally be considered as a periodic part of the heterogeneous structure that is sufficiently large to be a statistically representative of the composite, that is, to effectively include a sampling of all microstructural heterogeneities that occur in the composite [Kanit et al. 2003]. To obtain the homogenized effective material properties, periodicity must be ensured for the mechanical behavior of the RVE by introducing periodic boundary conditions between opposite surfaces. By constructing several load cases with selected traction loads and selected shear loads in one direction and preventing strains in the other directions, all effective elasticity coefficients can be calculated from the constitutive relations by an averaging technique. This procedure is described in detail in [Berger et al. 2005a; 2005b] and shall not be explained here.

**2.2.** ***Fiber generation by random sequential adsorption algorithm.*** Creation of an RVE with randomly distributed cylindrical short fibers which fulfill certain restrictions, such as nonoverlapping, ensuring periodicity and the like, is a difficult task. Due to the statistical distribution of inclusions, the RVE can be modeled as a cube with unit size. For automatic generation of such RVEs, a modified random sequential adsorption algorithm [Hinrichsen et al. 1986] is used. Several input parameters can be given, including the size of RVE, diameter and length range of fibers, minimum distance between neighboring fibers, and desired volume fraction. The algorithm starts by creating the cylinder axis of the first fiber at a random position, with random length and with random angle. Subsequently new fibers are created with random distribution values. If the new fiber matches the restriction of nonoverlapping and sufficient distance to the earlier one, it is accepted; otherwise it is deleted. Furthermore, to ensure periodicity, if any surface of the cylinder cuts any of the cubic RVE surfaces it is copied to the opposite surface with the RVE size length. In this case one also checks all the restrictions; if it fails, the original and copied fibers are deleted. Concerning the later finite element generation, we would also like to ensure that some practical limitations are fulfilled. For instance, the cylinder surfaces should not be very close to the RVE surface as well as to corners of the RVE in order to avoid highly distorted finite elements during meshing. The generation of new fibers is repeated until the desired volume fraction is reached or no more fibers can be placed due to the aforementioned restrictions. Figure 1 shows a sample of generated fibers before cutting on the RVE surface, after cutting, and an ensemble of four RVEs which demonstrate that periodicity is maintained.

By modifying the input parameters it is possible to create RVEs with different fiber arrangements, such as, for example, fibers of same diameter, fibers of same length, or only parallel alignment of fibers. Combining these arrangements opens the possibility of generating RVEs which represent different types of fiber reinforced composites such as those presented in this paper. The possible maximum fiber volume fraction plays an important role. In general, for fibers of identical size the algorithm can generate up to



(a) (b) (c)

**Figure 1.** Generation of randomly distributed short fibers: (a) uncut fibers, (b) cut fibers, (c) periodicity demonstrated with four RVEs.

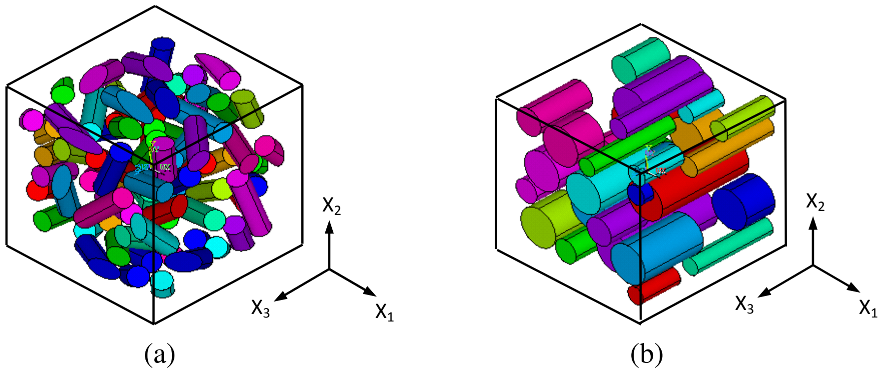



**Figure 2.** Types of composites: (a) ROF and (b) POF.

25% fiber volume fraction. For higher volume fractions, one must use fibers of different sizes, which can be generated by creating fibers with subsequently descending diameters. Using this approach, fiber volume fraction up to 40% can be achieved with minimum distortion of the finite elements.

For calculating effective material properties of randomly distributed short fiber composites, we investigate two types of fiber arrangements: randomly oriented fibers (ROF) and parallel-oriented fibers (POF); see Figure 2. For POF composites, the fibers in the models are aligned along the $x_3$-axis. This is denoted as the longitudinal direction, while the perpendicular $x_1x_2$ plane are the transverse directions.

**2.3. *Finite element modeling.*** All finite element calculations were performed with the commercial FE package ANSYS. The matrix and the fibers were meshed with 10 node tetrahedron elements with full integration. For the calculation of geometry of the fibers by random sequential adsorption algorithm, a special preprocessor was developed in FORTRAN programming language, which produces a partial input file for ANSYS. Cutting of the fibers on the RVE surfaces is carried out by geometrical modeling features of ANSYS. Figures 3 and 4 show samples of meshed RVEs for ROF and POF models.

To apply the periodic boundary conditions on the RVE, identical meshes are necessary on opposite surfaces. For this purpose a surface of the RVE is first meshed with blind plane elements; then this

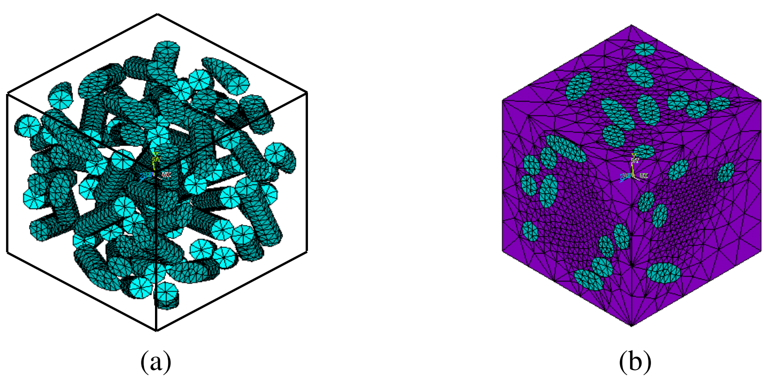
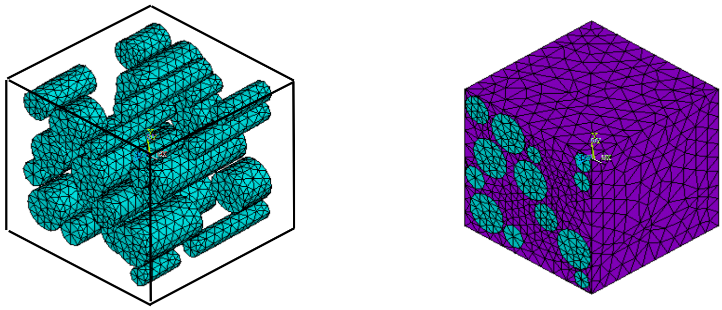



**Figure 3.** Sample for meshed RVE for ROF: (a) only fibers, (b) fibers and matrix.



(a) (b)

**Figure 4.** Sample for meshed RVE for POF: (a) only fibers, (b) fibers and matrix.

element configuration is copied to the opposite surface. Based on all meshed surfaces, three-dimensional meshing is carried out. In order to apply periodic boundary conditions, we must generate constraint equations between opposite nodal pairs. Here the ANSYS Parametric Design Language (APDL) is used to automate this process. This script language allows the common nodal pairs to be identified automatically by their coordinates. Furthermore, APDL is used to collect averaged stresses and strains from element solution as well as to calculate the effective elastic constants.

The combination of the FORTRAN preprocessor, APDL and ANSYS batch processing lets us automate the whole process. It also provides a powerful tool for the fast calculation of homogenized material properties for composites with a great variety of inclusion geometries.

## 3. Test models

We have investigated two types of short fiber composites: ROF and POF. In order to test the influence of various parameters, different RVEs were generated. Furthermore so that we can obtain statistically-averaged results for every configuration, five RVEs with different starting values for the random algorithm were generated. The material properties of the constituents used for the analysis to evaluate the effective material properties were taken from literature [Böhm et al. 2002] to verify the developed method with other solutions. Table 1 contains Young's moduli and Poisson's ratios for matrix and fibers.

The calculated results were compared with different analytical methods such as Hashin–Shtrikman two-point bounds (HS) [Hashin and Shtrikman 1963], Mori–Tanaka estimates (MTM) [Mori and Tanaka 1973], the self-consistent method (SCM) [Li and Wang 2005], and the generalized self-consistent method (GSCM) [Christensen and Lo 1979]. We also performed studies to determine the influence of aspect ratio length/diameter of fibers on the effective material properties of these composites.

| Constituent | Young's modulus | Poisson's ratio |
|---|---|---|
| Matrix Al2618-T4 | 70 GPa | 0.3 |
| Fiber SiC | 450 GPa | 0.17 |

**Table 1.** Material constants for constituents of the composite.

## 4. Results and discussion

**4.1.** ***Variation of volume fraction.*** Effective values of Young's modulus $E$, shear modulus $G$ and Poisson's ratio $\nu$ were evaluated for different volume fractions from 10% to 40% in steps of 10%; see Figure 5. Five samples of RVE models with randomly distributed short fibers (random angle of orientation, random diameter and length in a certain range) were generated for each volume fraction. In six particular load cases the RVEs were subjected to uniaxial tension as well as shear deformation along the three coordinate axes [Berger et al. 2005a; 2005b]. From these load cases nine material constants were calculated: $E_{11}$, $E_{22}$, $E_{33}$, $G_{12}$, $G_{13}$, $G_{31}$, $\nu_{12}$, $\nu_{23}$, $\nu_{31}$. Because of the statistically isotropy mean values $E$, $G$ and $\nu$ from all directions were used for comparison with other methods. Furthermore, due to the random distribution

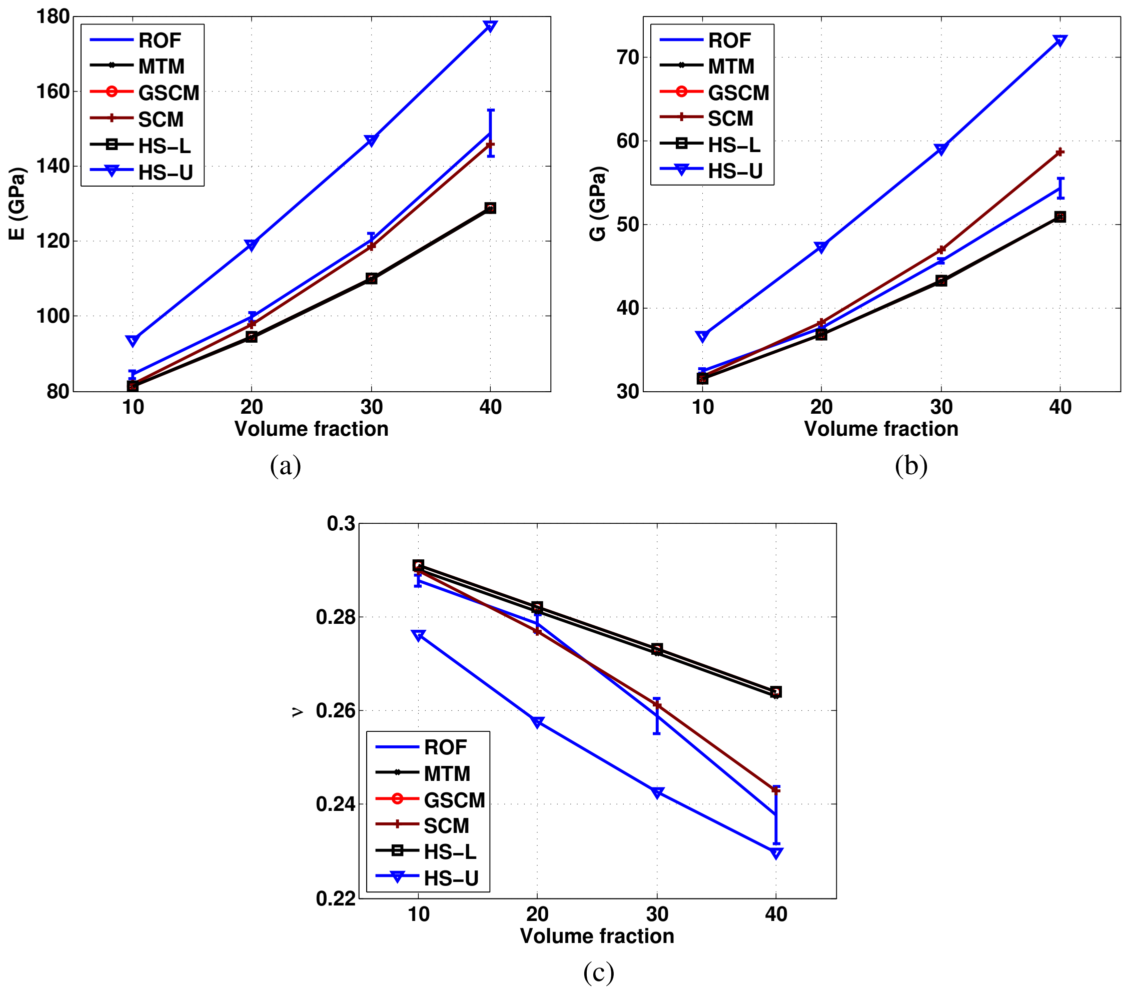



**Figure 5.** Variation of effective material properties for ROF composites with change in volume fraction and comparison with different analytical results: (a) Young's modulus, (b) shear modulus, (c) Poisson's ratio.

of fibers in each five samples, a certain variance can be observed for the effective values. The bounds of this variance are marked in the figures with vertical bars in the sense of a standard deviation.

The effective material properties, which were obtained for ROF composites using the presented numerical homogenization technique, lie within the lower (HS-L) and upper (HS-U) Hashin–Shtrikman bounds. The results of the analytical methods MTM and GSCM are always the same and are nearly identical with HS-L. The results of our solution (ROF) are nearer to the self-consistent method (SCM) for all volume fractions. The maximum difference between ROF and SCM is about 3%.

To show the nearly isotropic behavior of the ROF composite, in Figure 6 we plot effective Young's moduli in all coordinate directions as mean values from the five random samples for different volume fractions. Effective Young's moduli, which were obtained for the three coordinate directions, are nearly the same over the full investigated range of volume fraction; the maximum difference is less than 1.5%. This indicates a nearly isotropic macro behavior of the short fiber composite with randomly distributed fiber orientation.

Effective material properties obtained for POF composites were compared with ROF composites. Figure 7 shows the variation of effective Young's moduli for POF composites with change in volume fraction in three coordinate directions, and compares it with the results for ROF composites. The transverse Young's moduli of POF composites have slightly lower values compared to ROF composites. Nevertheless, along the longitudinal direction the POF effective material properties have higher values when compared with ROF composites. This is obvious because in case of POF composites, fibers are aligned along the longitudinal direction, which results in higher stiffness relative to the transverse directions. From Figure 7 it can also be seen that the effective Young's moduli $E_{11}$ and $E_{22}$ are nearly the same; this fact expresses transverse isotropy.

**4.2.** ***Variation of fiber aspect ratio.*** We have investigated the influence of aspect ratio length/diameter $L/D$ of fibers on their effective material properties for ROF and POF composites. As $L/D$ increases, the composite tends to a long fiber composite. The effective material properties were calculated at 10% volume fraction of fibers. Table 2 represents the variation of effective material constants $E_{11}$, $E_{22}$ and

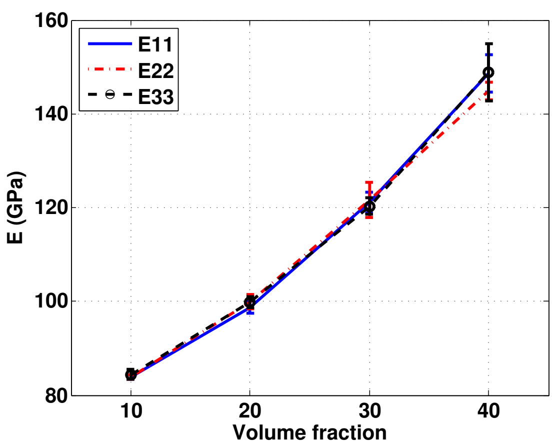



**Figure 6.** Isotropy of effective material properties expressed by Young's moduli in three directions for ROF composites.

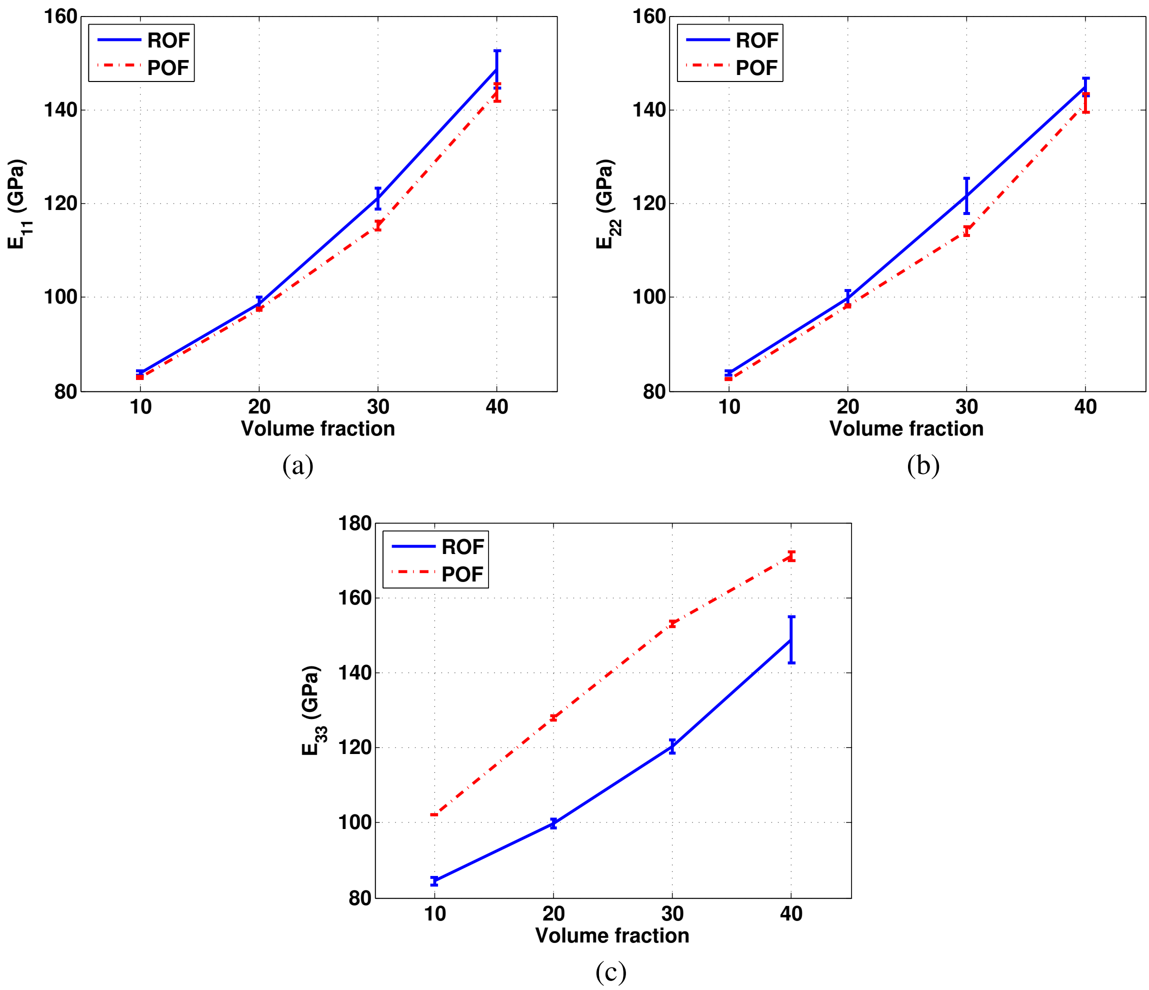



**Figure 7.** Variation of effective Young's moduli for all three directions with change in volume fraction for ROF and POF composites.

$E_{33}$ with change in aspect ratio $L/D$ of the fibers for ROF and POF composites. From Table 2 it can be observed that with respect to change in aspect ratio of fibers, there are no significant variations in effective Young's moduli along the three coordinate directions for ROF composites. This is not true for POF composites, which show a significant variation in $E_{33}$ with the increase in aspect ratio of fibers. Along the transverse direction, $E_{11}$ and $E_{22}$ of POF composites are slightly less than these parameters for ROF composites, but variations in the transverse Young's moduli with respect to the aspect ratio of fibers are not significant.

## 5. Conclusions

Numerical homogenization tools have been developed and presented for the evaluation of the effective material properties of short fiber reinforced composites. The effective material properties of randomly oriented fiber (ROF) and parallel-oriented fiber (POF) composites were obtained using these tools and

| Aspect ratio $L/D$ | $E_{11}$ (ROF) | $E_{11}$ (POF) | $E_{22}$ (ROF) | $E_{22}$ (POF) | $E_{33}$ (ROF) | $E_{33}$ (POF) |
|---|---|---|---|---|---|---|
| 1 | 83.73 | 83.53 | 83.79 | 83.21 | 83.85 | 83.95 |
| 3 | 83.81 | 82.68 | 83.77 | 82.34 | 84.80 | 92.96 |
| 6 | 84.57 | 82.54 | 84.27 | 81.98 | 82.94 | 98.85 |
| 9 | 85.17 | 82.16 | 83.53 | 82.19 | 84.44 | 103.98 |
| 12 | 83.74 | 81.96 | 83.85 | 82.01 | 83.92 | 104.36 |

**Table 2.** Variation of effective Young's moduli (in GPa) with change in aspect ratio of fibers length/diameter ($L/D$) for ROF and POF composites at 10% volume fraction.

compared with the results of different analytical methods. Our numerical predictions fit between the Hashin–Shtrikman bounds and are close to the results of the self-consistent approximation. We have also studied the influence of the aspect ratio of fibers on the effective material properties. These studies showed that there is no significant influence on effective material properties with increase of aspect ratio for ROF composites. However, POF composites show that along the longitudinal direction of the fibers the material behavior becomes stiffer as the aspect ratio increases.

Our investigation provides an insight into the more complex investigation of influencing factors for the macro behavior of fiber reinforced composites. We have shown that our method is reliable and offers the possibility for treatment of composites with arbitrary inclusions, for example, spheres and ellipsoids, with random distribution. Moreover, it allows the investigation of composites with more than two phases. The use of a modified random sequential adsorption algorithm allows the inclusions with different sizes to be generated so as to attain high volume fractions typical for many real composites.

The developed procedure, which combines a special geometrical preprocessor, ANSYS Parametric Design Language and ANSYS batch processing, provides a comprehensive tool for calculation of effective material properties of composites in a highly automated manner.

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Received 30 Jul 2006. Revised 2 Apr 2007. Accepted 20 Apr 2007.

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