Numerical Evaluation of the Effective Elastic Properties of 2D Overlapping Random Fibre Composites

W. Leclerc, P. Karamian, A. Vivet and A. Campbell

We present a numerical investigation of the elastic coefficients of random fibre composites with high contrast of properties. Here we consider a numerical study based on the generation of representative volume elements (RVEs) with overlapping random fibre network. Such a concept requires an important Monte-Carlo draw of patterns as well as an accurate determination of RVE size. In this paper, this latter is done by estimating the evolution of the standard deviation according to the number of realizations for given values of RVE size. We consider the use of an appropriate model for an automatic, reliable and fast generation of RVEs : the model with an n-order approximate geometry that allows the construction of complex overlapping fibre network. It is well-established that the morphology of the microstructure greatly affects the mechanical response of such kind material. Some morphological features, namely orientation, aspect ratio and dispersion are investigated by considering them as random variables in the design of RVEs. The results are subsequently linked to the percolation phenomenon that occurs when fibres overlap and form some pathways inside the soft phase. This phenomenon influences effective properties of heterogeneous media, particularly in the case of a high contrast of properties.

1 Introduction

This paper is devoted to the evaluation of elastic properties of heterogeneous media with overlapping short fibre inclusions. Here, the fluctuations of the microstucture and the high contrast of properties thwart the accuracy of the usual bounds as Voigt and Reuss, and Hashin-Shtrikman's ones (Hashin and Shtrikman, 1963). That is why our approach is based on a numerical investigation related to the generation of a large number of RVEs. This latter can be defined as a volume V large enough to take into account the microstructure of the media and sufficiently small to limit the calculation cost and respect a minimal scale ratio with the macroscopic material. We invite the reader to refer to the article of Drugan and Willis (1996) on this subject. The notion of RVE has a crucial importance in the field of heterogeneous media and requires an accurate determination depending on the material configuration. Thus, Kanit et al. (2003) set up a statistical approach to evaluate the RVE size for a given absolute or relative error ε in the case of Voronoï mosaics. According to authors, a unique large RVE can be chosen as well as several smaller ones providing that the dimensions avoid the bias related to the boundary conditions. It turns out periodical conditions yield the best results in RVE size convergence because the bias is reduced in comparison with kinematic or static uniform boundary conditions (KUBC or SUBC). Hence our choice was to perform a asymptotic evaluation of the properties by considering a large number of small and periodical RVEs according to the double-scale method described by Sanchez-Palencia (1980) and, Bensoussan et al. (1978).

We consider random short fibre composites with high contrast of properties. Such a kind material can be related to high technology composites reinforced in carbon nanotubes (CNTs). Early observations of carbon fibres and CNTs by Oberlin et al. (1976) and later by Iijima (1991) have aroused a big interest among the industrialists. Thus, for example, in the mechanical field their extraordinary stiffness associated to a low density could enable a use as reinforcement element for polymer-based composite materials. Among the first experiments made in order to conceive such materials, the works of Shaffer and Windle (1999) introduced the critical question of the morphology of the CNT network. The consequent scientific effort made to study the impact of CNT and CNT network morphology has highlighted 4 key points to master in order to optimize the properties of CNT-based composites. First, Odegard et al. (2003), among others, studied the effect of alignment. Their results show a sizeable effect of reinforcement in the preferential direction with a loss in transverse properties. Second, effect of waviness and decohesion was checked out by several authors whose Fisher et al. (2003) and Shao et al. (2009). Third, an important aspect ratio of inclusions is a well-known factor of reinforcement in fibre composites. This assumption stays true in the case of nanoparticles (see Odegard et al. (2003)). Finally, an important effect of

morphology is related to the dispersion of inclusions inside the soft phase. In the example of CNTs, Van Der Waals interactions tend to agglomerate them in bundles. The resulting inhomogeneous distribution turns out greatly affecting the mechanical response of the composite (see Villoria and Miravete (2007), and, Seidel and Lagoudas (2006)). However, consider a uniform distribution as undermining the reinforcement is a premature conclusion. Jeulin and Moreaud (2005, 2006b,a); Moreaud (2006) investigated the clustering phenomenon by a two-level Boolean scheme of spheres. Their purpose was to quantify the percolation phenomenon that occurs when pathways are formed by inclusions inside the matrix. Their results showed low percolation thresholds that highlighted an effect of reinforcement for a heterogeneous distribution of fibres.

In this work, first, we introduce a modelling adapted to take into account the overlapping phenomenon that is crucial to consider effects of percolation inside the matrix : the model with an n-order approximate geometry. The idea is to approximate the geometry of fibres by considering a grid of quadrangular elements and an adaptive mesh refinement process introduced by Berger and Colella (1989). The paradigm is adapted to an automated, reliable and fast generation of random RVEs taking into account overlaps. Some comparisons in time and results with a classical geometry are given as well. Second, we put up the RVE size determination by a statistical approach based on the variance estimate. Results in number of realizations are provided for different values of the absolute error. Third, a direct comparison of effective Young's, bulk and shear moduli is carried out with Voigt and Reuss, and, Hashin-Shtrikman bounds (Hashin and Shtrikman, 1963) and, self-consistent Halpin-Tsai estimates (Halpin and Kardos, 1976), (Wall, 1997). In a fourth step, we consider the investigation of different morphological parameters, namely orientation, aspect ratio and dispersion. In this last case, we use a two-scale Boolean scheme of circles to model the agglomerates. The investigation is done for agglomerates of a size equals to fibre diameter and a range of circle area fraction *f* between 60 and 100 % of the RVE. Finally, we link our results with the percolation threshold that is evaluated for different configurations of CNT network with the help of the model by classifying described by Jeulin and Moreaud (2007).

2 Numerical Modelling

The modelling we consider is based on a 2D periodical representative volume element (RVE). That deals with a representative pattern of an inhomogeneous material the size of which requires an accurate investigation. Indeed the pattern has to be small enough in comparison with the medium dimensions and sufficiently large to take into account enough informations on the microstructure and the network of fibres (Kanit et al., 2003). Here we considered periodic boundary conditions and the effective properties are evaluated by a Monte-Carlo draw of a large number of RVEs. The number of random draws greatly influences on the convergence of the homogenized properties and depends on the RVE size that will be subsequently investigated. The mesh and the geometry related to the representative patterns are created with the Cast3M software developed by the CEA. We consider plane and periodic RVEs for which the main morphological parameters of the inclusions namely, the fibre length, diameter, orientation and distribution are introduced as random variables. Each parameter can be fixed or follow a probability law as a Gaussian or a logarithmic-normal distribution. Each fibre considered in this article will be represented as a plane section of cylinder according to a straight or curved direction. In this section, RVE size is fixed to an adimensional value of 4, fibre length follows a Gaussian law around a mean value of 0.4 with a standard deviation of 0.08. Hence we have a mean scale factor of 10 between the dimensions of RVE and inclusions. The diameter of each fibre is fixed to 0.02 and we consider random oriented inclusions. Interactions between fibres are allowed and we suppose perfect bondings at the interface fibre/matrix.

2.1 RVE Model with Smooth Boundaries

First we consider a RVE model with smooth boundaries. This model respects the hypotheses introduced previously with a fibre represented as smooth section of cylinder. Figure 1 exhibits an example of RVE with the exact geometry built from a program which we have coded in Cast3M. We can observe in light (yellow) the polymer matrix and in dark (red) some fibres.



Figure 1. Periodical representative volume element of the CNT-reinforced polymer for the model with smooth boundaries

Some calculations performed with this model highlight some drawbacks related to the mesh construction. The first defect is the CPU calculation time which is too long to generate RVEs. For example if we want to create a representative pattern with a 5 percent fibre area fraction the calculation time is near to 1 minute with a processor Intel(R) Xeon(R) W3520 @ 2.67 GHz. That is a severe drawback to evaluate homogenized properties by putting into place a sample of several thousands of RVEs. Second, the mesh design becomes very difficult when we have numerous inclusions. Indeed the hypothesis of overlapping requires to recreate the connected interface around each aggregate formed by the intersected fibres. This step becomes very difficult to set up when we have a lot of inclusions with complex intersections inside the RVE and affects drastically the reliability and the automation of the design of a large sample of representative patterns. Another problem is related to the triangular elements which can be very elongated with the model with the exact geometry for which the mesh is created by triangulation around the interfaces. This kind of structural defaults in the mesh cannot be neglected because they generate ill-conditioned matrices in the calculation of the homogenized properties. We conclude that the RVE model with smooth boundaries is not suitable to perform a large generation of representative patterns and consequently to evaluate the mechanical properties of heterogeneous media. We must conceive a new, suitable and reliable model to avoid the different defaults highlighted here.

2.2 RVE Model with a 0-Order Approximate Geometry

In reality the boundaries of the fibres are often discontinuous. Thus, for a CNT fibre, the edge is made of a discrete lattice structure of C-C bonds. An idea is to conceive a model for which the inclusions are not represented with smooth boundaries but with an approximate geometry according to a structured grid of quadrangular elements and a local adaptive mesh refinement process (L.A.M.R., see Berger and Colella (1989)). Such a kind concept enables a tremendous diminishing in calculation cost and allows a totally reliable generation of overlapping fibres. This modelling is called RVE model with an n-order approximate geometry and depends on an n-order related to the degree of approximation of the geometry compared to the model with smooth boundaries. It corresponds to the ratio in power of 2 between the fibre diameter and the size of the quadrangular elements. Hence, on one hand, ∞ -order model is geometrically equivalent to the model with smooth boundaries. On the other hand, the 0-order provides a geometry for which the fibre diameter is equal to the size of elements, see Figure 2. This latter enables the fastest generation of RVEs and maintains a sufficient accuracy in the calculation of effective properties.



Figure 2. Periodical representative volume element of the CNT-reinforced polymer for the model with a 0-order approximate geometry

2.3 Construction of the RVE Model with a 0-Order Approximate Geometry

Our modelling depends on an initial grid of elements for which the size is not equal to the fibre diameter but is several times larger, up to a multiplicative factor parameter chosen by the user. The locations of the centres of gravity are either randomly drawn or distributed according to a probability law as the Gaussian law. All morphological parameters are set up in the same way. First, each inclusion is represented as a segment subdivided according to the fibre diameter. The next step consists in determining the elements of the coarse grid intersecting the straight segments. Thus we get coarse overlapping fibre that we refine locally according to a L.A.M.R. method to obtain elements of the size equivalent to the fibre diameter. The process is finished when we have gathered the refined elements with a fibre label inside the boundaries of the coarse nanoparticle. In the last step we subdivide each quadrangular element into two triangular elements and create the mesh of the matrix by triangulation around the boundaries of the hard medium and the RVE.

2.4 Comparative Study between Approximate and Smooth Geometry

Here, we set up a comparative study in results and calculation time between the models with smooth boundaries and an approximate geometry. For this purpose, we consider the 0, 1 and 2-orders and the model with smooth boundaries for which the convergence in mesh refinement is achieved. Table 1 exhibits the CPU time t^1 (in seconds) and the relative scatter of the effective Young's modulus (e_{rel}) obtained between the two models for the discussed orders.

	2%		4%		6%		8%		10%	
Model	e_{rel}	t								
0-order	1.62	0'02''47	4.07	0'04''26	6.11	0'06''05	7.45	0'07"88	8.91	0'09"85
1-order	0.456	0'11''82	2.33	0'23'16	3.98	0'35''47	4.75	0'49"53	5.34	0'65"'53
2-order	0.109	0'11"14	0.962	0'22'28	1.67	0'34''95	1.76	0'50"18	1.97	0'67"47
∞ -order	_	0'09''49	-	0'23''28	_	0'55''90	_	2'09''00	-	4'31''00

Table 1. Comparison in CPU time t (in seconds) and relative scatter of Young's modulus (e_{rel}) of the two discussed models

The results highlight an acceptable adequacy between the smooth and approximate geometries for a fibre area fraction less than 10%. The lower the order is, the greater the fibre area fraction is, the greater the relative scatter is. Thus, for an area fraction of 10%, we obtain a relative scatter of 8.91%. This value exhibits a sensitive effect of geometry which is diminished for a higher order. In the case of the CPU time, the results highlight the real contribution of the model with an approximate geometry. Thus, for a fibre area fraction fixed at 10% the calculation cost is decreased from 4 minutes and 31 seconds to only 9 seconds passing from smooth boundaries to the 0-order approximate geometry.

3 Determination of the RVE Size

The crucial issue of the RVE size is investigated in this section. We use a statistical approach that was developed by Kanit et al. (2003) in the framework of Voronoï mosaics but we consider random fibres composites with high contrast of properties. For this purpose, an important Monte-Carlo draw of RVEs for different sizes is set up in the framework of the isotropy and the model with a 0-order approximate geometry. The question of the appropriate number of realizations is studied by considering an accurate study of the variance parameter. Furthermore, we assume fibres as a hard continuous medium with an isotropic transverse behaviour and the matrix as an isotropic one. Here the fibre length follows a Gaussian law around a mean value of 0.4 with a standard deviation of 0.08. The diameter of each fibre is fixed at 0.02 and the inclusions are randomly oriented. Interactions between fibres are allowed and we suppose perfect bondings at the interface fibre/matrix. Moreover, in the case of fibres, the longitudinal Young's modulus is fixed at 4.2 and the shear one at 1.55.

¹Quadricore Intel(R) Xeon(R) W3520 @ 2.67 GHz

3.1 Effects of RVE Size

The RVE size must respect several conditions to respect the representativeness of the RVE in a homogenization process. First, a suitable RVE has to be large enough to take into account sufficient informations on the microstructure of the material. However a large RVE affects the calculation cost and loses its elementary aspect. Furthermore, an important drawback is related to the boundary conditions that introduce a bias in the calculation of the effective properties. The RVE area A can be linked to a given absolute error ε_{abs} and the standard deviation of the investigated effective property Y, $D_Y(A)$. Thus, for n independent realizations of area A, we have,

$$\varepsilon_{abs} = \frac{1.96D_Y(A)}{\sqrt{n}} \tag{1}$$

In other words, the calculation of the interval confidence for large samples of RVEs yields the suitable RVE size for given number of realizations and absolute error ε_{abs} . Therefore, a critical point is related to the following question, do we have to consider a small number of realizations of large RVEs or a large number of realizations of small RVEs to obtain the expected error ε_{abs} ? As regards the calculation cost the second assertion gives the best performances. However too small RVEs widely affect the accuracy of the effective properties because a bias is introduced by the boundary conditions (Sab, 1992), (Ostoja-Starzewski, 1998). This latter can be reduced in the case of periodic conditions (Kanit et al., 2003) but still exists. Figure 3 b) illustrates the evolution of the mean effective Young's modulus for different values of RVE size between 1.5 and 4 and an area fraction fixed at 5 %. The number of realizations for each RVE size is obtained so that the relative error ε_{rel} is less than 0.002. We observe a convergence of the effective property according to the RVE size around a mean value of 5.6. Besides, the standard deviation $D_Y(A)$ slightly decreases in the same time.

3.2 Number of Realizations and Calculation Cost

Figure 3 b) exhibits the evolution of the number of realizations according to the RVE size for an area fraction fixed at 5 %. Here, the relative error ε_{rel} is 0.005. The CPU time to carry out the corresponding realizations is illustrated on the same figure. We observe the greater the RVE is, the lower the number of realizations is, the greater the CPU time becomes. Thus the investigation of the calculation cost does not exhibit an optimal value of RVE size but a steady evolution according to the same parameter. Hence, the suitable size has to be chosen by considering the convergence of the effective property Y that describes the influence of boundary conditions. Here we have consciously limited our study to a RVE size of 4 for which, on the one hand, the convergence in Y is observed and, on the other hand, the calculation cost stays reasonable.



Figure 3. a) Parallel evolutions of the standard deviation and the Young's modulus according to the RVE size for a fibre area fraction fixed at 5%

b) Parallel evolutions of the number of realizations and the corresponding calculation time according to the RVE size for a fibre area fraction fixed at 5% and a relative error of 0.005

4 Comparison with Bounds

Analytical bounds provide a limited approximation of the effective properties as bulk, shear and Young's moduli in the framework of the linear elasticity. Indeed microstructure and statistical informations are difficult to take into account in a micromechanics model. However, Hashin-Shtrikman's bounds (Hashin and Shtrikman, 1963), (Benveniste, 1987) as well as Halpin-Tsai's self-consistent estimates (Halpin and Kardos, 1976), (Wall, 1997) enable to perform an interesting comparison with numerical results. Here, we consider a comparative study with bounds under the hypotheses previously presented and the assumption of an effective isotropic medium.



Figure 4. a) Evolution of the Young's modulus according to the fibre area fraction and comparison with Voigt and Reuss bounds and Halpin-Tsai estimates

b) Evolution of the bulk modulus according to the fibre area fraction and comparison with Hashin-Shtrikman bounds

c) Evolution of the shear modulus according to the fibre area fraction and comparison with Hashin-Shtrikman bounds

First, the effective Young's modulus is investigated in comparison with Voigt and Reuss bounds and Halpin-Tsai's estimates (see Figure 4 a)) which are obtained by considering extreme cases of longitudinal and transversal orientations of the material (Villoria and Miravete, 2007). We notice that the mean curve increases continuously according to the load rate of fibres inside the RVE. All data are localized between the bounds and the interval confidence is very narrow around the fitting curve obtained by a multiple linear regression. Second, we consider a similar study for the effective bulk and shear moduli which are compared to Hashin-Shtrikman's bounds. Figures 4 b) and c) illustrate the evolutions of the two moduli according to the area fraction of fibres. We observe that our results are all localized between the bounds as well. Therefore, the comparisons allow us to suppose our results are conform to the bounds.

5 Results and Discussion

In this section, the impact of some morphological features of fibres on the effective properties is studied. We consider the parameters of alignment, aspect ratio (or slenderness ratio) and distribution. According to several authors (Pötschke et al., 2003, 2004), (Jeulin and Moreaud, 2005, 2006b,a; Moreaud, 2006) the percolation phenomenon induces a significant improvement of effective properties. This phenomenon is related to the appearance of pathways inside the soft phase for a high load rate of fibres. This latter can be quantified by the statistical parameter of percolation threshold that corresponds to the required fibre area fraction to obtain 50% of RVEs for which the phenomenon is observed. Here, we evaluate both this parameter and elastic moduli for each discussed parameter. A final comparison of results is performed. It highlights a narrow link between percolation and reinforcement. Here, we consider RVEs for which both the representation and the material properties of fibres are the same as in the section 3.

5.1 Impact of Fibre Alignment

First, we suppose the fibres are not randomly oriented but perfectly aligned according to a preferential direction. In this case the composite material does not follow an elastic isotropic behaviour law anymore but an elastic orthotropic one according to the preferential direction. Contacts between inclusions are only allowed in their extremities. Figure 5 a) illustrates the evolution of the longitudinal Young's modulus according to the fibre area fraction, a comparison is made with the isotropic model and for three Gaussian models for which we consider a disruption of the alignment according to a Gaussian law. We remark that Young's moduli in the case of aligned fibres are drastically more important than for randomly oriented ones. Moreover, we can observe that the Gaussian models are scarcely affected by the amplitude of disruption (5, 15 or 25 degrees). The same figure exhibits the evolution for the shear modulus. In this case, the effective property is clearly diminished for aligned fibres and the disruption is much more significant. Thus the fibre alignment enhances the longitudinal effective properties to the detriment of transverse ones.



Figure 5. a) Evolution of effective Young's and shear moduli according to the fibre area fraction for aligned fibres

b) Evolution of the percolation rate according to the fibre area fraction for aligned fibres

An assessment of percolation rate was performed according to the method described by Jeulin and Moreaud (2006b) for the discussed models. A preliminary estimation was done in the case of an isotropic medium. The process consisted in generating a large data base of RVEs for which the percolation of the fibre network was subsequently evaluated. The results yielded a percolation threshold of 15.93 under the assumptions of randomly oriented fibres with aspect ratio 20. This value is near to different theoretical and empirical evaluations. Thus Sharma et al. (2006), in the framework of in-plane conductivity of spray metallic coatings, found a threshold close to 16. Other estimations done by Jeulin and Moreaud (Jeulin and Moreaud, 2006b, 2007) in the case of a 3D Boolean model of parallel cylinders gave percolation thresholds along axial and orthogonal directions of the axis of cylinders of 12.50 and 15.96. Their calculations for sphero cylinders with axis in the same plane and aspect ratio 5 yielded

percolation thresholds along axial and orthogonal directions of 12.94 and 16.125. Here, the estimations for aligned fibres give higher percolation thresholds except for the Gaussian model with a disruption of 25 degrees. Thus, the more the fibres are aligned the greater the percolation threshold is and the more the composite is strengthened along the preferential direction.

5.2 Impact of Fibre Aspect Ratio

We investigate the parameter of aspect ratio that is the ratio between the length and the diameter of fibres. For this purpose, we suppose an isotropic medium of randomly oriented fibres. A calculation was performed on 4 values of aspect ratio : 10, 20, 50 and 100. Large samples of RVEs were constructed in each case for different lengths (and corresponding diameters) and area fractions. Furthermore, the RVE size is fixed at 4 except for the last value for which it is 8. Figure 6 a) exhibits the influence of the aspect ratio on the Young's modulus for different fibre area fractions. We observe that the more the fibres are slender the more the composite is reinforced. Besides, we remark that the RVE size affects our results if not properly chosen. Thus, the calculation of the effective Young's modulus is undermined in the case of an aspect ratio of 100 for which the RVE size is 4 and the fibre length is fixed at 1. A new calculation performed with RVEs of size 8 yield results in agreement with the linear behaviour of the effective property according to the aspect ratio.





b) Evolution of the percolation rate according to the fibre area fraction for different aspect ratios

Figure 6 b) illustrates the influence of the aspect ratio on the percolation rate. The more the fibres are long and thin, the more the percolation phenomenon appears. Thus, the percolation threshold is multiplied by three, from 7.66 for aspect ratio of 50 to 22.05 for aspect ratio of 10. It turns out that the enhancement of effective Young's modulus is simultaneous to the appearance of percolation phenomenon.

5.3 Impact of Fibre Dispersion

A heterogeneous distribution of fibres inside the soft phase is well-known to influence the effective properties of fibre composites (Villoria and Miravete, 2007; Seidel and Lagoudas, 2006). The key issue is related to the real impact of the dispersion. Indeed, according to Jeulin and Moreaud (2007); Willot and Jeulin (2009, 2011), a suitable arrangement of 3D agglomerates inside the matrix enhances the effective properties of the material. Their works were based on a 2-scale Boolean scheme of spheres that models the distribution of clusters of fibres inside RVEs. Numerical estimations of percolation threshold performed by the authors in the case of heterogeneous media highlighted a simultaneous improvement of percolation and reinforcement. Here, we use the Boolean scheme to generate heterogeneous RVEs but we limit our study to circles with diameter equal to fibres' one. In other words, the scale factor between the inclusions and the agglomerates is fixed at 1. Figure 7 a) illustrates the scheme for which the RVE size is 4 and fibres are randomly oriented. The length of inclusions is fixed at 0.4 and the diameter at 0.02 so that the aspect ratio is 20. Figure 7 b) shows the corresponding final RVE with a mesh of 3-node triangular elements.



Figure 7. a) Boolean scheme of circles with centres of gravity of fibres b) Final RVE with mesh

In a first step the percolation threshold of the Boolean scheme of circles was evaluated under the assumption of a random distribution of overlapping circles. A value of $a_c = 62.045$ was found that is largely higher than the one estimated in the case of spheres in 3D (28.95 according to Rintoul and Torquato (1997)). However the assessment is close to the threshold estimated by Quintanilla and Ziff (2007) in the case of 2D overlapping circles (67.635). Thus, the dispersion of fibres was investigated for an area fraction of circles more than a_c so that the percolation phenomenon might be possible. Figure 8 a) shows the impact of the area fraction of circles on the evolution of the Young's modulus according to the fibre area fraction. We observe that the lower the area fraction of circles is the lower the effective Young's modulus is. Moreover, figure 8 b) illustrates the influence of the dispersion of fibres on the percolation thresholds yield values more than the one estimated in the case of a homogeneous distribution of inclusions. However the results obtained here are restricted to a scale factor fixed at 1 while the benefit of a fibre dispersion is only checked out for higher ratios according to Jeulin and Moreaud (2005, 2006b,a); Moreaud (2006).

6 Conclusions

The evaluation of effective elastic properties of 2D overlapping random fibre composites by Monte-Carlo draws of RVEs requires an accurate preliminary investigation. First, the RVE size can affect the results if not properly chosen. This one has to be sufficiently large to be representative of the heterogeneous material. Second, the minimal number of realizations has to be estimated by considering the evolution of the variance for a given expected error. Third, the representativeness of the pattern is related to the spatial arrangement, the morphology of fibres, the contrast of properties and the hypotheses of construction of the fibre network such as the authorization of overlaps. Therefore, the preliminary study must be repeated for each discussed configuration of fibres and fibre network.

The effective properties widely depends on the morphology of fibres. Thus, the alignment, the aspect ratio and the dispersion of fibres have a significant effect on the mechanical response. The dependance of properties on the configuration of fibres can be related to the percolation phenomenon which appears when fibres overlap and form some pathways inside the soft phase. This latter is quantified by the percolation threshold that is the required percolation rate to get 50 % of RVEs for which the phenomenon is observed. The calculation of the threshold for the discussed configurations highlight a narrow link between the enhancement of effective properties and the percolation. For example, long and thin fibres improve the phenonemon as well as they strengthen the material. However, this conclusion is only true for isotropic media. Thus, in the case of an alignment of fibres, the enhancement of longitudinal properties is simultaneous to an increase of percolation threshold.

The issue of the fibre dispersion is a key point to investigate. Here, we considered a Boolean scheme of circles to introduce a heterogeneous distribution of inclusions. A scale ratio between the RVE size and the diameter of circles was fixed at 10. Different parameters such as the scale factor between the size of agglomerates and the length of fibres, and the area fraction of circles inside each RVE affect the effective properties. Here the survey was restricted to a scale factor of 1 and an area fraction of circles from 60 % to 100 %. The results showed a sensitive

diminishing of effective properties as well as an increase of percolation threshold under these hypotheses. However, a 2D inhomogeneous dispersion of fibres is more suitably simulated by considering higher scale factors. Thus, an in-depth study of this parameter is required as well as a 3D setting of the model with an n-order approximate geometry to detect possible dimensional effects.



Figure 8. a) Evolution of the Young's modulus according to the fibre aspect ratio for different area fractions of circles

b) Evolution of the percolation rate according to the fibre area fraction for different area fractions of circles

Acknowledgement The authors wish to thank the regional council of Lower-Normandy for its financial support of Willy Leclerc's PhD.

References

- Bensoussan, A.; Lions, J.; Papanicolaou, G.: *Asymptotic analysis for periodic structures*. Springer Verlag, North Holland, Amsterdam Edn. (1978).
- Benveniste, Y.: A new approach to the application of mori-tanaka's theory in composite materials. *Mechanics of Materials*, 6, 2, (1987), 147 157.
- Berger, M. J.; Colella, P.: Local adaptive mesh refinement for shock hydrodynamics. *J. Comput. Phys.*, 82, (1989), 64–84.
- Drugan, W.; Willis, J.: A micromechanics-based nonlocal constitutive equation and estimates of representative volume element size for elastic composites. *Journal of the Mechanics and Physics of Solids*, 44, 4, (1996), 497 524.
- Fisher, F. T.; Bradshaw, R. D.; Brinson, L. C.: Fiber waviness in nanotube-reinforced polymer composites–i: Modulus predictions using effective nanotube properties. *Composites Science and Technology*, 63, 11, (2003), 1689 – 1703, Modeling and Characterization of Nanostructured Materials.
- Halpin, J.; Kardos, J.: The Halpin-Tsai equations : a review. *Polymer Engineering and Science*, 16, 5, (1976), 344 352.
- Hashin, Z.; Shtrikman, S.: A variational approach to the theory of the elastic behaviour of multiphase materials. *Journal of the Mechanics and Physics of Solids*, 11, 2, (1963), 127 140.
- Iijima, S.: Helical microtubules of graphitic carbon. Nature, 354, (1991), 56 58.
- Jeulin, D.; Moreaud, M.: Multi-scale simulation of random sphere aggregates application to nanocomposites. 9th European Congress on Stereology and Image Analysis, Zakopane, Poland, (2005).
- Jeulin, D.; Moreaud, M.: Percolation d'agrégats multi-échelles de sphères et de fibres application aux nanocomposites. Congrés matériaux, Dijon, (2006).

- Jeulin, D.; Moreaud, M.: Percolation of multi-scale fiber aggregates. S4G 6th international Conference, Prague, (2006).
- Jeulin, D.; Moreaud, M.: Percolation of random cylinder aggregates. Image Anal. Stereol., 26, (2007), 121 127.
- Kanit, T.; Forest, S.; Galliet, I.; Mounoury, V.; Jeulin, D.: Determination of the size of the representative volume element for random composites: statistical and numerical approach. *International Journal of Solids and Structures*, 40, 13–14, (2003), 3647 3679.
- Moreaud, M.: *Propriétés morphologiques multi-échelles et prévision du comportement diélectrique de nanocomposites.* Ph.D. thesis, Ecole des Mines de Paris, Centre de Morphologie Mathématique, Fontainebleau (2006).
- Oberlin, A.; Endo, M.; Koyama, T.: Filamentous growth of carbon through benzene decomposition. *Journal of Crystal Growth*, 32, 3, (1976), 335 349.
- Odegard, G. M.; Gates, T. S.; Wise, K. E.; Park, C.; Siochi, E. J.: Constitutive modeling of nanotube-reinforced polymer composites. *Composites Science and Technology*, 63, 11, (2003), 1671 1687, Modeling and Characterization of Nanostructured Materials.
- Ostoja-Starzewski, M.: Random field models of heterogeneous materials. *International Journal of Solids and Structures*, 35, 19, (1998), 2429 2455.
- Pötschke, P.; Alig, I.; Dudkin, S.: Dielectric spectroscopy on melt processed polycarbonate-multiwalled carbon nanotube composite. *Polymer*, 44, 17, (2003), 5023 5030.
- Pötschke, P.; Bhattacharyya, A. R.; Janke, A.: Melt mixing of polycarbonate with multiwalled carbon nanotubes: microscopic studies on the state of dispersion. *European Polymer Journal*, 40, 1, (2004), 137 148.
- Quintanilla, J. A.; Ziff, R. M.: Asymmetry in the percolation thresholds of fully penetrable disks with two different radii. *Phys. Rev. E*, 76, (2007), 051115.
- Rintoul, M. D.; Torquato, S.: Precise determination of the critical threshold and exponents in a three-dimensional continuum percolation model. *Journal of Physics A.*, 30, (1997), 585 592.
- Sab, K.: On the homogenization and the simulation of random materials. *European Journal of Mechanics*, 11, 5, (1992), 585 607.
- Sanchez-Palencia, E.: Non-homogeneous media and vibration theory, 127 (1980), Berlin.
- Seidel, G. D.; Lagoudas, D. C.: Micromechanical analysis of the effective elastic properties of carbon nanotube reinforced composites. *Mechanics of Materials*, 38, 8-10, (2006), 884 907, Advances in Disordered Materials.
- Shaffer, M.; Windle, A.: Fabrication and characterization of carbon nanotube/poly (vinyl alcohol) composites. *Advanced Materials*, 11, 11, (1999), 937 941.
- Shao, L. H.; Luo, R. Y.; Bai, S. L.; Wang, J.: Prediction of effective moduli of carbon nanotube-reinforced composites with waviness and debonding. *Composite Structures*, 87, 3, (2009), 274 281.
- Sharma, A.; Gambino, R. J.; Sampath, S.: Anisotropic electrical properties in thermal spray metallic coatings. Acta Materialia, 54, 1, (2006), 59 – 65.
- Villoria, R. G. D.; Miravete, A.: Mechanical model to evaluate the effect of the dispersion in nanocomposites. Acta Materialia, 55, 9, (2007), 3025 – 3031.
- Wall, P.: A comparison of homogenization, hashin-shtrikman bounds and the halpin-tsai equations. *Application of Mathematics*, 42, 4, (1997), 245 257.
- Willot, F.; Jeulin, D.: Elastic behavior of composites containing boolean random sets of inhomogeneities. *Interna*tional Journal of Engineering Science, 47, 2, (2009), 313 – 324, dedicated to Valery Levin's 70th Birthday.
- Willot, F.; Jeulin, D.: Elastic and electrical behavior of some random multiscale highly-contrasted composites. *International Journal of Multi-scale Computational Engineering*, 9, 3, (2011), 305 326.

Address: Willy Leclerc, Philippe Karamian, Alexandre Vivet and Alain Campbell,

University of Caen Lower-Normandy, Mathematics laboratory Nicolas Oresme, Campus 2, Bld maréchal Juin, 14032 Caen.

email:willy.leclerc@unicaen.fr; philippe.karamian@unicaen.fr