

OPTIMIZATION OF ELASTICITY OF UNIDIRECTIONAL NON-OVERLAPPING FIBER REINFORCED MATERIALS

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Abstract

The aim of this work is to efficiently select samples of non-overlapping parallel fiber reinforced composites with regard to their elasticity and their fiber distribution in the composite cross-section.

The samples were built with the help of the simulated annealing technique according to chosen Radial Distribution Functions. For each sample the fields of local stresses were simulated by finite element method, then homogenized by volume averaging in order to investigate their elastic properties. The effect of RDF shape on elastic properties was quantified. The more the fiber distributions deviate from Poisson's Law the higher the effective elastic moduli are. A method to select samples of real fiber reinforced composites according to their elasticity is proposed.

Keywords: Fiber-reinforced materials; Finite elements ; Homogenization ; Microstructure ; Simulated annealing; Elasticity.

1. Introduction

Elasticity of materials built with longitudinally arranged fibers in a matrix (Fiber-reinforced composites) can be sensitive to the fiber distribution. The aim of this work is to provide an efficient elasticity criterion of selection for real materials with regard to their fiber distribution.

Determination of the laws of their macroscopic linear elasticity requires, in addition to knowledge of the laws of the behavior of each individual component, an averaging of local properties or homogenization. In this work, numerical homogenization was applied to digital samples. The change on effective elasticity was evaluated with regard to the second order correlations of the fiber distribution which were modified with the help of simulated annealing. At low volume fraction; $V_f < 20\%$ effective elasticity is known to be barely sensitive to fiber localization while at high volume fraction $V_f > 40\%$, closer to jamming limit, the possibilities to modify fiber distributions are restrained. Therefore

results presented here, deal with a moderate volume fraction of fibers $V_f = 30\%$.

2. Morphology

Initially, the fibers were located by a process of random sequential adsorption within a frame of square section that avoids fiber overlapping through a repulsion criterion $|r_{ij}| > 1$ where r is the dimensionless position vector such as $|r_{ij}|$ is equal to 1 at contact between fibers i and j .

2.1 Radial Distribution Function

In addition of volume fraction V_f , microstructures of fiber reinforced composites can be characterized statistically by different types of correlation functions^[1]. In case of isotropic composites built with similar non-overlapping fibers of identical circular section, the Radial Distribution Function (RDF) $g(r)$ ^[2] is the easiest one. The physical interpretation of $g(r)$ is the number of fiber centers located in an annulus of radius r and thickness dr centered on a test fiber, divided by the number of fibers given by a uniformly distributed fiber field.

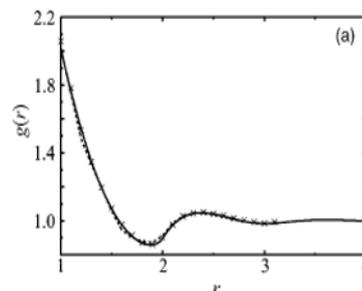


Fig1. The correlation function $g(r)$ computed from the PY equation for $V_f = 36.29\%$

Naturally, the non-overlapping condition implies that for $r < 1$ $g(r) = 0$. Then approximately for $1 < r < 1.5$, $g(r)$ always exhibits a peak (except for very low volume fractions or perfect-gas-like distribution of fibers) denoting frequent occurrences of close-together fibers followed by a deficient of RDF, as shown on Fig.1^[3].

2.2 Simulated Annealing

The simulated annealing method [4][5][6] consists of rearranging the particles initially in a given microstructure in order to evolve toward a desired new configuration. Technically, the ensemble of fibers is assimilated to a canonical ensemble in which fibers were moved in order to reach a state of lower energy. A randomly chosen fiber was displaced by a random distance Δr in a random direction, both provided by a Poisson law. The maximum value of Δr was adjusted to optimize the efficiency of the global process. Δr must never exceed the value of the mean free path in statistical physics. At each move of a fiber, a change in energy of the system ΔU was evaluated and called on a probabilistic law of accepting the move (ΔU) :

$$P(\Delta U) = \begin{cases} 1 & , \Delta U \leq 0 \\ e^{-\beta \Delta U} & , \Delta U > 0 \end{cases}$$

in which β is the Boltzmann factor that is the second parameter to be adjusted. Both ΔU and β are not necessarily real energies. The process was repeated until the desired state is reached.

Here, we focus on increasing the peak of $g(r)$ within the range of $1 < r < 1.5$.

According to statistical physics, the averaged energy of the system can be related to $g(r)$ by:

$$U \propto -\ln[g(1 < r < 1.5)]$$

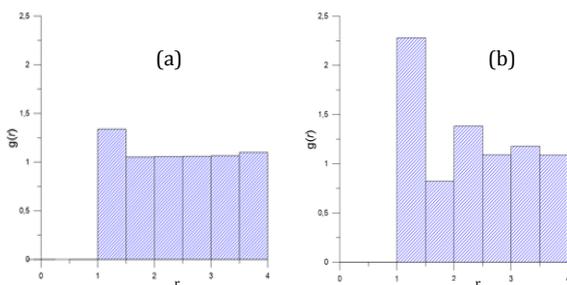


Fig.2 $g(r)$ for $V_f=30\%$ at (a) initial state and (b) after 20000 moves

Fig.2 shows the increase of the values of $g(1 < r < 1.5)$ with the number of moves by simulated annealing.

Due to the convergence difficulties, $g(r)$ is not presented as curves but as histograms with steps of 0.5.

3. Homogenized values

The homogenization method consists of applying finite element calculations of linear elastic behavior on different samples (Fig.3). The boundary conditions are the usual periodic conditions (PBC).

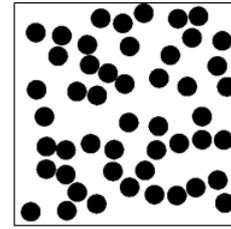


Fig.3 Non-overlapping sample cross section at $V_f = 30\%$

The images samples studied were of 49 inclusions at a volume fraction of 30%. Young's moduli and Poisson's ratios were respectively for the matrix and the fibers:

$$E_m = 10GPa, E_f = 1000GPa, \nu_m = \nu_f = 0.3$$

Fig.4 describes the evolution of the effective values of bulk and shear moduli with regard to the peak of RDF $g(1 < r < 1.5)$. Because 49 inclusions are not enough to reach RVE, the effective properties resulted from averaging on 25 samples. These results always agree with the lower second order bounds HS⁻ of Hashin and Shtrikman [7]. As expected, they tend to be closer to the lower bound HS⁻ that is known to well fit the behavior of common random fiber reinforced composites.

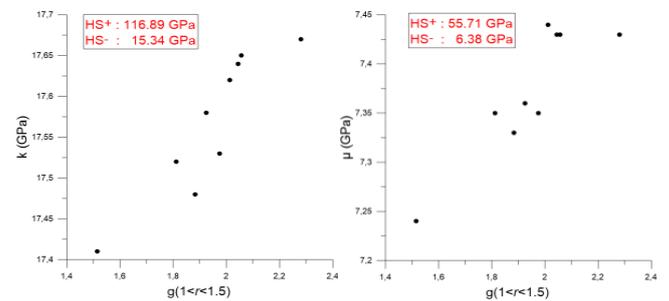


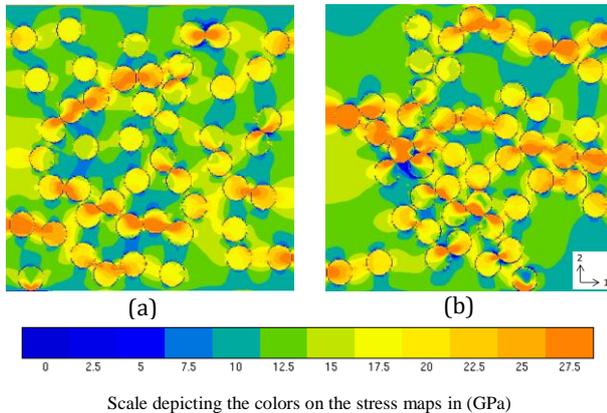
Fig.4 Evolution of macroscopic bulk (k) and shear (μ) moduli with regard to $g(1 < r < 1.5)$

In spite of a light dispersion due to a number of inclusions reduced to 49 on only 25 samples, the overall evolutions on Fig.3 clearly show an increase of effective physical properties with the height of $g(r)$ peaks.

From $g(1 < r < 1.5) = 1.5$ to $g(1 < r < 1.5) = 2.3$ the bulk modulus increases of 1.5% and the shear modulus of 2.6% . It can simply be explained: as the $g(r)$ peak increases, a higher rate of close-together fibers is observed which creates paths of high stresses.

Fig.5 shows maps of normal stresses obtained by numerical simulations on the two samples of different values of $g(r)$. The paths of high stresses always form line segments aligned in the direction of stresses under consideration. These lines are built by succession of jumps from one fiber to the closest and generate high

stresses not only in the stiff fibers but in the inter-fiber spaces as well.



4. Conclusion

The set of numerical results presented here reveals that homogenized elasticity on the overall samples of unidirectional non-overlapping fiber reinforced composites is sensibly influenced by second order correlations such as RDF. Even a small fiber rearrangement can increase or decrease stiffness.

The simulated annealing method (SA) applied in this study is a numerical process and so cannot be used in production of practical composites, such as fiber reinforced resins. However it is easy to extract RDF from snapshot of real composite section by image processing [8]. Then the values of $g(r)$ at short range ($1 < r < 1.5$) could be a good indicator of the relative stiffness between different samples and so lead to the optimization of production processes.

From a modeling perspective, the local behavior exhibited by stress maps suggests that pertinent scaling for fiber reinforced material stiffness cannot be reduced to volume fraction. Similar observations have already been reported by J. Botsis et al [9] about strength. The volume fraction macroscopic scale has to be supplemented by a micro-scale such as nearest neighbors distance that is able to capture occurring of small area of high stresses. When fibers start to agglomerate, a third scale might be required to take into account the formation of large pores where lower stresses reduce the effective values as suggested by M.-D. Rintoul and S. Torquato [10].

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