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Morphological Modeling and Simulation of Random Microstructures for Physical Applications

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Materials and biological microstructures show heterogeneity at various scales. This can be handled through a probabilistic approach, which enables us to model and to simulate the microstructures, in order to be able to estimate spoiled or missing data, or physical properties of heterogeneous media.

A first step in this approach deals with a *random structure characterization*. For instance, when considering two-phase materials, we use a model of random set A [1,2,3], fully characterized from a probabilistic point of view by its Choquet capacity T(K) defined on the compact sets K, from equation 1 below, where *P* denotes a probability:

$$T(K) = P\{K \cap A \neq \Phi\} = 1 - P\{K \subset A^c\} = 1 - Q(K)$$

In practice, T(K) can be estimated by area fraction measurements on images (from true microstructures, or from simulations), after morphological dilation of the set A by the set K, or calculated for a given theoretical model. Equation 1 is used for the identification of a model (estimation of its parameters, and test of its validity).

A second step is to build *random morphological models* at the micro scale. We use models defined in the Euclidean n dimensional space, with usually good stereological properties (the identification can be made on 2D or 1D sections). Starting from the Poisson point process, different types of grain models were proposed: the Boolean model [1,2], generated by the union of random grains located on the Poisson germs; the sequential dead leaves model [3,4] can provide multiphase textures. These random sets models have their counterpart as random functions models (scalar or multivariate, to generate multi-spectral textures) [2,4]: the Boolean random functions were initially developed to generate rough surfaces. The dead leaves model provide a good process of simulation of perspective views, which can be used for the morphological analysis of powders from SEM images [5]. More complex microstructures can be modeled and simulated by combinations of basic models. For instance multi-scale models, using union or intersections of Boolean models, were proposed to reproduce the distribution of carbon black in nanocomposites materials [6]: the model generates aggregates of nanoparticles, and zones of repulsions between aggregates. Its identification is made from TEM micrographs obtained on thin slices, and account for their thickness. FIG. 1 shows a 3D simulation. Starting from 3D images of composite materials obtained by microtomography, it was possible to propose a model of sphere stacking respecting the statistics of their centers in 3D boxes [7]. Finally, a different class of models, based on reaction-diffusion models, which are solutions of parabolic non-linear stochastic partial differential equations, generate many realistic classes of 3D textures, which evolve with time according to a chemical and to a transport process [8].

In the last step, models can be used in the *prediction of the average macroscopic response of random media from their microstructure*. This point, also called homogenization, is very useful in order to be able to design specific microstructures with given physical properties (thermal or electrical conductivity, dielectric permittivity, elastic moduli, optical properties, etc.). From a partial knowledge of the microstructure (namely from correlation functions of second or third order), it is possible to provide bounds of the effective properties depending on the properties of its components

[9,10]. These bounds can lead to the definition of so-called "optimal materials" with respect to given properties. More recently, 3D microstructures (real or simulated) are introduced into a numerical solver in order to solve the homogenization problem. This opens the door to so-called "*digital materials*". For instance, we could predict the effective dielectric permittivity of carbon black nanocomposites by solving the Gauss equation (div D = 0, D being the dielectric displacement) on 3D simulations of the multi-scale material. The resolution is made by iterations of Fourier transforms, since the problem can be formulated as an integral equation involving a convolution product [11,12]. Similarly, the effective elastic moduli of random media were calculated using finite elements on 3D simulations of complex microstructures [13]. The following points must be addressed for this approach to be successful: (i) one needs to know the *local physical properties* of the components of the medium, and therefore local measurements are required (even on a microscopic scale, as for the dielectric permittivity in [12]); (ii) since numerical simulations are always performed with a finite size with respect to the microstructure, an assessment of the statistical representativity of the prediction must be given. This can be done by a probabilistic approach of the so-called RVE (*Representative Volume Element*) [10,13].

References

[1] G. Matheron, *Random Sets and Integral Geometry,* J. Wiley, New-York, 1975.
[2] J. Serra, *Image Analysis and Mathematical Morphology,* Academic Press, London, 1982.
[3] D. Jeulin (ed), *Advances in the Theory and Applications of Random Sets*, World Scientific, Singapore, 1997.
[4] D. Jeulin, *Modèles morphologiques de structures aléatoires et de changement d'échelle*, Thèse de Doctorat d'Etat, University of Caen, 1991.
[5] D. Jeulin, *J. Microscopy* 172 (1) October (1993) 13.
[6] L. Savary et al., *Acta Stereologica*, 18 (3) (1999) 303.
[7] A. Delarue and D. Jeulin, *Image Anal. Stereol.*, 20 (3) (2001) 186.
[8] L. Decker and D. Jeulin, *Acta Stereologica,* 18 (2) (1999) 247.
[9] D. Jeulin, In: *Mechanics of Random and Multiscale Microstructures*, D. Jeulin and M. Ostoja-Starzewski (ed.), CISM Lecture Notes N° 430, Springer Verlag, Berlin, 2001.
[10] D. Jeulin, In: *Tribute to Georges Matheron*, F. Meyer and M. Schmitt (ed.), Springer Verlag, Berlin, 2005.
[11] A. Delarue and D. Jeulin, In "*Proc. Matériaux 2002* » (Tours, France, 21-25 October 2002).
[12] S. Paciornik et al., *Eur. Phys. J. App. Phys*., 21 (2003) 17.
[13] T. Kanit et al., *Int. J. solids and structures*, 40 (2003) 3647.

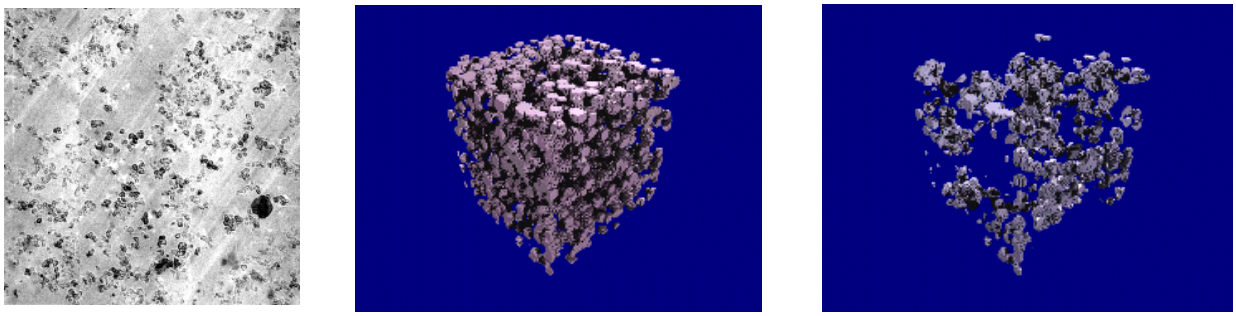

FIG. 1. 3D Simulation of a three-scales nanocomposites carbon black-resin (center and right) from TEM micrographs (magnification 17100 (1,5x x1,5 μm^2)) (left) [6,11,12].

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