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Numerical modeling of the flax fiber morphology variability



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ABSTRACT

This paper provides a methodology for the numerical modeling of the scattering observed in the geometry of plant fiber cross-sections. It is well known that the observed random microstructures are expected to have a significant impact on the calculation of their effective properties. The solution proposed here to model randomness in the fiber boundary contour, which has never been done in the past to the author's knowledge, is based on a randomized version of the Fourier expansion of its complex coordinate function. The involved random variables have been identified from a large set of 2D optical micrographs and the methodology has been applied both to elementary fibers and bundles which are simultaneously observed on composite sections. This model is found to be sufficiently relevant to render the morphometric factors of the observed fibers in a statistical sense. This contributes to the microstructural modeling of composites reinforced by natural fibers.

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1. Introduction

Environmental and sustainability issues prompt the industrial community to reconsider its modes of design and manufacture. In this context, most industrial sectors are nowadays engaged in an "eco-design" approach. This includes a reduction in their consumption of petrochemical resources and a progressive transition toward renewable resources.

In the field of materials science, a large amount of research work is currently being undertaken to propose high-performance materials that comply with the new environmental regulations. Fully green composites based on natural resources for both matrices and reinforcements appear attractive for a wide range of applications [1,2] but much more work is still needed before they can be extensively used in structural applications [3,4]. Natural fibers to reinforce either renewable or fossil carbon matrices as an alternative to synthetic fibers are therefore widely investigated by the research community, see, for example, surveys on bast fibers [4-9]. Among the latter, there is a growing trend to employ flax fibers in composite materials due to their competitive specific characteristics compared to those of glass fibers [10]. These plant fibers exhibit low density, a high aspect ratio, relatively high specific mechanical properties, good vibration and sound absorption properties, with a good environmental footprint and ready availability. Nevertheless, the commercial success of long flax fiber reinforced polymers for high performance structural applications will depend on the reliability of their final mechanical properties. So far, one of the major drawbacks to flax composites results from a marked variability in their properties [6,10,11].

The composition and properties of both long flax fibers and derived composites have up to now mainly been attained through experimental approaches, see, for example, Refs. [10,12-16]. The nature of plant fiber reinforced composites makes difficult micromechanical modeling based on analytical approaches. Recourse to numerical simulations may appear to be a more suitable alternative to experimental work. Micromechanical calculations have become more and more affordable in recent years and should therefore be viewed as cost-effective and powerful tools for a better understanding and prediction of the materials' behavior. They are expected to provide information on the correlation between the material microstructure and the material macroscopic properties and to enable the simulation of local damage phenomena.

Researchers who develop computational techniques and homogenization theories for such purposes agree with the need to accurately model the randomness in microstructures revealed by optical or electronic micrographs. So far, very few works have however been devoted to numerical modeling of long flax fiber reinforced polymers, see, for example, Refs. [17,18]. Most methodologies have recently been developed for synthetic fiber reinforced composites and metal materials, see, for example, Refs. [19-30]. Some of these works focus on suitable tools that enable a quantitative characterization and the simulation of the spatial dispersion of microstructural features [19-24,27,29,30]. Some methodologies propose homogenization procedures and Finite Element (FE) simulation techniques [20-22,25-27] whilst others assess the influence

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of microstructure on macroscopic properties [19,20,23,28]. Efforts have also been made to incorporate the size and orientation distributions of particles of regular shapes into the numerical models [19,24,28].

These micromechanical studies do not usually address the shape distribution modeling of material features because the considered materials do not always require such levels of detail. This is generally true for plastics reinforced by synthetic fibers which show quasi-perfect circular shapes and therefore no morphology dispersion. Singh et al. [24] propose to account for the complex shapes of SiC particles embedded in an aluminum alloy matrix through FE analyses. No modeling of their morphology scattering is suggested. The strategy solely lies in the collection of real images of these SiC particles and their random distribution in the simulation space. Even if this work does not permit the simulation of new particle shapes representative of real ones but not yet spotted, this emphasizes the need to take into account the dispersion in particle morphology.

Contrary to synthetic fibers with well-defined cross-sections and no diameter variation along the fiber length, flax fibers and, more generally, biofibers have a much more complex structure. The geometry of natural fibers, which depends on their growing harvesting and processing conditions, might exhibit large dispersions [11]. Thomason et al. [31] emphasizes through statistical analyses that the randomness in natural fiber shape may have a significant impact on the characterization of the mechanical properties of their composites. The research community should therefore be aware that the influence of randomness in the geometry and spatial distribution of these fibers (due to their composition and manufacturing process conditions) on the variability in the final mechanical behavior of reinforced composites may be substantial, even if this has not yet been thoroughly assessed. This calls for the expansion of new numerical strategies during the design process which should include such sources of variability in order to control their effects on the quality and reliability of the resulting composite structures. More generally speaking, these approaches should belong to the overall concept of virtual testing whose objectives are to give a better prediction of the constitutive laws of materials, give new schemes for the design of such materials and gain insights into the effects of microstructural details on their properties.

The present work contributes to this research area by focusing on the uncertainty quantification in flax fiber morphology. This represents an essential step towards a realistic description of the microstructure of composites reinforced with flax fibers, which will in turn serve to identify the most influential microstructural parameters by carrying out sensitive analyses on its macroscopic properties. Here, the objective is to propose an original procedure to model randomness in the flax fiber cross-section so as to allow the simulation of virtual fibers with the same geometrical and statistical properties. In this work, we only model the outer boundary of the flax fiber cross-section. We therefore do not represent the lumens and we make the assumption that bundles form an homogeneous material whose mechanical properties differ slightly from those of elementary fibers [17]. The approach is based on a randomized version of the Fourier expansion of the complex boundary coordinate function. Hundreds of embedded flax fibers have been observed and measured to adjust the coefficient distributions of the Fourier representation with theoretical Probability Density Functions (PDF). Monte Carlo Simulation (MCS) is then performed to produce virtual fibers whose geometrical properties are compared with those of observed fibers. Usual shape factors (area, perimeter, convexity, etc.) are computed for this purpose. The methodology is applied both to elementary fibers and to bundles also called "technical fibers" which are simultaneously observed in flax reinforced polymers.

2. Materials and image processing

2.1. Description of material and image acquisition

The flax considered in this study was supplied by Safilin in the shape of long tows of retted, scutched and hackled fibers. A dozen tows which gather both elementary fibers (*i.e.* single fibers) and bundles (*i.e.* technical fibers) are embedded longitudinally in an epoxy resin and cut transversally with a glass knife. Composite sections are then stained with toluidine blue and captured using an optical microscope. A sufficiently high resolution is required to identify correctly fiber sizes and shapes, see, for example, Fig. 1(a). By scanning and analyzing 10 images, approximately 850 elementary fibers and 175 bundles are gathered.

2.2. Image processing and boundary contour extraction

Contrast issues (optical marks and traces of the stem bark in the resin presenting the same gray values as some fibers, fibers or lumens exhibiting different gray values, etc.) hinder the direct use of automatic algorithms which aim to extract the boundary contours of flax fibers and bundles. Several manual pre-processing steps are required. A "home-made" procedure is therefore proposed to progressively convert the 10 observed images into images that can be automatically processed. The main steps read as follows:

- Clean the digital images using a manual pixel-by-pixel approach: carefully erase flaws, stem bark and burred pixels on the outline of the fibers. Also remove fibers crossing the image boundaries.
- 2. Enhance the brightness contrast of grayscale images prior converting to binary. A threshold value of approximately 190 on the grayscale (0–255) is here found to allow sufficiently differentiation and is therefore used for all pictures.
- Fill the holes which represent either the lumen of elementary fibers or the pectic cement inside the bundles.
- 4. Then, smooth the fiber contours by applying an opening operation. This consists in removing outgrowths of the boundaries smaller than a preset element, the so-called "structuring element". We here choose a 2 × 2-pixel square structuring element. The reader should refer to Refs. [32,33] for details on basic definitions and tools used in image analysis and mathematical morphology.

The open source GNU Image Manipulation Program Gimp 2.8 is used for the first step. This free software allows high magnification and offers accurate drawing tools. Steps 2–4 are then performed using ImageJ, a public domain Java-based image processing software, and the Image Processing toolbox of Matlab.

The detection of fiber and bundle 2D-outlines is then automatically performed using an in-house developed code based on the *bwboundaries* Matlab function. The shape boundaries gathered in the 10 images are one pixel thick and their coordinates are stored in text files. Fig. 1(b) plots the fiber and bundle outlines automatically retrieved by the program.

2.3. Statistical properties of the morphology of observed flax fiber cross-sections

2.3.1. Morphometric features

The morphology of the collected flax fiber cross-sections is statistically studied in this section. Seven morphometric features are introduced for this purpose. They feature:

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