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Regeneration of surface roughness by the Langevin equation using stochastic analysis on AFM image of a carbon fiber

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ABSTRACT

A new method was developed using AFM images of a fiber surface to regenerate the surface roughness in 3D geometry, such as the cylindrical shape of a "model" fiber. The Langevin equation was used to derive the fluctuations of a carbon fiber surface image. The equation contains two quantities, $D^{(1)}(h)$ and $D^{(2)}(h)$ which in physics represent drift and diffusion coefficients. Knowing this coefficient and adding a proper noise function, a similar surface of larger dimension with the same statistical properties of the initial data was created. The generated surface was mapped into cylindrical coordinates, then a mesh generated. The resulting reconstructed surface, input over the geometry of a cylindrical shape, can be implemented for finite element analysis of a single fiber surrounded by matrix and generalized to a many fiber model.

1. Introduction

Because of its stiffness, dimensional stability, corrosion resistance and low weight, carbon fiber epoxy composites become predominate in space application namely for support structures, antenna and dishes [1,2]. In aerospace and marine industries, carbon fiber composites have been replaced with structural materials like aluminum or titanium to reduce weight and increase fuel efficiency. Carbon fibers are also used in the automotive industry [3], as gas storage cylinders, for robot arms, turbine blades, and sporting goods. Manufacturers can generally reduce the total weight and utilize the stiffness of carbon fiber. Cost was an issue preventing application of carbon fibers in smaller industries, but recently by decreasing the price of such composites, there is an increasing appearance of carbon fiber composites for new applications [4]. Recent fiber reinforced composite technology success benefits from improvement in analytical models for optimization of fiber to matrix volume fraction, fiber size, orientation, and distribution along with experimental efforts on fiber surface treatments to increase interface adhesion and strength [5]. Recently, long thin diameter fibers have become available which have a high ratio of surface to unit volume. This large ratio of surface-to-volume increases the value of development of new methods in the field of composite analysis which considers the surface properties of the fiber/matrix interface. The fact that failure may initiate from a weak or defective fiber/matrix interface and consequently reduce ultimate performance, increases current interest in improving and understanding interfacial bonding of the fiber with matrix [6]. Remarkable improvement in the mechanical properties and performance of composites have been achieved using nanofiller-modification in the polymer matrix, which increases the interfacial stress transfer efficiency, and reduces the local stress concentration in the interface between the fiber and matrix [7,8]. Similar enhancement is also obtainable using one of various available surface treatments [9]. Statistical analysis on atomic force microscopy (AFM) images of carbon fibers during the surface treatment is an effective tool that can be used to characterize the treatment [10–12]. A problem with this technique is the near impossibility to scan the entire surface of a typical fiber by AFM to produce a profile of surface height in different positions. Since the fiber has a cylindrical curvature, a difficult full range of 360° scan would be sought. However, just scanning a representative portion of the fiber is possible. This encourages finding a way to reproduce the surface using representative information. To be representative, the regenerated surface must retain the statistical properties of the original. In the current work statistical analyses were done on AFM images to create 3D models of fibers having surface roughness similar to the actual fibers. One can implement this model to predict the mechanical response of an interface area between fiber and matrix, required for simulating realistic surface geometries. Similar work has been done to input real dental crown geometry for FEA (finite element analysis) analysis using Abaqus software [13]. The change in idea here is using AFM images to reconstruct the geometry instead of using X-ray tomography to reconstruct the accurate body.

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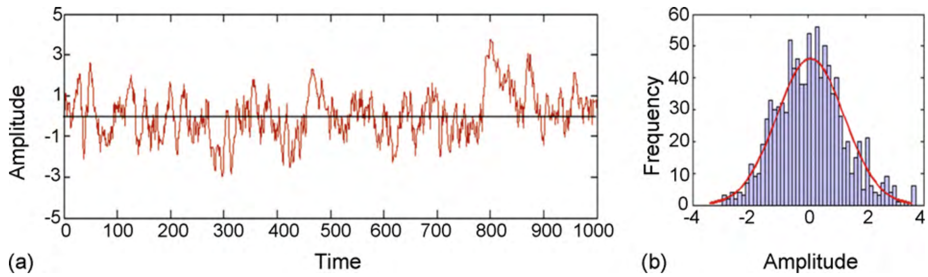

Fig. 1. (a) Random noise numbers with zero mean for ±4 range. (b) Gaussian distribution corresponding to random noise used in (a).

2. Method of stochastic analysis using Langevin equation

A typical surface topography of a carbon fiber consists of the global geometric dimensions with diameters in the range of 5–7 μm. The surface is made up of sub-micron features consisting of troughs and grooves which typically range from +100 nm to −100 nm in height from the basal surface. A conventional optical light microscope with 100× magnification is only capable of resolving the macroscopic micron sized features. However observations using high magnification techniques such as Scanning Electron Microscopy (SEM) or AFM reveal the sub-micron features. The surface of a carbon fiber is smooth when looking under the optical microscope at 100× magnification, but the same surface will be rough when looking under a SEM or by AFM where magnifications are orders of magnitude greater.

Characterization of the morphology depends on the scale of observation and resolution of the system employed. Recently, the size of fiber diameters has reduced, even carbon nano-tubes of nanometer size are commonly considered for reinforcement [14,15]. When the size of a fiber diameter reduces, the effective surface area for a constant volume fraction increases and surface morphology effects on the strength of composite material becomes significant. Atomic force microscopy, which is one of the powerful and practical techniques to obtain surface geometry, at sub-micrometer to micrometer scales, is generally implemented to obtain topography of flat or curved surfaces.

One way to regenerate a surface is to find statistical coefficients of the surface using the Langevin equation as in the following [16].

$$\frac{d}{dx}h(x) = D^{(1)}(h) + \sqrt{D^{(2)}(h)f(x)} \tag{1}$$

Using Eq. (1), one can readily regenerate a surface statistically similar to the original surface [17,18]. In Eq. (1) $D^{(1)}$ (h,r) plays the role of a deterministic component of the regenerated surface while the $D^{(2)}$ (h,r) coefficient generates and controls the noisy nature of the surface height fluctuations which are introduced by the $f(x)$ noise function. In fact, $f(x)$ is a random zero mean with a Gaussian distribution. Unlike applications in electronics, noise here is not completely a result of external sources and undesired detected signals. The concept of noise here is small random fluctuations of the real surface, which carries physical meaning and has statistical properties. Fig. 1a illustrates a 1000 random noise number with a zero mean in the ±4 interval produced by a Matlab program which has a Gaussian distribution (Fig. 1b).

The probability density function (PDF) is a function that describes the density of probability at each point in the collected data space. An AFM image data, containing the spatial information pertaining to the location and roughness forms the matrix for the PDF. By convention P $(h_1; r_1; t_1; h_2; r_2; t_2, \ldots, h_n; r_n; t_n)$ denotes the probability of finding a point located in r_1 (x, y) position in an image matrix at time t_1 at a height h_1 and r_2 at a height h_2 at the later time t_2 and so forth up to r_n at a height h_n at time t_n. In our case PDF is a time independent function. If we calculate all possibilities for the probability density functions ($i = 1$ to 256 and $j = 1$ to 256), we obtain complete stochastic information for a given AFM image. For any given process without memory called Markov process [19] a simple Chapman–Kolmogrove equation can be used for $r_1 < r_2 < \cdots < r_n$. The n-scale joint PDF functions can be expressed by a multiconditional PDF function.

$$\begin{aligned} &P(h_1; r_1, h_2; r_2, \ldots, h_n; r_n) \\ &\quad = P(h_1; r_1 | h_2; r_2, \ldots, h_n; r_n) \\ &\qquad .P(h_2; r_2 | h_3; r_3, \ldots, h_n; r_n) \ldots P(h_{n-1}; r_{n-1} | h_n; r_n). \end{aligned} \tag{2}$$

where $P(h_i;r_i|h_j;r_j)$ denotes a conditional probability, which is defined as the probability of finding r_i height h_i under the condition that at r_j the value h_j was found.

The Chapman–Kolmogrove equation formulated in differential can take the Fokker–Plank equation [16].

$$\frac{d}{dx}p(h, r) = \left[-\frac{\partial}{\partial h}D^{(1)}(h, r) + \frac{\partial^2}{\partial h^2}D^{(2)}(h, r) \right] p(h, r) \tag{3}$$

In the Fokker–Plank equation the term $D^{(1)}$ (h,r) describes the deterministic part of the process and is denoted as a drift term, and $D^{(2)}$ (h,r) is the variance of a Gaussian noise as a diffusion term. The $D^{(1)}$ (h,r) and $D^{(2)}$ (h,r) can be estimated directly from the data and moment of conditional probability distributions,

$$M^{(k)} = \frac{1}{\Delta r} \int dh'(h' - h)^{(k)} p(h', r + \Delta r | h, r) \tag{4}$$

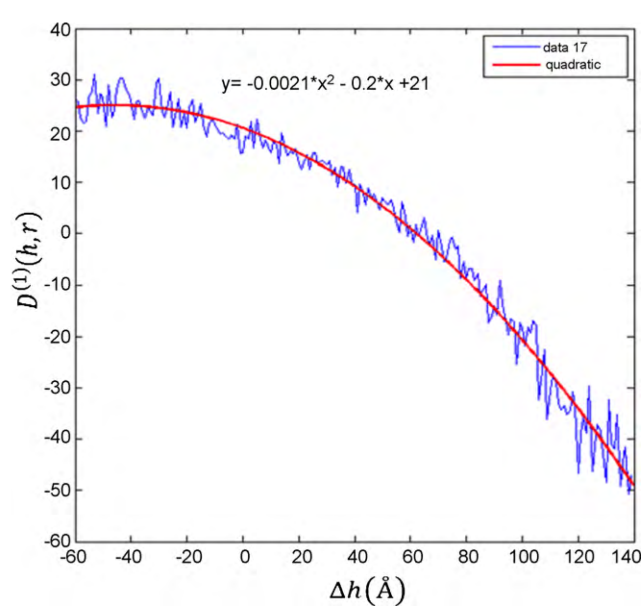

Fig. 2. Drift coefficient $D^{(1)}$ (h,r) for $r = 4$ nm as function of Δh.