Fractal Analysis of AFM Data Characterizing Strongly Isotropic and Anisotropic Surface Topography

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Abstract. This study discusses changes in angle-dependent fractal parameters determined for surfaces with different anisotropy ratios. The studied surfaces were PG (Bruker), TGT1 and TGZ1 (NT-MDT) calibration standards as models of isotropic and anisotropic surfaces. Surface topography was scanned using Atomic Force Microscopy (AFM). The obtained results indicate that fractal parameters (fractal dimension, topothesy) can be easily derived in each case, and that changes in their angle-dependent characteristics can be associated with the anisotropy ratio.

Introduction

There are many examples of scaling-law behavior that can be seen in time-dependent and/or spatial properties of natural objects. This includes the formation of solid surfaces, the evolution of geographic object contours, morphology of molecular clusters, aggregates, fibrous and porous materials. Since their fractal properties extend over an infinite range of scale lengths, they are referred to as self-similar fractals and are described solely by the fractal dimension (F). In contrast, man-made objects are subjected to further restrictions due to a finite range of material. In this case, surface morphology is fully described by two parameters: fractal dimension (F) and topothesy (K), which simultaneously characterize scalable surface features at different levels: from the smallest details to the longest wavelength components. Such objects are referred to as self-affine fractals.

Every manufacturing process leaves its unique fingerprint on the surface by forming it in a specific manner which can be studied by means of fractal parameters. Hence, fractal analysis enables the tracing of each manufacturing process back to the original surface state [1, 2]. In order to achieve that goal, however, it is necessary to determine whether and how fractal properties of isotropic and anisotropic surfaces change with surface orientation at a given stage. The aim of this study was to analyze angle-dependent characteristics of fractal parameters as a function of the surface anisotropy ratio.

Methods

Several methods of calculating fractal parameters have been developed for self-affine surfaces [1-3]. Among them, a method that relies on the calculation of the areal autocorrelation function (AACF) prior to the calculation of the structure function (SF) appears most effective. The AACF is defined as:

$$R(\tau) = \left\langle z\left(x\right) \cdot z\left(x+\tau\right) \right\rangle \tag{1}$$

where: τ is the delay (lag) between two points in the plane of the analyzed surface, and > denotes the mean value.

Following the determination of the AACF, the structure function can be calculated as a function of the lag τ according to:

$$S(\tau) = 2 \left| R(0) - R(\tau) \right| \tag{2}$$

A plot of the profile structure function on a log-log scale exhibits characteristic features: it increases linearly at the shortest wavelengths, but it is asymptotically saturated at the longest wavelengths. It can be shown [1] that for any self-affine fractal profile, $S(\tau)$ is determined by fractal parameters according to the formula:

$$S(\tau) = K\tau^{2(2-F)} \tag{3}$$

The above indicates that fractal dimension and topothesy along a given surface orientation can be easily determined from the slope and the intercept of the structure function drawn on a log-log scale.

Angle-dependent surface properties give rise to the surface anisotropy. Stout et al. [4, 5] quantitatively described anisotropy using parameter S_{tr} (also referred to as the anisotropy ratio), defined as the ratio of two extreme separation lengths τ_{min} and τ_{max} corresponding to the fastest and the slowest decay of the AACF value from 1 to 0.2, respectively:

$$0 < S_{tr} = \frac{Min\{\tau : R(\tau, \theta) \to 0, 2\}}{Max\{\tau : R(\tau, \theta) \to 0, 2\}} \le 1$$

$$\tag{4}$$

where: $R(\tau, \theta)$ is the AACF expressed in polar coordinates. Thus, it is possible to establish two main anisotropy axes on the surface, a_1 , and a_2 , which are parallel to the directions of the fastest (τ_{min}) and the slowest (τ_{max}) AACF decay, respectively.

In order to determine angle-dependent fractal parameters, two-dimensional AACF and SF functions were calculated based on AFM topography scans of three calibration standards: TGT1, TGZ1 (NT-MDT) and PG (Bruker). AFM measurements were carried out using Multimode 8 (Bruker) microscope in the contact mode (ScanAsyst-Air (Bruker) SPM tip, diameter 2 nm, spring constant 0.4 N/m). The scanned areas ($10x10 \ \mu m^2$) were sampled at 512 equidistant points at a low scan rate of 1 Hz. The resulting topographic images with their 2-dimensional AACFs are presented in Fig. 1.

Results and Discussion

The main axes of anisotropy (a_1 and a_2) are shown in AACF maps. Angles θ_{a1-a2} between the axes were determined at 77⁰, 45⁰ and 90⁰ for TGT1, PG and TGZ1, respectively. The obtained values of the anisotropy ratio S_{tr} reached 0.9 (TGT1), 0.916 (PG) and 0.073 (TGZ1), respectively. Since the extreme value of S_{tr} could reach 1 (perfectly isotropic surfaces) and 0 (highly anisotropic surfaces), the analyzed surfaces represented two extreme cases of surface lay. It should be noted, however, that the PG sample appeared isotropic in terms of S_{tr}, although upon close inspection, it seemed to have crossed lay.

To determine angle-dependent fractal properties, profiles of structure functions observed at angle θ relative to direction a_1 were drawn, and from each plot, fractal dimension F and topothesy K were determined according to Eq. (3). The results are shown in Fig. 2. When the direction was changed from a_1 to a_2 , the fractal dimension of TGT1 varied between 1.1 and 1.2, and it reached minimum value at $\theta = 40^{\circ}$, whereas in the PG sample, fractal dimension varied between 1.2 and 1.3, reaching a minimum at 15° . In Fig. 1, the directions of minimum F were marked as a_{1+40} and a_{1+15} , respectively. As a rule, the angle at which F reached its minimum was that of the longest repetition period, both in topography images and in AACF maps. Conversely, anisotropic standard TGZ1

exhibited fractal dimension F that monotonically increased from 1.3 (a₁ axis) to 1.5 (a₂ axis and surface lay). The changes observed in this case could be explained by a power-law dependence. It should be noted, however, that although F values for the PG sample were placed between the corresponding values for TGT1 and TGZ1, the angular characteristics of F were indicative of isotropic surfaces regardless of its crossed lay. On other hand, the reported F values are smaller than those given by Thomas et al. [3], in whose study, the majority of fractal dimensions of machined surfaces ranged between 1.3 and 1.6. The above authors observed that F was invariant with orientation for an isotropic surface, but it remained constant in every direction, excluding parallel, to the lay for a highly anisotropic surface [3]. The above discrepancy can be attributed to surface formation mechanisms (scratching vs. point etching for machined surfaces and AFM calibration standards, respectively). It could also be explained by the fact that AFM images resulted from a convolution of the actual surface topography and the AFM tip.



Fig. 1. Surface topography images (upper row) and corresponding spectra of the autocorrelation function (lower row) of the calibration standards (respectively): (A) TGT1, (B) PG, (C) TGZ1.



Fig. 2. Changes in fractal dimension (left), and topothesy (right) with respect to the main anisotropy axis a_1 of the studied samples.

Changes in topothesy K as a function of observation angle with respect to the a_1 axis are shown in Fig. 2b. In general, topothesy reached a very small value with the order of 10^{-4} µm, although it behaved in a different manner depending on the anisotropy ratio. TGT1 and PG samples (isotropic surfaces) exhibited higher K values which reached a maximum at the same angle at which the fractal dimension reached its minimum. In contrast, the topothesy of a strongly anisotropic surface (TGZ1) remained constant at a very low level regardless of the observation angle. Our results are, however, inconsistent with the findings of Thomas [3] in whose study, the topothesy of isotropic surfaces appeared to be higher in comparison with anisotropic surfaces. In the cited work [3], the topothesy for anisotropic surfaces was rather sensitive to orientation, and a smooth but marked decrease was noted as it approached the a_2 lay direction. Once again, due to similar measurement methods, the observed discrepancy could be attributed to different surface formation mechanisms.

Conclusions

The method for evaluating fractal parameters based on the 2-dimensional autocorrelation function and the structure function is straightforward to compute, and it reveals important information about the topography and history of the surface. Our results indicate that angle-dependent fractal dimension is very sensitive to surface orientation for anisotropic surfaces, but it is less sensitive for isotropic surfaces. In the latter case, however, F approaches the minimum in the direction of the longest repetition period of surface topography, whereas in the former case, the fractal dimension increases monotonically upon turning from direction a_1 to a_2 .

An analysis of fractal parameters' suitability for characterizing surface anisotropy revealed that only the topothesy of samples with pronounced lay appears to be insensitive to orientation. This observation creates new opportunities for applying fractal analysis and AFM methods in studies that investigate changes in surface topography caused by, for example, internal stress. When fractal parameters of a stress-free and loaded surface are compared in terms of sample distortion, the degree of plastic deformation could be possibly determined.

Unfortunately, the proposed approach to the characterization of surface anisotropy seems to produce results that are inconsistent with those given by other authors. In our opinion, those discrepancies result mainly from differences in surface formation mechanisms. The results of our study contribute valuable observations that fractal analysis is not only sensitive to surface isotropy/anisotropy, but it is also highly influenced by surface treatment, and that the behavior of angle-dependent fractal characteristics could vary significantly subject to surface finish.

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