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Model to estimate fractal dimension for ion-bombarded materials

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ABSTRACT

Comprehensive fractal Monte Carlo model ITMC-F (Hu and Hassanein, 2012 [1]) is developed based on the Monte Carlo ion bombardment simulation code, i.e., Ion Transport in Materials and Compounds (ITMC) code (Hassanein, 1985 [2]). The ITMC-F studies the impact of surface roughness on the angular dependence of sputtering yield. Instead of assuming material surfaces to be flat or composed of exact self-similar fractals in simulation, we developed a new method to describe the surface shapes. Random fractal surfaces which are generated by midpoint displacement algorithm and support vector machine algorithm are combined with ITMC. With this new fractal version of ITMC-F, we successfully simulated the angular dependence of sputtering yield for various ion-target combinations, with the input surface roughness exponent directly depicted from experimental data (Hu and Hassanein, 2012 [1]). The ITMC-F code showed good agreement with the experimental data. In advanced, we compare other experimental sputtering yield with the results from ITMC-F to estimate the surface roughness exponent for ion-bombarded material in this research.

1. Introduction

Fractal is a concept introduced by Benoît Mandelbrot in 1975. It is based on the mathematical assumption of

$$(\text{line})^{\frac{1}{1}} = (\text{area})^{\frac{1}{2}} = (\text{volume})^{\frac{1}{3}} \tag{1}$$

From Eq. (1), if a rough surface has a dimension D greater than 2, it should obey the modified relationship [3]:

$$(\text{area})^{\frac{1}{D}} = (\text{volume})^{\frac{1}{3}} \tag{2}$$

In fractals, the property that same pattern repeats itself for all observing scales is called self-similarities. Basically, there are three groups of fractals. These are exact self-similarity, quasi-self-similarity, and statistical self-similarity. Exact self-similarity fractals appear exactly the same under any scales. Usually this kind of fractal is defined from iterated function. Quasi-self-similarity fractals appear in distorted or degenerated forms in different scale. Usually they are defined by recurrence relations. The last one is the statistical self-similarity fractals. These fractals preserve the same statistical properties across scales. The representation for this group is Brownian motion.

The next question is how to calculate this type of non-integer dimensions. Mathematician Felix Hausdorff made two important concepts to fractal dimensions, the Hausdorff measure and Hausdorff dimension. Here is a plain interpretation: if a given object will double its size with three copies, the dimension for this object is $d = \frac{\log 3}{\log 2} = 1.44427$ which is not an integer. More generally speaking, if C copies are needed with the size becomes "a" times for a "d" dimension object, the fractal dimension is therefore $d = \frac{\log C}{\log a}$.

For the mathematical definition of Hausdorff dimension, we need to introduce Hausdorff measure. Assuming an arbitrary subset $F \in R^n$ with $\{U_i\}$ is a δ-cover for F. Given nonnegative real s, $\delta > 0$, we define

$$H^s_\delta(F) = \inf\{\sum_{i=1}^{\infty} |U_i|^s : 0 < |U_i| < \delta, \forall i\} \tag{3}$$

where the infimum (the largest element which is smaller than all the elements in the set) is taken over all sequences of sets $\{U_i\}_{i=1}^{\infty}$.

If we let $\delta \to 0$, we can construct the s-dimensional Hausdorff measure by

$$H^s(F) = \lim_{\delta \to 0} H^s_\delta(F) \tag{4}$$

For Hausdorff measure definition, supposed that $t > s$ so that $t-s > 0$, and that $\{U_i\}$ is a δ-cover for F. Then we get

$$\sum |U_i|^t \leqslant \delta^{t-s} \sum |U_i|^s \tag{5}$$

and by taking infima we get

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$$H^t_\delta(F) \leqslant \delta^{t-s} H^s_\delta(F) \tag{6}$$

If $\delta \to 0$ and $H^s_\delta(F)$ is finite, it can be seen that $H^t_\delta(F) \to 0$. Also if $H^t_\delta(F)$ is finite, it means $H^s_\delta(F) \to \infty$. The interpretation of this result is that there is a critical value of s at which $H^s_\delta(F)$ changes from $\infty \to 0$. For $F \in R^n$, we define this unique value to be the Hausdorff dimension of F and denote it $\dim_H F$, where

$$\dim_H F = inf\{s : H^s(F) = 0\} = sup\{s : H^s(F) = \infty\} \tag{7}$$

It is difficult to determine Hausdorff dimension in experiments. Thus the practical way is to use the so called box-counting method. The idea of box-counting is to implement the fractal onto a uniformly divided mesh and count how many grids are needed to cover the fractal. By observing the relation between grid size and number of grids needed, box-counting dimension can be defined by these two parameters. For the mathematical definition, again we assume an arbitrary subset $F \in R^n$ with $\{U_i\}$ is a δ-cover for F. Let $N_\delta(F)$ be the smallest possible number of sets in any δ-cover of F. We define the lower box and upper box dimension by

$$\underline{\dim}_B = \underline{\lim}_{\delta \to 0} \frac{\log(N_\delta(F))}{-\log(\delta)} \tag{8}$$

and

$$\overline{\dim}_B = \overline{\lim}_{\delta \to 0} \frac{\log(N_\delta(F))}{-\log(\delta)} \tag{9}$$

If $\underline{\dim}_B = \overline{\dim}_B$ then we call the common value simply $\dim_B(F)$ or the box-counting dimension

$$\dim_B(F) = \lim_{\delta \to 0} \frac{\log(N_\delta(F))}{-\log(\delta)} \tag{10}$$

Here the terms "lower" and "upper" indicate the lower and upper limit concept in math.

So what exactly is the relationship between Box-counting and Hausdorff measure? Consider for a sufficiently small δ, such that $H^s_\delta \geqslant 1$, so for all such δ-covers U_i of F, we have

$$1 \leqslant \sum_{i=1}^{\infty} |U_i|^s \tag{11}$$

Thus in any δ-cover of F,

$$1 \leqslant \delta^s N_\delta(F) \tag{12}$$

By arranging the equation, we have:

$$0 \leqslant \log N_\delta(F) + \log \delta^s = \log N_\delta(F) + s \log \delta \tag{13}$$

$$\frac{\log N_\delta(F)}{-\log \delta} \geqslant s \tag{14}$$

So we can see that

$$\underline{\dim}_B(F) \geqslant s = \dim_H(F) \tag{15}$$

Since we always have $\overline{\dim}_B(F) \geqslant \underline{\dim}_B(F)$, the relation between Hausdorff dimension and box-counting dimension is

$$\overline{\dim}_B(F) \geqslant \underline{\dim}_B(F) \geqslant \dim_H(F) \tag{16}$$

Based on box-counting idea, numerous techniques are developed for different research topics. In 1983, Peter Pfeifer with David Avnir and Dina Farin used this concept to measure the fractal dimension of material surfaces [4,5]. They used different sizes of molecules adsorbed on material surface as shown in Fig. 1, and used Braunauer–Emmett–Teller (BET) method to measure the number of molecules adsorbed. By calculating the relationship between molecule sizes and quantity, they can determine surface roughness, and more details can be found in reference [6].

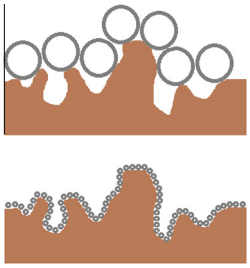

Fig. 1. Schematic of gas adsorption method.

Instead of using the relation between surface areas versus molecule cross section, in 1990s scientists started to use Scanning Tunneling Microscopy (STM) in experiments to measure the root-mean-square (rms) roughness which is defined by:

$$\sigma = < [h(x,y) - h]^2 >^{\frac{1}{2}} \tag{17}$$

where h is the average height.

Krim's group [7] used the relation of average rms roughness versus scanning size to determine fractal dimension, because the rms surface roughness increases with the sample length L following the relation $\sigma \propto L^H$. Here H is called the roughness exponent and has a value $0 < H < 1$, which relates to fractal dimension by $D = 3 - H$. There are several other methods to determine surface roughness other than gas adsorption and STM. Atomic Force Microscopy (AFM), Reflection High-Energy Electron Diffraction (RHEED), High Resolution Low Energy Diffraction (HRLEED), helium atom scattering, Transmission Electron Microscopy (TEM), as well as Scanning Electron Microscopy (SEM) all have been utilized to measure fractal dimension.

For simulation aspect, in 1989, D. Ruzic implemented a model in a code named VF-TRIM [8] to model surface roughness by adding the fractal geometry into TRIM, which is a binary-collision computer program for calculating material sputtering. The rough surface implemented in the model is composed by an exact self-similarity fractal. Snell's refraction law is considered when an incident ion entering a surface, and the fraction relation between initial incident angle α and the new angle angle α' is:

$$\sin^2\alpha' = \frac{E_0}{E_0 + E_{sb}} \sin^2\alpha \tag{18}$$

In the equation, E_0 is the incident energy and E_{sb} is the surface binding energy. This equation is actually the measure of refraction for a particle hitting the surface. And from α' the characteristic fractal dimension D is defined as:

$$D = \frac{\log(R\frac{P_{max}\tan\alpha' + P_{max}}{P_{max}/\cos\alpha'})}{\log(R)} = \frac{\log(R(\cos\alpha' + \sin\alpha'))}{\log(R)} \tag{19}$$

This has the similar form with the fractal dimension in the mathematical definition.

Another simulation result is from the Yamamura's group in 2005. Their group added the fractal dimension parameter into the ACAT code, which is based on Monte Carlo simulation [9]. They used Fourier Filtering method to describe surface roughness and set the fractal dimension equals 2.1 to fit the experimental data and compared to planar ACAT.

In conclusion, experimental methods are similar to box-counting concept and simulation methods have used both exact and random fractal to describe the surface. There are numerous experimental and simulation research in this area, but they are not well-connected together by fractal dimension and thus are not yet able to predict the surface roughness exponent.