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F-TRIDYN: A Binary Collision Approximation code for simulating ion interactions with rough surfaces

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ABSTRACT

Fractal TRIDYN (F-TRIDYN) is a modified version of the widely used Monte Carlo, Binary Collision Approximation code TRIDYN that includes an explicit model of surface roughness and additional output modes for coupling to plasma edge and material codes. Surface roughness plays an important role in ion irradiation processes such as sputtering; roughness can significantly increase the angle of maximum sputtering and change the maximum observed sputtering yield by a factor of 2 or more. The complete effect of surface roughness on sputtering and other ion irradiation phenomena is not completely understood. Many rough surfaces can be consistently and realistically modeled by fractals, using the fractal dimension and fractal length scale as the sole input parameters. F-TRIDYN includes a robust fractal surface algorithm that is more computationally efficient than those in previous fractal codes and which reproduces available experimental sputtering data from rough surfaces. Fractals provide a compelling path toward a complete and concise understanding of the effect that surface geometry plays on the behavior of plasma-facing materials. F-TRIDYN is a flexible code for simulating ion-solid interactions and coupling to plasma and material codes for multiscale modeling.

1. Introduction

Plasma-material interactions (PMI) are crucial to the operation of all plasma devices, including experimental fusion reactors. In fusion experiments, interactions with the wall are responsible for drastic changes in plasma performance and confinement, including radiation losses via impurities. Energetic ions are primarily responsible for many phenomena important to fusion reactor performance, including sputtering and tungsten fuzz growth [1]. In addition to semi-empirical formulas for calculating sputtering yields such as the Yamamura formula [2], the two main strategies for studying ion-solid interactions are Molecular Dynamics (MD) and Binary Collision Approximation (BCA) simulations [3].

While semi-empirical equations for sputtering yields can be used for simple systems, simulations allow one to study a significantly larger volume of the many-dimensional parameter space for ion-solid interactions. Simulations provide information, such as implantation depth profiles and Frenkel pair damage profiles, that cannot be captured in a single equation. MD simulations directly integrate the equations of motion for a number of interacting atoms. This direct integration, generally relying on ab initio or experimentally derived pair interaction potentials, is computationally difficult. MD simulation of timescales relevant to ion-solid interactions in the fusion community requires access to high-performance computers and, in some cases, prohibitively long computational times. For this reason, MD codes are not practical to use as directly coupled components of multiscale codes. BCA codes, on the other hand, treat the ion-solid interaction as a combination of elastic two-body ion-atom collisions and inelastic electronic stopping [4]. BCA codes are fast enough to run on-line with other codes and are statistically and physically accurate for a wide range of materials and ion energies [5].

While SRIM, based on the TRIM code, is arguably the most popular BCA code in use today, it has been shown to be inaccurate, especially for sputtered atom angular distributions and the angular dependence of sputtering yields [6]. TRIDYN, and its successor SDTrimSP, do not share the inaccuracies present in SRIM. They are upgraded versions of TRIM to include a more accurate interaction potential and features such as dynamic surface composition [5]. Fractal TRIDYN (F-TRIDYN) is a new, further upgraded version of TRIDYN to include explicit fractal surface roughness and additional output modes. Fractal surface roughness was first implemented in a

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BCA code in FTRIM [7], [8]. FTRIM, in addition to being based on the older TRIM code, utilized a fractal surface algorithm that was of $O(N^2)$, where N is the number of points that comprise the fractal surface, making it prohibitively expensive to use for large-scale contemporary simulations. The new surface algorithm implemented in F-TRIDYN, however, is of $O(N)$. In addition to the new fractal surface algorithm and the inherent advantages in accuracy of using TRIDYN as a base code, F-TRIDYN adds features that FTRIM does not have, including output lists of stopped projectile locations, stopped Primary Knock-on Atom (PKA) and Secondary Knock-on Atom (SKA) locations, Frenkel pair damage locations, and energy-angle distributions of the sputtered particles, all in three dimensions. These additional output features in particular make F-TRIDYN suitable for coupling to a wide variety of plasma and material codes as a wall boundary condition for energetic ions.

2. Fractal surface roughness

Fractals are mathematical objects that possess either self-similarity or self-affinity. Self-similarity is the property that elements of an object at different scales are exactly or approximately the same. Self-affinity is a weaker quality that allows for an object to scale differently along different spatial dimensions. Fractals can be characterized by a so-called fractal dimension. Fractal dimensions describe how the size of the space fractals occupy relates to the size of the space within which they are embedded. In particular, the fractal dimension of a curve describes how its total measured length changes depending on the length scale of the measurement. For example, smooth curves will be measured to have the same total length regardless of the length scale considered. Therefore, the space smooth curves occupy scales according to a power law of order equal to their topological dimension. Measurements of the length of fractal curves, however, will scale according to a power law of order greater than their topological dimension, meaning that their total length is not well-defined and depends on the observed length scale. In particular, they will scale according to a power law of order equal to their fractal dimension [9]. Intuitively, fractal dimension can be seen as a measure of the complexity or roughness of a curve. Determination of the dimension of simple geometric objects, such as points, lines, and planes is trivial. For fractals, however, there are multiple methods of measuring their dimensions, which are not, in general, equal. Throughout this paper, the fractal dimension referred to will be the box-counting dimension [10] as described hereafter.

Calculation of the box-counting dimension is straightforward. For a given curve, separate the space it occupies into boxes of side length L. The number of boxes that are at all occupied by any portion of the fractal curve are counted as N. If one plots on a log-log scale the number of occupied boxes versus the box side length, the slope of any linear section of the resulting line will be equal to the negative fractal dimension in that region. Some curves may exhibit fractal behavior over a limited range of length scales. Outside of this range the box-counting plot will either have slope zero or be nonlinear [9]. The range of length scales for which a curve has a measurable, non-zero fractal dimension will be referred to as the fractal length scale. In Fig. 1, the Koch Snowflake and its box-counting plot are shown.

Many natural objects and physical phenomena are fractal at some length scale [10]. Particularly, fractals provide a consistent and realistic model for rough molecular surfaces [11], [12]. For surfaces such as these, the roughness can be characterized by just two parameters, the fractal dimension and the fractal length scale. This allows complex geometry representative of the rough surface to be generated on the fly for any arbitrary fractal dimension. Additionally, fractal dimension is practically measurable in-situ. For

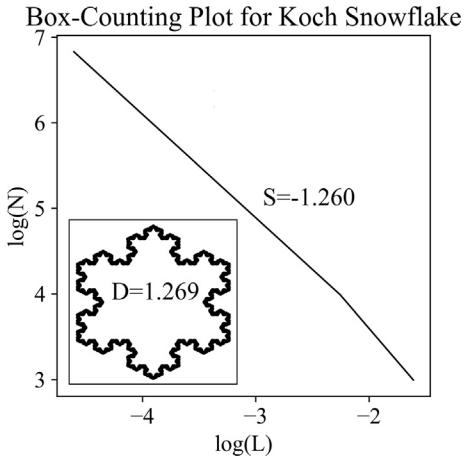

Fig. 1. The Koch snowflake (inset) and its corresponding box-counting plot. After extracting points from a rendered image of the Koch snowflake, the box-counting algorithm was used to measure the slope of the log-log plot of the number N of boxes of side length L occupied by the curve for a range of side lengths. The negative slope of the line, found via least squares linear regression, is equal to 1.260. The actual fractal dimension of the Koch snowflake is 1.269.

most PMI experiments, it is not possible to measure surface morphology directly without breaking vacuum. Using the methods of Fractal BET adsorption theory [13] [14], the fractal dimension of a rough surface can be determined via the amount of adsorption onto the surface of differently sized gas molecules. This offers a compelling methodology to study the effect of rough surfaces on ion-solid interactions in a single machine by measuring surface roughness, performing ion irradiation, and performing subsequent surface diagnostics.

3. Generation of fractal surfaces for F-TRIDYN

Fractal surfaces in F-TRIDYN are composed of two orthogonal cross-sections. Because a fractal surface will have an overall fractal dimension equal to the sum of the dimensions of each of its cross sections, two-dimensional fractal surfaces of dimension $2.0 \leq D_{2D} \leq 3.0$ can be represented by a combination of a dimension 1.0 cross-section and a dimension $D_{2D} - 1.0$ cross section. For this reason, fractal surfaces in F-TRIDYN are represented using a single fractal cross section, spanning the $Y - Z$ plane (see Fig. 2). As long as the fractal dimension of a surface is homogeneous across

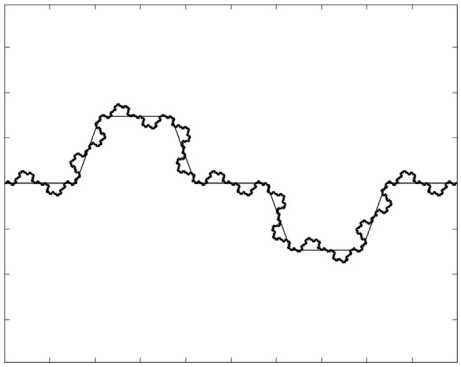

Fig. 2. An example of the default fractal generator in F-TRIDYN and its subsequent iterations with fractal dimension $D = 1.18$. This fractal generator is used because it is qualitatively similar to molecular surfaces and because it can span, without self-intersections, the widest range of fractal dimensions (up to approximately $D = 1.8$) of all tested fractal generators.