Computational Materials Science 149 (2018) 301–306

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

F-TRIDYN simulations of tungsten self-sputtering and applications to coupling plasma and material codes☆

Jon Drobny*, Davide Curreli

Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana Champaign, Urbana, IL 61801, United States

ARTICLE INFO

Keywords:
Binary Collision Approximation
Fractal
Surface roughness
Ion-solid interactions
Plasma Material Interactions
Code coupling

ABSTRACT

Fractal-TRIDYN (F-TRIDYN) is an upgraded version of the Monte Carlo, Binary Collision Approximation code TRIDYN for simulating ion-surface interactions. F-TRIDYN adds an explicit model of surface roughness and additional output modes for coupling to both plasma and material codes. Code-coupling represents a compelling path toward whole-device modeling, especially for future fusion reactors. Whole device models need to span length and time scales of many orders of magnitude. Atomic processes in materials that occur on the order of picoseconds, such as changes to surface morphology, will have an effect on fusion plasma performance over many hours of operational time. Conversely, interactions with the plasma will drive chemical, thermal, and morphological processes in the material. Simulating this complex interaction between the plasma and the plasma-facing material demands fast interfaces between material and plasma codes. F-TRIDYN is a flexible code for simulating atomic-scale ion-surface interactions, which are responsible for interactions between plasma and surface such as sputtering and implantation. F-TRIDYNs surface roughness model allows the effect of surface roughness on ion-surface interactions to be simulated. Surface roughness can significantly alter sputtering yields and other ion-surface interaction quantities. Understanding the role surface roughness plays in Plasma-Material Interactions will be crucial to modeling the performance of future fusion reactors such as ITER. F-TRIDYN is also suited for the simulation of a wider range of plasma-surface interactions where surface morphology may play a role, including those utilized for sputter-coating and plasma treating applications.

1. Introduction

Plasma-Material Interactions (PMI) are fundamental to plasma device operation. Plasma species can interact with surfaces in radically different ways depending on the plasma operating conditions and the material structure and composition. Among the most economically and scientifically important PMI are ion-surface interactions. Ion-surface interactions include sputtering, reflection, implantation, chemical and morphological changes, and damage. Sputtering, the process in which ions incident upon a target expel atoms from the surface via atomic collisions, is of significant importance to plasma-surface interactions because it is one of the main responsible for plasma contamination. Sputtering is measured quantitatively using the sputtering yield, measured as the ratio of target atoms released to the number of incident ions. Sputtering yields for a given ion incident upon an atomically smooth target depend on the incident angle and energy of the ion. Sputtering yields are zero below a threshold energy, known as the sputtering threshold. At very high energies, when incident ions penetrate deeply into the bulk, sputtering yields decrease as less energy is transferred to more readily sputtered surface atoms. At low angles of incidence, that is, angles close to the surface normal, the sputtering yield increases with increasing angle of incidence due to an increase in energy transfer to atoms nearer the surface. At high angles of incidence, that is, angles nearly parallel to the surface, energy transfer to target atoms is less efficient and the sputtering yield decreases. Because of the wide and diverse realm of possible ion–solid interactions, especially when considering surface morphology and composition, they are difficult to capture completely with empirical models or analytic methods. However, ion-surface interactions can be handled fully with computer simulations. Two popular simulation techniques for ion-surface interactions are Molecular Dynamics (MD) codes and Binary Collision Approximation (BCA) codes [1]. MD codes numerically integrate the equations of motion for a large number of interacting particles. Interaction potentials for MD codes are validated using density functional theory [2]. Although MD codes offer a complete view of atomic scale particle dynamics at a large range of energies, this technique does not scale easily and often requires High-Performance Computing to handle large atomic systems. BCA codes, alternatively, track incident

☆ This article belongs to the special issue: Radiation Effects.

* Corresponding author.
E-mail address: drobny2@illinois.edu (J. Drobny).

https://doi.org/10.1016/j.commatsci.2018.03.032
Received 8 September 2017; Received in revised form 24 February 2018; Accepted 16 March 2018
Available online 26 March 2018
0927-0256/

projectiles through a series of discrete, binary collisions.

2. Binary Collision Approximation codes

The Binary Collision Approximation (BCA) is a set of simplifying assumptions used for simulating ion-surface interactions. Although binary collisions can be assumed in many physical systems where multi-body interactions are rare, in the context of PMI the BCA refers to a specific physical model with the following assumptions:

- Ions interact with atoms in the material via a series of discrete, two-body collisions
- Nuclear collisions occur at mean-free-path distances and are calculated using a classical scattering integral
- Electronic stopping is calculated at the distance of closest approach of each collision
- Atoms in the material are set into motion only if the collisional energy transfer is greater than a material-specific threshold energy
- Particles set into motion in the simulation are stopped if their kinetic energy falls below a material-specific cutoff energy

Because of these simplifying assumptions, BCA codes provide a computationally efficient, highly parallelizable approach to the problem of fast ion-material interactions. As long as the incident ion energy is far greater than thermal energies and chemical and other thermal effects in the material can be neglected, BCA codes are accurate and well-tested against experiments. Some BCA codes, such as MARLOWE, include an explicit atomic lattice within which particle dynamics are modeled and allows for particles to undergo simultaneous collisions with multiple target atoms [4]. MARLOWE also includes a recombination distance for vacancy-interstitial pairs that increases the validity of damage estimates in the BCA [5]. F-TRIDYN, however, approximates materials as amorphous. This common assumption allows collision partner positions to be generated from a distribution on the fly. Physical processes that depend on an explicit lattice structure, such as ion channeling, cannot be reproduced with the amorphous approximation, but in general, when such effects are weak or otherwise not relevant, it provides good agreement with experiment. Improvements to amorphous BCA codes to increase their validity have been made. TRIDYN includes the ability to include the effect of surface binding energy on tracked particles [6]. TRIDYN also includes a weak collision loop, which includes the effects of up to 3 additional collision partners on scattering events, effectively extending the BCA to a 4-body code [7]. Since particle trajectories in Monte Carlo BCA codes are independent, they can be run in parallel to significantly increase computational speed. BCA codes like F-TRIDYN provide an efficient alternative to MD codes for simulating ion-surface interactions.

BCA codes in common use include TRIM [8] and SRIM [9], FTRIM and VFTRIM [10,11], TRIDYN [6], MARLOWE [4], and SD.TRIM.SP [12]. TRIM and SRIM are among the most widely used BCA codes. SRIM includes a graphical user interface and large libraries of physical parameters, material compositions, and more. However, SRIM has been found to produce inaccurate results, especially for sputtered particle angular distributions; this may lie in the use of the ZBL interatomic potential in TRIM and SRIM. More recent BCA codes use different interatomic potentials, such as the Kr-C potential, and produce more accurate results [13]. FTRIM and VFTRIM were upgraded versions of TRIM to include a fractal model of surface roughness [14]. FTRIM's fractal model of surface roughness has been reproduced in F-TRIDYN with improved algorithms for generation and implementation in the code [15]. TRIDYN is an upgraded version of TRIM that uses the Kr-C interatomic potential and contains a 1D, layered model of dynamic surface composition that tracks displaced atoms and changes the composition accordingly through a diffusion-type model [6]. MARLOWE is a BCA code that includes crystalline structure. SD.TRIM.SP is an upgraded version of TRIDYN for modern computers and there exist versions thereof with various 2D and

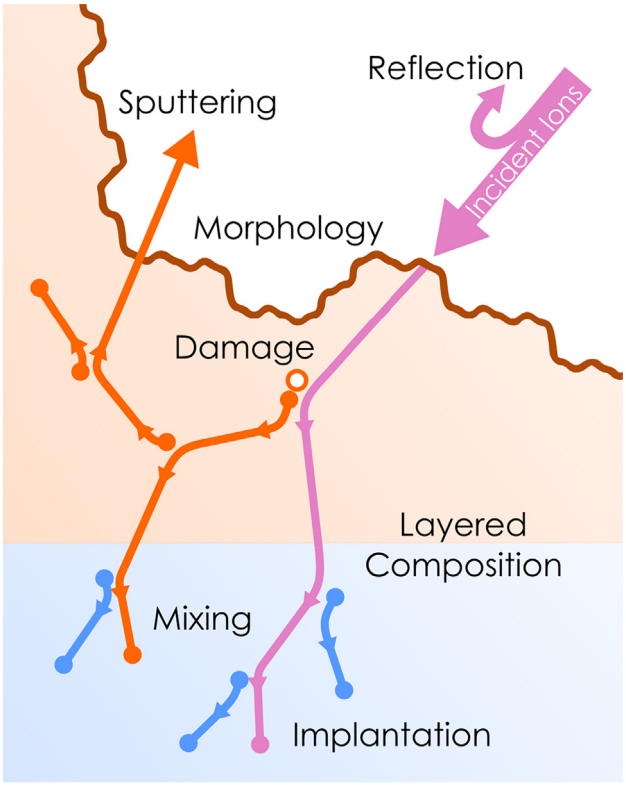

Fig. 1. A diagram showing the physics included in F-TRIDYN. F-TRIDYN includes surface morphology and dynamic composition, sputtering, reflection, implantation, and damage.The two trajectory colors represent the species of the two layers of the material, one blue and the other orange. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3D implementations of surface morphology [16,17]. Advancements to the BCA model include hybrid MD-BCA codes, which combine the advantages in speed of BCA codes with the n-body interactions of MD codes. Examples of hybrid MD-BCA codes include MD-TRIM [18], a coupling of TRIM and MolDyn, and CMDC [19], which activates and deactivates local MD simulations on the fly to simulate collision cascades. De Backer et al. used BCA simulations to find areas of deposited energy to study cascade fragmentation [20]. F-TRIDYN is a BCA code developed with PSI and surface roughness in mind. A diagram illustrating the PSI physics included in F-TRIDYN is shown in Fig. 1. These strategies for improving the validity of BCA codes overcome some of the limitations of the BCA. Future development of BCA codes may lie in increasing the number of active particles, such as in hybrid MD-BCA codes, or in improving the validity of components of the BCA such as interaction potentials or electronic stopping power.

3. Fractal-TRIDYN

F-TRIDYN is based on the BCA code TRIDYN. TRIDYN itself is an improved version of TRIM, one of the earliest BCA codes, upgraded to include a dynamic composition model and to use the Kr-C potential instead of the ZBL potential to model interatomic forces [7].The dynamic composition model of TRIDYN simulates the 1D compositional changes induced by target atom displacement and ion implantation [6]. The Kr-C potential produces more accurate results than the ZBL potential, especially for simulating the angular distributions of sputtered atoms at non-normal angles of incidence, an important process for coupling plasma and surface codes [13]. F-TRIDYN uses the same base collision model as TRIDYN. However, F-TRIDYN includes an explicit model of surface roughness and Python libraries for fractal surface