Simulation of Sputtering Damage of Tungsten Coating Layer on First Wall Materials of a Fusion Reactor

Hyunmyung Kim, Ho Jung Lee and Changheui Jang*
Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology
*Corresponding author: chjang@kaist.ac.kr

1. Introduction

First Wall (FW) structural materials of fusion reactors, such as International Thermonuclear Experimental Reactor (ITER), are subjected to transient loads (disruptions, ELMs, and VDE) resulting in the loss of integrity from erosion/deposition processes. The dominant mechanism for erosion of Plasma Facing Component (PFC) materials is sputtering by which atoms from the surface of solid are ejected due to interaction with energetic plasma ions. Simulation of such trajectories of ions is used to calculate sputtering yields further estimating lifetime of materials.

Tungsten coating on FW materials such as tungsten (W) and Carbon Fiber Composites (CFC) has been considered to compensate for this loss of eroded materials. In this study, a computational simulation of sputtering of W coating on W and CFC target was performed to incorporate physical interpretation of impact of coating density and surface binding energy (adhesion) on target damage behaviors.

2. Methods

2.1. Basics of TRIM

TRIM (The Transport of Ions in Matter) 2013 is a part of the SRIM 2013 (Stopping and Range of Ions in Matter) software package distributed by J. F. Ziegler and J.P. Biersack [1]. TRIM simulates ion bombardment with input parameter as following: physical properties of target and ion elements, incidence energy, and incidence angle. Physics underlying TRIM are described [2] using binary collision approximation (BCA) Monte-Carlo calculations to make detailed calculations of the energy transferred to every target atom until incident ions and recoils have s small enough energy to induce sputtering.

2.2. Relation of density and surface binding energy to sputtering yield of coating

Key input parameters being considered in TRIM calculation of target materials are the following: Width, density, lattice displacement energy, surface binding energy, and lattice binding energy. Among these parameters, while the density has no bearing on sputtering rate, higher density targets last longer and have fewer voids or inclusion providing a better resistance to sputtering. Therefore, a direct relation of material density to its sputtering yield can be safely considered as a reference value for determining the thickness of material removed during the sputtering process.

Granted the density plays an important role in affecting sputtering yield of the material, the sputtering yield is indirectly proportional to the surface binding energy in linear cascade regime [3]. A physical expression for the surface binding energy is safely assumed to be related to adhesion of materials in contact. Therefore, changing the surface binding energy as one of the input parameters in TRIM calculation would definitely influence the sputtering yield of coating.

2.3. TRIM setup and calibration of input parameters

TRIM setup window commands ion and target input variables for a series of calculations (Fig. 1). The high energy ion condition simulates the transient loads in which the most of significant mass loss takes place. Among the wide-area convolution of D, T, and He sputtering, He ion plays the most significant role in affecting to sputtering yield as compared to the other two ions at the same energy [4]. Since noticeable W erosion will mainly occur with 1.6 MJ/m^2 or higher, 2.5 MeV He ion is intentionally chosen for physical interpretation of ITER with some experimental data conducted by EU-RF collaboration available at 2.5 MJ/m^2 [5].

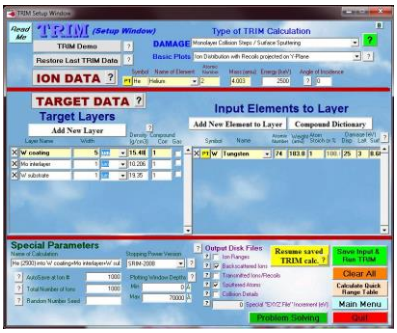

Fig. 1. TRIM setup window in which ion data and target data command.

As target parameters, 3 layers (W coating/Mo interlayer/W substrate) with each pure composition element are being considered. Two individual extreme cases are made as in comparison of the W coating with 1) an ideal density of nominal W density (19.35 g·cm^{-3}) and 2) 80% density (15.48 g·cm^{-3}) of bulk W mentioned

in [6] which is plasma-sprayed (PS) W with droplet (porous) formation.

Along with target density variation, surface binding energy of W coating is also considered as to see the effect on the sputtering yield of the coating layer. Granted the surface binding energy of the most materials is in the range of 1 – 10 eV, with Mo and W having 6.86 and 8.68 respectively, modifications of W coating and Mo interlayer surface binding energy from 1 to 10 eV for both low and high density cases are performed in every single eV interval.

3. Results and Discussion

3D target damage plots and sputtering yields with low density (15.48 g·cm^{-3}) and high (19.35 g·cm^{-3}) density are calculated. A clear distinction is shown between the two cases shown in Fig. 2

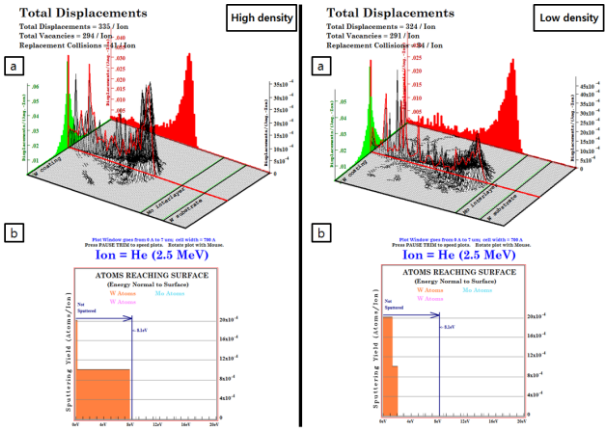

Fig. 2. TRIM calculation results under 2.5 MeV He^+ ion of low density (left column) and high density W (right column) coating: a) 3D target damage plots and b) sputtering yield.

A high sputtering yield in low density can be readily recognized by looking at 3D target damage of total displacement in Fig. 2a representing a physical cascade of the target. The boarder and deeper region of the W coating is more being affected from the ion bombardment for low density (15.48 g·cm^{-3}) coating layer compared to the high density. The average ion range of the high density is 3.44 um while that of the low density is 4.28 um. Sputtering yield is shown in Fig. 2b displaying sputtered atom yield versus energy. Even with a low energy, the same amount of sputtering (the area of colored area, integral method) takes place in low density case.

In variation of the surface binding energy, all the results seem to be very much alike regardless of the change from 1 to 10 eV. This can be physically interpreted as follow: Adhesion of coating can be ignored when it faces to transient loads because regardless how well the coating is in contact with the substrate (high surface binding energy), it would simply penetrate the coating deep enough to induce erosion.

Therefore, in consideration of both density and surface binding energy factors, an optimization between the coating density and adhesion either using PS (in general for thickness) or PVD (for high density) should be conducted in future. It would be beneficial to use PVD for high density coating. On the other hand, PS would be better in achieving thick coating layer, and then the adhesion factor could be ignored as long as a certain degree of coating density is achieved.

4. Conclusion

1. In variation of tungsten coating density, TRIM simulation on 3D target damage on tungsten substrate is carried out.
2. For the higher coating density, the less target damage occurs.
3. Surface binding energy modification seems to have no effect on sputtering yield of coating at all.
4. Balancing of coating density and adhesion needs to be optimized

Experimental validation of such results is to carry out for FW candidate target materials such as CFC and W by PS and PVD coating technique.

Acknowledgement

This work was supported Technology Follow-up and Development for ITER Plasma Facing Material by grant funded by National Fusion Research Institute (NFRI) (Project No. N04130013)

REFERENCES

[1] J. P. Biersack and W. Eckstein, Sputtering Studies with the Monte Carlo Program TRIM.SP, Appl. Phys. A34, p. 73, 1984

[2] J.F. Ziegler, J.P. Biersack, and U. Littmark. The stopping and Range of Ions in Solids, Pergamon ISSN 0891-5490, 1985

[3] P. Sigmund, Sputtering by Ion Bombardment: Theretical Concepts, Heidelberg:Springer-Verlag ISBN 978-3-540-38514, p. 9-71, 1981

[4] L. Pranevicius, Magnetron-Sputter Deposition of W Coatings for Fusion Applications, Mat. Sci., Vol. 15, p. 212, 2009.

[5] J. N. Brooks, D. N. Ruzic, D. B. Hayden, Sputtering erosion of beryllium coated plasma facing components – general consideration and analysis for ITER detached plasma regime, Fus. Eng. And Des. Vol. 37, p.455, 1997

[6] A. Loarte, Report on EU-PWI SEWG on Transient Loads and Future Work, EU plasma-WallInteraction Task Force Meeting – CIEMAT, 2007

[7] J. Rapp, G. De Temmerman, G.J. Van Rooij, P.A. Zeijlmans Van Emmichoven, A. W. Kleyn, Plasma-facing Materials Research for Fusion Reactors at FOM Rijnhuizen, Rom. Journ. Phys., Vol. 56, Supplement, p. 30, 2011.