Applied Surface Science 439 (2018) 456–461

Contents lists available at ScienceDirect

Applied Surface Science

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

Full Length Article

Note on the artefacts in SRIM simulation of sputtering

V.I. Shulga

Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, 119991 Moscow, Russia

ARTICLE INFO

Article history:
Received 23 December 2017
Accepted 4 January 2018
Available online 8 January 2018

Keywords:
Ion bombardment
Surface sputtering
Sputter yield
Silicon
Computer simulation
Program SRIM

ABSTRACT

The computer simulation program SRIM, unlike other well-known programs (MARLOWE, TRIM.SP, etc.), predicts non-zero values of the sputter yield at glancing ion bombardment of smooth amorphous targets and, for heavy ions, greatly underestimates the sputter yield at normal incidence. To understand the reasons for this, the sputtering of amorphous silicon bombarded with different ions was modeled here using the author's program OKSANA. Most simulations refer to 1 keV Xe ions, and angles of incidence cover range from 0 (normal incidence) to almost 90°. It has been shown that SRIM improperly simulates the initial stage of the sputtering process. Some other artefacts in SRIM calculations of sputtering are also revealed and discussed.

1. Introduction

Knowledge of sputtering properties of solids under ion bombardment is necessary for many applications ranging from the nuclear power and aerospace industry to a variety of nanotechnologies. In recent decades, a high priority in ion sputtering studies is given to atomic scale simulation, providing a fairly accurate description of collision cascades in solids in terms of the binary collision approximation or by molecular dynamics. Atomic simulation allows one to bypass many limitations of analytical models of sputtering, use realistic interatomic potentials, take into account, if necessary, the crystalline structure of the irradiated material, changes in its composition during ion bombardment, effects of surface topography, etc. [1].

One of the computer programs simulating the sputtering process is the program SRIM-2013 [2], which is freely available and is very convenient for practical use. The program implements the Monte-Carlo scheme for calculating collision cascades in solids in the binary collision approximation and allows one to calculate various characteristics of ion-solid interactions, including the sputter yield Y, i.e. the average number of sputtered atoms per incident ion. It was found, however, that SRIM-2013 (and earlier versions of SRIM) can greatly distort the yield at normal and especially at glancing incidence [3–8]. Serious discrepancies with experiment were detected in the angular distributions of reflected particles [9]. These artefacts were explained by errors in the trajectory calculations presumably caused by inappropriate approximations of scattering events and non-random target-atom spacing [3]. Some authors questioned about the interatomic potential used in SRIM [7], the algorithm for searching potential collision partners when the incident ions approach the surface [8], and ignoring extremely small scattering angles in elementary collision events [9].

Close inspection of the SRIM results suggests, however, a simpler explanation of the above artefacts, at least some of them. Fig. 1 plots the SRIM-calculated ion trajectories of 100 eV Xe ions in a Si target at normal incidence. The trajectories are represented by points separated by a free flight path which is taken as $\lambda = N^{-1/3}$, where N is the atomic density of the target (for silicon $N = 0.0498$ atoms/Å^3 and $\lambda = 2.7$ Å). From the figure it can be concluded that at normal incidence the first ion-atom collision occurs at a distance λ from the surface. This means that all the projectiles start from the surface, i.e. from zero depth. The same is expected at oblique incidence. Obviously, all this can greatly affect the sputtering process, especially at glancing incidence, when many bombarding ions are reflected from the surface and carry away energy that could initiate sputtering.

The aim of this paper is to verify the above assumption. The calculations were carried out using the program OKSANA in the version described in [10]. By analogy with SRIM, an amorphous target having a smooth surface is considered. Most of the calculations refer to silicon bombarded with 1 keV Xe ions, and the angle of ion incidence α is varied from 0 (normal incidence) to almost 90°.

2. Simulation model

Let us recall the main characteristics of the OKSANA program, the first version of which was developed in the mid-1980s [11]. The program is designed to calculate the sputtering of crystalline

E-mail addresses: shulga@anna19.msu.sinp.ru, vish008@yandex.ru

https://doi.org/10.1016/j.apsusc.2018.01.039
0169-4332/

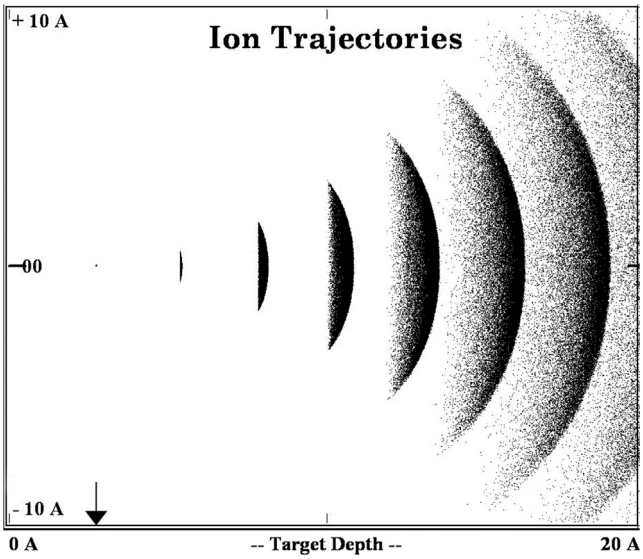

Fig. 1. Trajectories of 100-eV Xe ions in a Si target at normal incidence on the surface (the left boundary of the figure), calculated using the SRIM-2013 program. The trajectories are represented by points separated by a free flight path determined by the average interatomic distance $\lambda = 2.7$ Å. Note that in all cases the first ion-atom collision occurs at the depth λ (marked by arrow). The point above the arrow is somewhat enlarged to be better visible.

and amorphous targets during ion bombardment. The amorphous target is modeled by the rotation of a crystalline atomic block; the rotation procedure is repeated for each new collision in the same way as in the MARLOWE program [12]. Classical scattering in ion-atom and atom-atom collisions is described by a screened Coulomb potential. As in SRIM, the Ziegler-Birsack-Littmark (ZBL) interatomic potential [13] is used. Inelastic energy losses in particle collisions are described as default by the Firsov formula [14]. The remaining parameters of the model correspond to the standard version of the program described in [15].

The direction of ion bombardment is specified in a rectangular coordinate system, the X' and Y' axes of which lie in the surface plane of the target, and the Z' axis is directed into the target. The initial point of the ion trajectory has a coordinate $Z' = z_0$, where z_0 can vary ($z_0 = 0$ corresponds to the target surface). In the standard version of the program, the value of z_0 is taken equal to -2λ or distributed randomly between -2λ and -3λ. The collision partner is chosen from the atoms of the first coordination sphere of the crystal lattice. If an atom has a coordinate $Z' < 0$, the scattering on this atom does not happen and the search for a partner begins again among the atoms located in front. This procedure allows us to take into account the effect of weak collisions when particles approach the surface. For a correct comparison with SRIM, the target surface is considered to be smooth.

The atom is considered to be sputtered if it overcomes a flat surface potential barrier of an E_S height equal to the sublimation energy of the target material (4.7 eV for Si). The bulk binding energy E_B is usually taken to be 0, but in this work we use the SRIM value $E_B = 2$ eV. It was assumed that recoiling atoms begin their motion in the target with a reduced (by E_B) energy and overcome the surface barrier with the surface binding energy reduced by the same amount. Note, however, that such a variation of E_B has little effect on the results, at least in the cases studied (see below).

The physical model underlying SRIM is described in [13,16]. In the context of this work, it is important to note the following. In SRIM, collision partners are selected from atoms that lie in a plane located at a distance λ from the scattering centre. To obtain the given atomic density N, the maximum impact parameter of a collision is limited to the value $p_{max} = \pi^{-1/2}\lambda$; for silicon, $\lambda = 2.7$ Å and $p_{max} = 1.5$ Å. The next collision partner is chosen similarly, but taking into account the new direction of ion motion.

The radius of the first coordination sphere d in the silicon lattice is related to the average interatomic distance λ by the relation $d = 3^{1/2}\lambda/2 = 2.3$ Å. Since $d < \lambda$, it is clear that in the model underlying the program OKSANA, the atoms of the first coordination sphere can be located at the distance λ from the surface (as in SRIM) only at a small positive value of z_0. Fig. 2 illustrates this in the case of normal incidence. It is easy to show that in this case the adjustable value of z_0 should not exceed $z_{max} = \lambda - d[1 - (p_{max}/d)^2]^{1/2}$; for silicon $z_{max} = 0.93$ Å, which is close to $\lambda/3 = 0.91$ Å. For another limiting case, $\alpha = 90°$, a similar analysis gives the interval of adjustable values of z_0 ranging from 0 to $p_{max}/2 \approx \lambda/4$. At $\alpha = 90°$ the quality of the fit can be improved by varying d or N, but this is unacceptable from a physical point of view. Analysis of the ion trajectories generated by the SRIM program suggests, as a rough approximation, the angular dependence $z_0 = (\lambda/3)\cos\alpha$, which more or less satisfies both limiting cases.

3. Results and discussion

3.1. Normal and oblique incidence

Fig. 3 shows the sputter yield of an amorphous Si target bombarded with 0.1–100 keV Xe at normal incidence as a function of the initial ion energy E_0 ranging from 0.1 to 100 keV. The figure compares the results of OKSANA and SRIM simulations with each other and with the experimental data [7,17–20]. The OKSANA-calculated results are given for the values of $z_0 = -2\lambda$ and $\lambda/3$. It will be recalled that the first of these values is standard for OKSANA, and the second one is suggested to bring together the results of OKSANA and SRIM simulations. It can be seen from the figure that this really occurs in the whole energy range and that the relative difference between the OKSANA and SRIM results decreases with increasing energy. The latter is due to the fact that at higher energies surface effects lose their significance, especially at normal incidence. Note the good agreement of the OKSANA-calculated yields ($z_0 = -2\lambda$) with experimental data. An exception

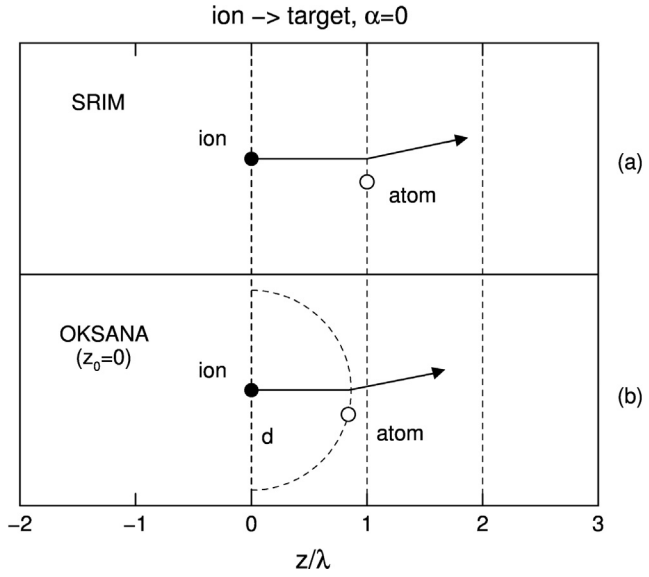

Fig. 2. Schemes of ion trajectories simulated by the SRIM (a) and OKSANA (b) programs (normal incidence). In both cases the ion starts from the surface ($z = 0$). λ is the free flight path average interatomic distance, d the radius of the first coordination sphere (for silicon $\lambda = 2.7$ Å and $d = 2.3$ Å).