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Sputtering of cubic metal crystals by low-energy xenon-ions

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ABSTRACT

Ion thrusters are playing an increasingly important role on-board satellites, largely because of their high fuel efficiency. As a result, there has been strong interest in improving their performance and extending their operational lifetimes. A key factor limiting these lifetimes is the sputtering of atoms from thruster components. Ion thrusters generally use molybdenum grids, however it is thought that non-standard grid materials may prove more robust to this damage. High manufacturing costs and lengthy testing times limit the ability of researchers to investigate this experimentally. Computational methods provide an alternative mechanism for assessing potential alternative grid materials. Atomistic simulations of sputtering have been shown to be accurate for a number of systems, and so in this work we attempt to establish this effectiveness for a much wider range of materials. Atomistic simulations additionally have the potential to elucidate the dynamics of sputtering better than other simulation methodologies. To this end, we used atomistic simulations to compute sputter yields for 12 different metals under bombardment by xenon-ions with kinetic energies of between 100 eV and 1 keV. We found that the method showed great promise, but that the sputter yield is dependent on the exact choice of interatomic potential. We went on to examine sputtering of molybdenum in greater detail and compared our results with commonly used empirical models, the TRIM simulation program and experimental data from the literature. Some similarities and some differences were observed, however atomistic simulations are shown to generally produce accurate yields and a more realistic representation of the dynamics of sputtered particles.

1. Introduction

Low-energy ion thrusters are an increasingly utilized form of spacecraft propulsion which electrostatically accelerate xenon-ions through molybdenum grids to generate thrust. Not all ions exit the thruster cleanly however. Some collide with the screens instead, causing erosion through sputtering. This damage is the primary factor limiting a thruster's operation lifetime. To address this, researchers are investigating the usefulness of alternative screen-grid materials. High manufacturing costs and lengthy testing times limit the ability of researchers to experimentally investigate the sputtering of heavy ions on metallic crystals. Thus, molecular dynamics modeling of low-energy ion bombardment will assist in screening candidate materials for further development.

Many different types of sputtering model have been developed in the past. These include analytical models [1,2], empirical models [3,4] and models based on the binary collision approximation [5]. These models suffer from a range of issues including inaccuracy for low-energy ions and a dependence on experimentally determined parameters. This first issue has particular relevance for modeling ion thruster erosion since most sputtering events in this system occur at low ion energies. The second issue has relevance more broadly, as experimental sputtering data shows a wide spread in the measured yield [6]. Recently increasing computational power and high-level interatomic potentials have allowed atomistic simulations of sputtering to rapidly progress. These have the advantage of providing better accuracy for low-energy ion-crystal interactions and allow for multi-body effects, thus avoiding the limitations inherent in the binary collision approximation.

Atomistic sputtering simulations are generally performed using a combination of embedded atom method (EAM) interatomic potential and a screened nuclear repulsion potential for short interatomic separations. This combination has been successfully applied to low-energy xenon-ion bombardment of nickel [7], and high-energy xenon-ion bombardment of gold, silver and

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molybdenum [8,9]. The method is robust across a wide variety of systems since screened nuclear repulsion potentials can be calculated for most atom pairs and the EAM potential has been determined for a large number of metals and alloys. Demonstration of the efficacy of the method for a large range of systems at low ion energies has not yet been carried out however. At a more detailed level, there has been little examination of the accuracy of atomistic simulations in producing realistic distributions of sputtered atoms.

In this work, we apply atomistic simulations to the sputtering of 12 elemental metallic crystals under bombardment by low-energy xenon-ions. Sputter yields are computed from these simulations and compared with experimental results taken from the literature [10,4,6]. As molybdenum grids are the current industry standard material, we then go on to compute a number of sputtering statistics in greater detail for the xenon–molybdenum system. These include the sputter yield as a function of ion incidence angle and the kinetic energy distributions of the sputtered atoms and probability density functions for their trajectories.

2. Method and materials

2.1. Molecular dynamics model

Our atomistic sputtering model consisted of two types of atom: a crystalline metal 'target' formed from a pure element and a number of bombarding 'projectile' ions. Target surfaces were chosen as the lowest energy plane for each crystal studied. These are the {110} surface plane for body-centered-cubic (bcc) crystals and the {111} surface plane for face-centered-cubic (fcc) crystals [11]. Other crystal structures are not considered in this study. The target was made of $12 \times 12 \times 8$ crystal cells, with periodic boundary conditions applied to the x- and y-axis boundaries and free boundary conditions applied to the z-axis boundaries.

Atoms within the interatomic potential's cutoff distance from the bottom of the simulation were held fixed to prevent the crystal from shifting and to approximate the inter-atomic forces of a target with an infinite extent for the mobile atoms above. Between here and the top two crystal layers, atoms had a Langevin thermostat at 20 °C applied to them (with a relaxation time of 1 ps). This thermostat emulates heat conduction into the surrounding material (not simulated) [8]. The uppermost two crystal cell layers were completely free. It was found that having two free layers was sufficient to prevent the thermostat from affecting sputter yields. As shown in Fig. 1, the average sputter yield for two projectile energies converges on a similar value for a number of different free layers.

Simulations began with a 5 ps equilibration period during which the target was set to room temperature. Next, a number of projectile atoms were sequentially impacted with the target at randomized locations. All projectiles have the same kinetic energy and impact the target at a chosen incidence (or altitude) angle, with randomized azimuthal angles. The time between subsequent impacts was 1 ps, which was observed to be sufficiently long for most sputtering events to have occurred. The number of projectile atoms that were impacted in each simulation was chosen to provide a flux of 0.04 atoms/Å^2, matching simulations conducted by Zhou et al. [7]. Following the simulation, the final coordinates and velocities of the atoms are used to compute a range of statistics.

2.2. Interatomic potentials

For our simulations two interatomic potentials are required, one between atoms within the target and one between projectile ions and target atoms. Interactions between multiple projectiles are ignored.

For interactions between atoms within the target, we use the embedded atom method (EAM) potential [12,13]. This gives the potential energy between two atoms as

$$E_i^{EAM} = F_\alpha\left(\sum_{j\neq i}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}^{EAM}(r_{ij}). \tag{1}$$

Here, ρ is the atomic electron density used to compute the embedding energy F_α, which represents the energy required to embed an atom i of type α into the electron cloud of an atom j of type β. The $\phi_{\alpha\beta}^{EAM}$ term is a pair potential between atoms of type α and β and r_{ij} is the distance from atom i to atom j. Although shown here in an analytic form, these potentials are often provided in tabular formats. EAM potentials are determined using fitting processes such that they accurately reproduce a chosen set of physical properties for a given material. The EAM potential is widely used for metal systems since its embedded energy term accounts for multi-body interactions. This is important in crystal structures and provides a realistic model of free surfaces.

For interactions between projectile ions and target atoms, we use the Ziegler–Biersak–Littmark (ZBL) universal potential [14]. This potential represents screened coulombic repulsion between atomic nuclei and is used to simulate high-energy collisions between atoms. Here, the potential energy between two atoms i and j at a distance r_{ij} is given by

$$E_{ij}^{ZBL} = \frac{1}{4\pi\epsilon_0}\frac{Z_i Z_j e^2}{r_{ij}}\phi^{ZBL}(r_{ij}/a) + S(r_{ij}), \tag{2}$$

$$a = \frac{0.46850}{Z_i^{0.23} + Z_j^{0.23}}, \tag{3}$$

$$\phi^{ZBL}(x) = p_1 e^{q_1 x} + p_2 e^{q_2 x} + p_3 e^{q_3 x} + p_4 e^{q_4 x}, \tag{4}$$

where $\mathbf{p} = [0.18175, 0.50986, 0.28022, 0.02817]$, $\mathbf{q} = [-3.19980, -0.94229, -0.40290, -0.20162]$, e is the electron charge, ϵ_0 is the electrical permittivity of a vacuum, and Z_i and Z_j are the nuclear charges of the two atoms in electron charge units. $S(r)$ is a switching function that ramps the potential to zero between an inner and outer cutoff distance. Ideally, we would also combine this potential with an EAM potential to give accurate low-energy projectile–target interactions, however these are not readily available for common projectile–target pairs.

2.3. Data sources and models used for comparison

To demonstrate the accuracy of the results presented in this paper, we compare the yields computed for normally incident ions to a variety of experimental results. We use three main sources for these. The first are the results of Rosenberg and Wehner [10], who measured sputter yields for 30 different elemental targets under bombardment by three different ion types at normal incidence angles and low kinetic energies. The second set of results come from Yamamura and Tawara [4], who collated a large number of experimentally measured sputter yields for normally incident ions at kinetic energies from tens to hundreds of thousands of electron-volts. We were unable to get these results in a tabulated format and instead have digitized them from plots (using PlotDigitizer [15]). We acknowledge that inaccuracies will arise from this process since it was done by hand. Lastly, Nakles [6] provides experimentally measured sputter yields for molybdenum under low-energy xenon-ion bombardment collated from a number of sources (see 10,16–22).

We also provide a comparison of our results with two other numerical models. The first model comes from Yamamura and Tawara [4], and consists of a number of formulae which are shown in Appendix A. These can be used to compute sputter yields for ions at a range of incidence angles and energies, and can give an