

Suppression of sputtering in tungsten fuzz: Interplay of porosity and surface roughness

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We present a comprehensive study on the sputtering behavior of tungsten fuzz structures under deuterium and argon ion bombardment using three-dimensional simulations. We employed SDTrimSP-3D to investigate porosity as a predictor for the sputtering behavior, complementary to the well-established effects of surface roughness, with simulations conducted across multiple ion energies (500 eV–2000 eV) and incidence angles (0°–85°). Fuzz structures were algorithmically generated with varying porosities, and sputter yields were systematically calculated. The findings reveal a universal linear relationship between sputter yield and porosity/volume filling, demonstrating that porosity significantly suppresses sputtering. Importantly, the zero-porosity limit is given by the sputter yield of a rough, but solid surface rather than a flat target. This linear behavior holds consistently across the different ion types and energies for a wide range of incidence angles. When normalized to the rough-surface sputter yield, the slope of the porosity dependence is nearly constant, indicating a common underlying suppression mechanism. The study enhances fundamental understanding of sputtering in porous nanostructures and provides a simple, predictive framework with implications for material design, particularly in nuclear fusion research, where erosion of tungsten fuzz impacts reactor component lifetimes.

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I. INTRODUCTION

Sputtering by ion bombardment is a process ubiquitous in surface science, technical applications, and nature. A standard tool in sample preparation, sputtering is often used to clean specimen surfaces on an atomic level. On the other hand, as a means of physical vapor deposition, it is employed to grow films and coatings of several nm to μm thickness for fine-tuned applications in industry, such as to increase wear resistance or to change optical properties [1,2]. Besides its utilization in science and technology, sputtering occurs naturally on plasma-exposed surfaces such as on rocky bodies in space bombarded by solar wind ions. In this case, the continuous ion barrage can lead to weathering and erosion of the surfaces of planets, such as Mercury, or the Moon [3–5]. In nuclear fusion research, the erosion of reactor wall materials by the plasma ions is undesired and should be minimized, as it impairs both the reactor lifetime as well as the efficiency of the fusion reaction [6,7].

In many of these contexts, sputtering is still discussed and modeled assuming idealized, flat target surfaces. For such surfaces, the sputter yield, defined as the number of atoms ejected per incident ion, is a well-established function of ion energy, incidence angle, and projectile-target mass ratio. Theoretical descriptions exist since the foundational work by

Sigmund [8], whereas more recently, computational methods such as molecular dynamics or the binary collision approximation (BCA) have gained traction [9]. For rough surfaces, the description is slightly more involved, as additional effects emerge: the local ion incidence angle depends on the position on the sample and might differ from the nominal incidence angle. Moreover, shadowing and redeposition of sputtered recoils further impact the sputter yield. The influence of these effects have been studied experimentally, numerically, and analytically, and a main conclusion in the literature body is that modifications to flat-surface sputter yields can be accurately described solely by taking into account these geometric effects, with a special focus on the distribution of local inclination angles [10–13].

While the effects on sputtering due to a mesoscopic surface roughness can now be considered well understood, it remains unclear if or how porosity, e.g., open, winded channels between potentially overhanging surface features, affects the sputtering behavior. In porous nanostructures, ions can penetrate deeper into the material, potentially shifting the energy deposition away from the surface and increasing the probability of redeposition of sputtered atoms. This raises the fundamental question of whether alterations in the sputter yield in such systems can be understood solely in terms of surface roughness, or whether porosity introduces an additional suppression mechanism that must be treated separately. Tungsten nanocolumns, for example, exhibit lower sputter yields that depend on their spacing in a way that cannot be attributed to surface corrugation alone [14,15]. Plasma-exposed metal foams show a considerable sputter yield reduction across various ion energies [16,17]. Moreover, the loose, porous dust blankets on the Moon and planets significantly affect both

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the solar wind sputter yields and ion backscattering [4,18–21]. Lastly, tungsten (W) has been shown to form porous, spongelike nanofibers when exposed to He plasmas [22,23]. These structures, often called fuzz, can potentially impair the otherwise advantageous mechanical and surface-thermal properties of tungsten in the context of a wall material for thermonuclear fusion reactors. Therefore, also their sputtering behavior under fuel or seeding gas ions is of interest, and has been studied either at low energies [24–26] or at energies and fluences high enough to investigate dynamical erosion and morphology changes [27].

In this work, we systematically investigate how the sputter yield of tungsten fuzz evolves as a function of porosity, elucidating on the interplay of surface roughness and porosity. Sputtering of fuzz structures was simulated at three different energies for two projectiles, Ar and D, under various incidence angles for algorithmically prepared surfaces of varying porosity. We show that the yields follow a linear dependence on the volume filling, and that this holds universally for a large parameter space. The parameters of this linear model are uniquely determined by the rough-surface sputter yield. The linear dependence of the sputter yield on the volume filling factor makes porosity a suitable predictor for the sputtering behavior.

II. METHODS

A. Sputtering simulations

SDTrimSP [28,29] and SDTrimSP-3D [30,31] form a popular simulation package commonly used to calculate various effects of ion-solid interactions. The codes provide information on reflection coefficients and sputter yields as well as depth distributions of implanted ions, damage production, or the energy and angular distributions of sputtered particles and reflected ions. Also dynamic effects such as compositional changes with ion fluence, surface erosion, or layer intermixing can be described.

We used these two codes to simulate the sputtering of flat W surfaces as well as fuzzy structures under ion bombardment. These codes apply the binary collision approximation (BCA) and a Monte Carlo simulation approach to efficiently calculate quantities related to ion beam irradiation. In the BCA, collisions are assumed to happen solely between two partners and multibody influences are neglected. For this case, the energy transfer to the recoil as well as the scattering angle of the projectile can be determined numerically from the classic scattering integral as a function of the impact parameter. The impact parameter is in turn chosen randomly, as is the azimuthal angle. Between these elastic collisions, inelastic energy losses are accounted for. After the first generation of recoils is set in motion, the subsequent collisional generations are tracked as the collision cascade forms. If a surface atom surpasses the surface binding energy, it is finally counted as sputtered. In addition to the sputter yield, this procedure allows us to track ion implantation, damage production, ejecta angular, and energy distributions and other quantities, as well [9,28,32].

While the above described concepts hold for the BCA in general, one important distinction between SDTrimSP and

SDTrimSP-3D is their treatment of the target geometry, especially apparent in the surface morphology. As the names imply, the former considers only one-dimensional, i.e., flat, targets, while the latter allows for arbitrary sample structures in three dimensions. We used flat-sample simulations as a benchmark, in particular because for this case, the dependence of the sputter yield on the ion incidence angle is well understood [33]. Moreover, the particular combination of both Ar and D ions impinging on W is of high relevance in nuclear fusion research and has been extensively investigated. A large literature body on sputter yield data and refined models exists [34,35].

The three-dimensional (3D) version is especially useful to study the influence of roughness and porosity in varying degrees. A numerical approach is highly relevant since fuzz samples with well-defined and varying porosities are hard to manufacture. Additionally, typical sputter yield quantification processes for W fuzz rely on plasma exposure of the sample until the fuzz layer is entirely eroded. The sample mass before and after erosion is then compared, and a yield is obtained [24,36]. This process is, however, inherently destructive and does not enable us to study the desired (co)dependence on porosity and roughness, as both are dynamically changed during the measurement. Furthermore, the conditions necessary for W fuzz growth prohibit the use of a quartz crystal microbalance, a highly sensitive technique that utilizes the piezoelectric properties of a quartz resonator to resolve mass changes due to ion irradiation [37]. It would be well suited for nondestructive experiments, but the high temperatures in which W fuzz is produced would trigger a phase transition in the quartz crystal, impeding its resonant piezoelectric response and thus rendering this *de facto* standard method for measuring sputter yields useless for this application.

In SDTrimSP-3D, the geometrical information for arbitrary samples structures is handled by a uniform three-dimensional grid of filled or empty voxels. Just like a pixel is the smallest element in a bitmap image, a voxel is the generalization in the third dimension. In SDTrimSP-3D, the voxels are cubes that define the irradiation target. In principle, sample composition can be varied voxel by voxel, even though for this study, the entire sample consists solely of W. Each voxel has atomically flat faces and its composition is assumed to be homogeneous and amorphous. Therefore, what we describe as roughness in this article is given mesoscopically by the relation of the voxels ($5\text{ nm} \times 5\text{ nm} \times 5\text{ nm}$) to each other rather than nanoscopically as per, e.g., atomic-scale displacements of nearest neighbors.

For this study, we simulated both Ar and D bombardment of fuzzy W surfaces at three different energies (500 eV, 1000 eV, 2000 eV) at nine (nominal) incidence angles with respect to the sample surface normal (0° , 15° , 30° , 45° , 60° , 70° , 80° , 82° , 85°). While these energies are high for plasma-exposed components in model fusion reactors, they are often used in other fields of surface science and technological applications. Choosing these energies thus enables to draw more fundamental conclusions relevant even beyond the initial motivation of nuclear fusion research. For the same reason, we used the static simulation mode: to have the sputter yield modifications due to surface morphology untangled from any potential fluence-dependent surface modifications. For every

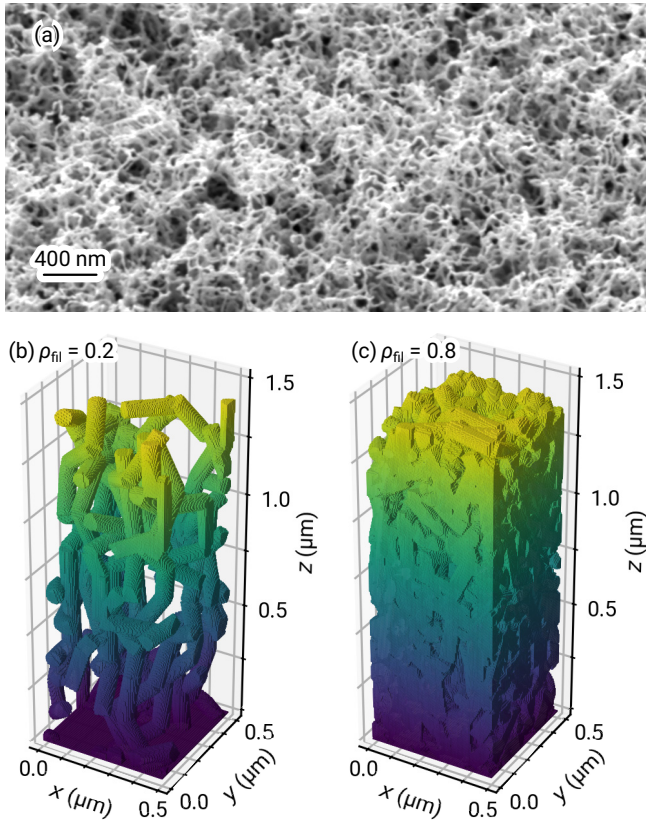


FIG. 1. Visualization of tungsten fuzz. (a) SEM micrograph of a fuzzy W sample. Image provided by M. Rasinski, Forschungszentrum Jülich GmbH. (b) 3D render of a computer-generated fuzz structure with a volume filling $\rho_{\text{fil}} = 0.2$ used in this study. (c) Same as (b), but with 80% volume filling.

parameter combination, we simulated 2×10^5 (Ar) or 5×10^5 (D) impacting ions, respectively, to account for higher statistics necessary for lighter particles. Other model parameters for the BCA simulations were the following:

- (i) KrC interaction potential [38].
- (ii) Surface binding model 1 of SDTrimSP, set via $\text{isbv} = 1$. In this model, the surface binding energy is approximated by the energy of sublimation. Every involved species is assigned a constant value. For W, $E_{\text{SBE}} = 8.79$ eV is used.
- (iii) Inelastic (electronic) energy loss according to the average of the Oen-Robinson model [39] and the Lindhard-Scharff model [40] for Ar and W, and the “H, D, T” model [41] for D.
- (iv) Gaussian quadrature for numerical integration.
- (v) Eight pivot coefficients for the numerical integration.

For the sake of reproducibility, we provide an exemplary input file, cf. section “Data Availability.” Further explanations of the underlying models are given in the SDTrimSP documentation [28].

B. Fuzz generation

As is visible in Fig. 1(a), the W fuzz comprises a network of individual interconnected filaments. The models used for the 3D simulations were generated following the algorithm

presented and tested by Stadlmayr *et al.* [27]. In this random-walk process, the starting point of an individual fuzz filament is randomly determined starting on a flat surface. Each fuzz filament is composed of several cylinders. Every cylinder has a constant length of 250 nm and a diameter of 50 nm. The growth direction of the first cylinder is given by an azimuthal and a polar angle. The former is drawn between $[0, 2\pi)$ from a uniform distribution. To ensure upwards-oriented growth, the latter can take values from $[0, \pi/2)$, again uniformly distributed. At the end of this cylinder, the next one is created with a different growth direction, using the same limitations and random number distributions. Once the highest point of the next cylinder would exceed the upper limit of the simulation cell, the process is aborted and the filament is terminated. When leaving the simulation cell on one side, the fuzz filament reenters from the opposite side, ensuring periodic boundary conditions already at the stage of surface generation. In the same manner, the next filament is grown. The total number of filaments is defined by the desired porosity. In a final step, the fuzz strings are mapped onto a discretized simulation cell. For this purpose, the cell is set up with 100 voxels in both lateral dimensions and 300 voxels in height. The bottom of the simulation cell is terminated with one layer (5 nm thick) of filled voxels. Should two filaments intersect, the number of voxels corresponding to their joint set is filled. The process was repeated three times for every given porosity and three distinct fuzz samples were created.

An overview of the W fuzz structures is given Fig. 1. Figure 1(a) shows an electron microscopy image of a real fuzz sample, while Figs. 1(b) and 1(c) present renders of the computer-generated structures for 20% and 80% volume filling, respectively.

In our fuzz models, one voxel is defined to have sides of 5 nm length. This length was chosen as a compromise between resolution and computational efficiency: While more voxels with smaller volumes would increase the fidelity in reproducing the sample geometry, they would also raise the computational demands. The general recommendation is to have the voxel dimensions below a typical size of the collision cascade of the ions in the solid [30]. While this is certainly the case for the D ions with mean projected ranges of approximately 8 nm, 13 nm, and 20 nm at energies of 500 eV, 1 keV, and 2 keV, respectively [42], this is, however, not necessarily the case for Ar (projected ranges of roughly 1.1 nm, 1.6 nm, and 2.4 nm). On the other hand, the collision cascade typically extends farther than just the mean projected range and our chosen voxel size has already shown to produce results in 3D BCA modeling for Ar that were verified with experimental observations [27,43]. In all of the following work, we use the volume filling factor ρ_{fil} as a descriptor for the porosity of a fuzz structure. We define it as the ratio of filled voxels over the number of total voxels in the simulation cell. Therefore, small ρ_{fil} correspond to highly porous samples, whereas the limit of $\rho_{\text{fil}} = 1$ gives a solid structure without hollow crevices underneath the surface.

We considered this limit in a slightly different way, since the above described algorithm would result in a solid block without structure for a volume filling of unity. Much rather, we took the structure generated for $\rho_{\text{fil}} = 0.9$ and extracted only its surface by evaluating the voxel with the highest

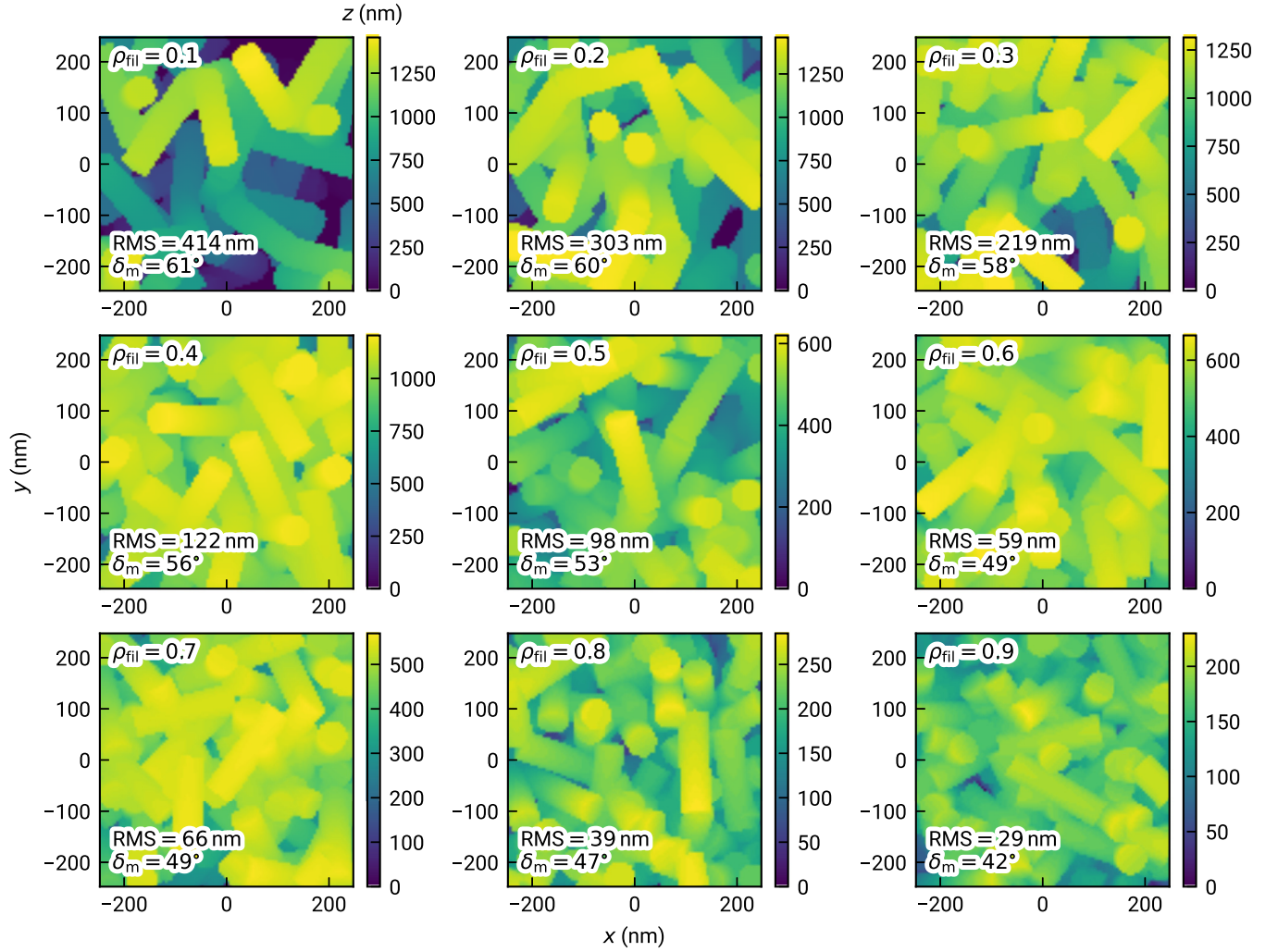


FIG. 2. Top views of the surfaces extracted from the fuzz structures for all nine porosity cases. For every panel, the x and y axes give the lateral extensions, while the color bar on the right represents the elevation.

z coordinate for each pair (x, y) of lateral coordinates. The result is a solid, nonporous surface that does preserve structure and roughness from the fuzz filaments. For the case of $\rho_{\text{fil}} = 0.9$, we used the resulting sputter yield as the sputter yield of a corresponding rough surface, Y_r . For the other porosity cases (ρ_{fil} varying from 0.1–0.8), we used the same procedure to shed light on the synergies between surface roughness and porosity. A top view of surfaces created in this manner is given in Fig. 2. The text insets in the bottom left corners give two quantities to characterize the surface roughness: the root-mean-square roughness (RMS) and the mean of the surface inclination angle distribution (δ_m).

III. RESULTS

The data obtained are presented with the aim of highlighting the interplay of surface roughness and porosity and their effect on the sputter yield of tungsten fuzz. Subsequently, we demonstrate that the introduction of porosity leads to a pronounced and systematic suppression of sputtering, which can be described by a simple linear dependence on the volume filling factor over a range of ion energies, projectile species

and incidence angles. Due to the large parameter space covered in this study (several projectiles, energies, angles, and porosities), we will show exemplary, illustrative results in the following. We have verified that the qualitative trends at hand are observed throughout the entire dataset. Additionally, we provide all data necessary to perform the analyses presented here for all other parameters [53].

As a first step, we examine the angular dependence of the sputter yield for flat and fuzzy (porous) tungsten surfaces. Figure 3(a) shows sputter yields Y of 1 keV Ar ions as a function of the incidence angle α with respect to the nominal sample normal. The flat-surface sputter yield (orange line) follows a well-known behavior with a pronounced maximum at approximately 60° , beyond which it falls sharply. In contrast, for fuzzy surfaces (green, red, and blue lines for volume fillings of 0.2, 0.5, and 0.8, respectively) show a suppressed dependence on α and are mostly constant, with small deviations from this trend only in the region of very grazing incidence ($\alpha > 80^\circ$). While the general trend of the flattening of the $Y(\alpha)$ curve is observed for all fuzz porosities, the absolute offset depends on the volume filling factor ρ_{fil} and the projectile species. For the Ar case in Fig. 3(a), all fuzz-derived curves start below the

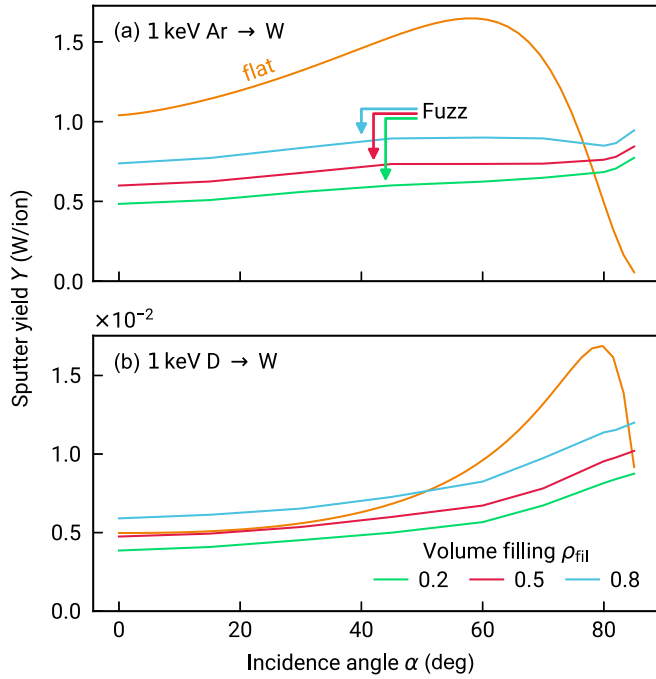


FIG. 3. Sputter yields Y for 1 keV (a) Ar and (b) D impinging on W as a function of incidence angle α with respect to the surface normal. Data from SDTrimSP for a flat surface are given in orange, while exemplary curves for three different fuzz porosities are shown in green, red, and blue, respectively.

flat-surface sputter yield. On the other hand, with D impactors, fuzz yields from $\rho_{\text{fil}} \gtrsim 0.5$ start above the flat-surface curve and the trend only reverses for more grazing incidences.

To quantitatively assess the influence of porosity beyond the angular effects illustrated in Fig. 3, we now examine the sputter yield as a function of the volume filling factor ρ_{fil} for all investigated porosities. Figure 4 summarizes this dependence for both Ar and D bombardment and forms the basis for identifying a simple scaling relation between sputter yield

and porosity. Figure 4(a) shows the sputter yields in W atoms per incident ion for the case of Ar bombardment over volume filling ρ_{fil} (left vertical axis, black). The corresponding data for D ions is shown in Fig. 4(b). As literature often gives simulated sputter yields of rough samples with respect to the flat surface sputter yield, we do the same on the right-hand vertical axis of both panels (gray axis). The corresponding flat surface yield is shown using the orange symbol, labeled Y_f in both panels and annotated with an arrow in Fig. 4(a). In both panels of Fig. 4, we used a linear function to fit the sputter yields Y as a function of ρ_{fil} :

$$Y(\rho_{\text{fil}}) = m \times \rho_{\text{fil}} + b. \quad (1)$$

The fit is shown by the blue solid line. We give both the slope (m) and the intercept (b) in the annotations of the figure, as well as the coefficients of determination. The fit is derived only from the data obtained for samples with volume fillings ranging from 0.1 to 0.9. Yet when extrapolated to a solid target (gray, dashed vertical line; $\rho_{\text{fil}} = 1.0$), the fit coincides with the sputter yield for a rough sample (red dot, Y_r) rather than the flat surface data shown in orange. This is the case both for Ar as well as D, even though for the presented cases in Fig. 4, the qualitative relation between Y_f and Y_r is different between the projectiles: $Y_f > Y_r$ for Ar, whereas $Y_f < Y_r$ for D under the given energy and incidence angle.

IV. DISCUSSION

A. Sputter yield modification

The sputter yields as presented above suggest two main findings: First, sputter yields are modified when changing the sample surface from flat to rough and subsequently reduced when hollows are introduced. This modification from flat to rough can take two forms as seen in Fig. 3: either an increase or a decrease, depending on the impactor and the incident angle. For Ar, $Y(\alpha)$ of a flat surface rises only moderately such that the maximum is only about 50% higher than the sputter yield at normal incidence. In this case, redeposition and shadowing seem to outweigh the variation of the local

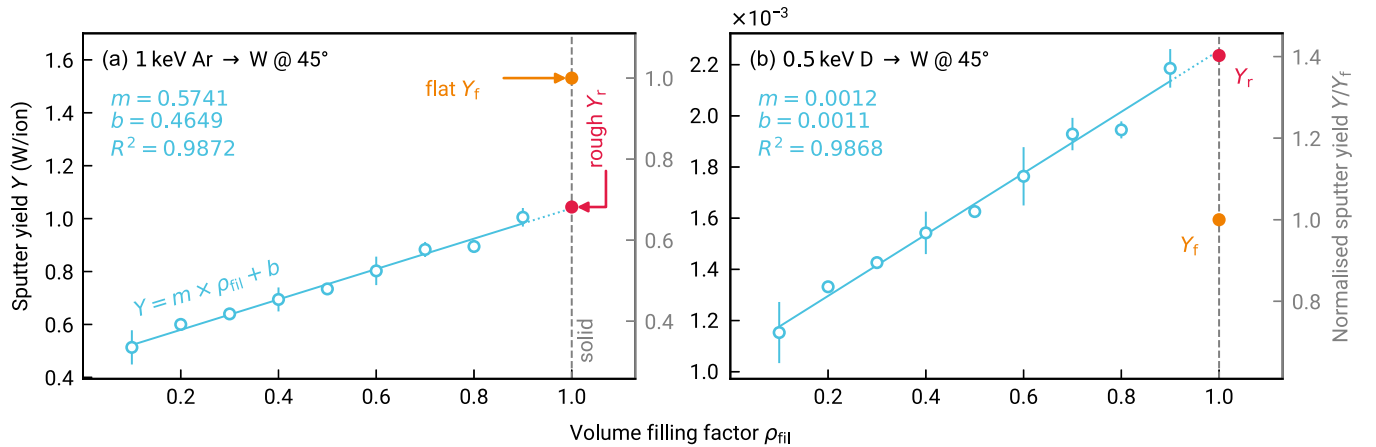


FIG. 4. Sputter yields Y of W fuzz at volume fillings corresponding to different porosities. (a) 1 keV Ar impinging under 45° . (b) 500 eV D impinging under 45° . In both subfigures, sputter yields are shown in blue circles alongside a linear fit (solid line). Fit parameters and coefficients of determination are given in the inset. In the limit $\rho_{\text{fil}} \rightarrow 1$ (solid target), the fit approaches the sputter yield values for rough, but solid targets (red circle, annotated), rather than a flat surface (orange, annotated). Note the exponential factor for the left vertical axis of (b).

incidence angle, and the sputter yield is effectively decreased. D, on the other hand, can also show an increased sputter yield compared to a flat surface. Here, the dependence of Y on α is much more pronounced, and it is increased threefold at its maximum compared to 0° incidence. Thus, the yield enhancement by an increased surface inclination is stronger than the potential redeposition.

Second, this suppression can be predicted well with a linear model. It should be noted that the intercept defining the fit in the limit of solid target is given by a similarly rough sample rather than a flat one. This holds true regardless whether the sputter yield for the rough surface is increased or decreased compared to the flat surface. In our case, similarly rough means filling all hollow spaces while preserving the surface envelope. In other studies, the distribution of the surface inclination angles and its mean have been established as measure for surface roughness that is well suited to describe the effect of surface roughness [11,13]. In both of these works, surface roughness has been attributed to modify the sputter yield due to geometrical effects, most notably the presence local inclinations as well as shadowing and the possibility to redeposit sputtered ejecta. Depending on the parameters at hand (energy, target-projectile combination, incidence angle), this modification can lead to either a yield increase or decrease. We observe this as well in Figs. 3 and 4, where in the D case the flat-surface yield is lower than for the rough fuzz envelope.

For the linear model, we point out that it likely will not hold for very small porosities, and as a result the parameter b is finite and nonzero. In the extreme case of volume fillings significantly smaller than 0.1 and sufficiently thick fuzz layers, one would expect further sputter yield reductions. Contrarily, in our simulation workflow the sputter yields for a flat surface would be recovered for the limit $\rho_{\text{fil}} \rightarrow 0$ due to the filled bottom layer of one voxel thickness. We thus restricted the simulations to a parameter space where we do not expect this problem to occur. As can be seen in Fig. 2, even for $\rho_{\text{fil}} = 0.1$, the bottom layer is not visible as indicated by the maximum extent of the color bar being below the full simulation cell height. For these reasons, we also refrained from extrapolating our findings towards $\rho_{\text{fil}} = 0$ in Fig. 4.

In contrast to the two possibilities for yield alteration when considering initial roughness, the further introduction of porosity always reduces the sputter yield, starting from the rough-surface yield. Once the roughness is accounted for, the hollows in the sample allow the ions to penetrate deeper. As a consequence, the energy deposition takes place farther away from the surface, and the particles sputtered have a higher chance of redeposition and will escape less likely. Due to their relatively low energies (on the eV scale [44]) below the sputtering threshold, these ejecta will not cause further sputtering themselves, thus effectively reducing the sputter yield. Only when the ion incidence becomes too grazing does the ions' initial momentum component directed into the sample get small enough that the influence of the porosity diminishes: The fuzz bands in Fig. 3 lie closer together for $\alpha > 80^\circ$, while their spacing is more constant throughout all the smaller angles. In a similar approach, Chang *et al.* [45] already investigated sputter yield data of Mo fuzz structures using a simple geometric description in which they accounted for the decrease in projectile and ejecta populations with increasing

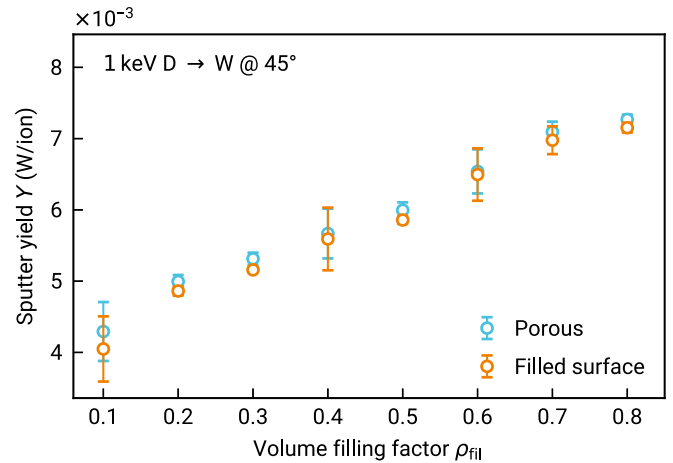


FIG. 5. Comparison of the sputter yields for the porous fuzz samples (blue) and the corresponding rough surfaces.

porosity and increasing fuzz layer depth. Their findings support the interpretation of porosity in a deep layer facilitating redeposition. Based on these assumptions, they formulated an analytical model with only a porosity-dependent mean-free path as a single parameter, and were able to qualitatively reproduce experimental sputter yield data.

Similarly, Fig. 2 already demonstrated an increasing RMS roughness for higher porosities, corroborating the interpretation of sputtering events happening deeper into the simulation cell. Moreover, also the roughness as described by the mean inclination angle increased. Both of these measures suggest that the sputter yield should also decrease when considering only the filled surfaces. We show these data for the remaining porosity case using example of 1 keV D under 45° incidence in Fig. 5. The sputter yields coincide within the error bars and only minimal scatter is present. This observation indicates that the sputter yield reduction can already be explained to a large extent by the modified surface envelope resulting from different filament spacings. Thus, within the present BCA framework, porosity primarily acts through its influence on the effective surface morphology rather than requiring an additional porosity-specific sputtering mechanism.

Nonetheless, when looking at the distributions of surface inclination angles as shown in Fig. 6, there is a significant difference compared to work in which the mean surface inclination angle δ_m was established as a quantitative descriptor for the sputtering behavior of rough surfaces [11,13]. In all the distributions in Fig. 6 (corresponding to the different underlying porosity cases), there are two distinct features: one peak at about 45° and another peak towards very grazing incidences. The former is presumably linked to the cylindrical shape of the fuzz filaments themselves, as it is present in a similar shape and height for all investigated porosities. The latter, on the other hand, is particularly pronounced for the high-porosity structures and almost vanishes with high volume filling. It therefore corresponds to steep flanks and trenches into the fuzz that are carried over into the large RMS values for low ρ_{fil} seen in Fig. 2.

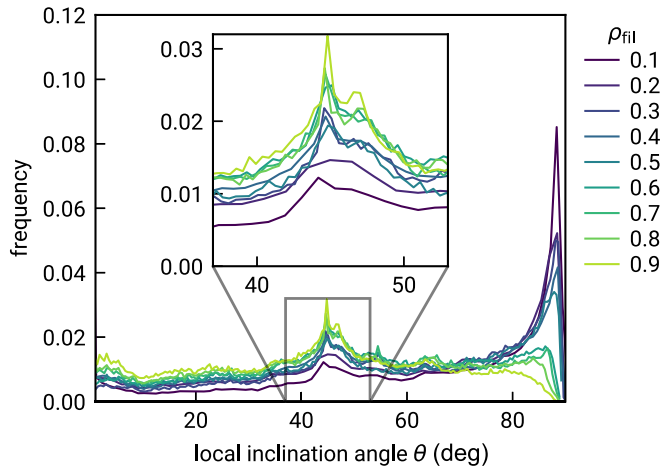


FIG. 6. Surface inclination angle distributions of the enveloping surfaces of fuzz structures for all porosity cases. The inset provides a zoomed-in view of the feature around 45° .

Since the inclination angle distribution for these artificial structures is so distinct, we do not expect the predictive, analytical framework from Ref. [13] to hold. It was developed under the assumption of surface elevations distributed according to a Gaussian normal distribution, and the resulting slope distributions have one single peak that is—depending on the RMS roughness and autocorrelation length—much broader. Similarly, all the experimental and simulated surfaces in Ref. [11] were characterized or created with a Gaussian height distribution. Therefore, while surface roughness may qualitatively explain the sputter yield reductions, the established quantitative models are not applicable. On the other hand, the linear fit over ρ_{fil} as given by Eq. (1) and illustrated in Fig. 4 was suitable over the entire investigated parameter space. In the following, we will explore its abstraction by means of a simple scaling law.

B. Generalization of the linear model

While the absolute slopes of the porosity-dependent sputter yields differ substantially between projectile species and ion energies, this variation largely reflects the corresponding differences in energy transfer and absolute sputter yields. To assess whether a common underlying behavior governs the porosity dependence across different projectiles and energies, we therefore normalize the slopes by the rough-surface sputter yield Y_r . Figure 7 reveals that, once normalized to Y_r , the slopes collapse onto a narrow band for a wide range of ion energies (0.5 keV to 2 keV; blue, orange and green lines) and for both projectile species (solid and dashed lines) investigated. Up to incidence angles of approximately 45° , the normalized slope m/Y_r remains nearly constant, with a mean value of about 0.54 (black line in Fig. 7) and only weak scatter (two standard deviations given by the light gray band therein). This behavior indicates that the suppression of sputtering by porosity follows a common scaling law that is largely independent of projectile mass and ion energy within this angular range. The finding highlights the importance of the rough surface yield and implies that once this Y_r is known,

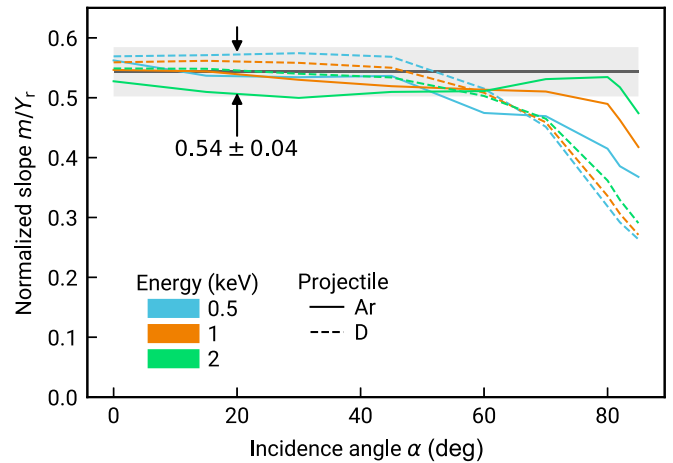


FIG. 7. Slopes m of the linear fits through the porosity-resolved sputter yields from Fig. 4 normalized per the respective rough surface sputter yield Y_r . For a wide range of incidence angles α up to $\approx 45^\circ$, m/Y_r is roughly constant for the investigated energies (blue, orange, and green lines) and projectiles (solid and dashed lines).

the entire porosity dependence of the sputter yield is defined, at least up to incidence angles of $\approx 45^\circ$. From a practical perspective, this implies that the volume filling factor may serve as a convenient morphological descriptor for predicting sputter yields, while the underlying physical origin remains closely linked to the corresponding surface roughness.

C. BCA limitations and comparison to fuzz literature

A potential limitation of this study is the reliance on simulated data obtained within the binary collision approximation. While simulation suites based on the BCA are widely used and typically provide a practical estimate on the sputter yield and related quantities, quantitative precision can deviate by several 10% compared to experimentally verified values. This is particularly true for combinations of light ions and heavy target species. As a consequence, the choice of physical input parameters remains an active area of research [35,46–48]. This is the reason why we provide an exemplary simulation input file [53]: should an updated default with better accuracy emerge for SDTrimSP, our results can be easily reevaluated. On the other hand, similar investigations aiming to untangle the effects of surface morphology on the sputter yield concluded that three-dimensional BCA simulations capture this influence with a high fidelity. This holds under the condition that the sample structure is adequately discretized, and that a potential initial yield offset is accounted for; that is, the relative effect is well described [4,11,27,30]. We therefore show the gray axis (units of flat-surface sputter yields) in Fig. 4. This is customarily done in literature (e.g., [24,36,45]) and enables verification with other works, as potential quantitative errors in absolute units should cancel out. We conduct such comparison in the following paragraphs.

Our lowest recorded relative sputter yield across the entire data set is $Y/Y_r \approx 28\%$. Nishijima *et al.* [24] show that the sputter yield reduction ranges from $\approx 40\%$ down to roughly 10% depending on the fuzz layer thickness at Ar energies up to 100 eV. For higher energies, they note that due to changed

angular emission characteristic of sputtered particles, this reduction could potentially saturate at higher relative yields Y/Y_f . Moreover, they also observed a proportional scaling of the relative sputter yield with the sample porosity, well in line with our findings. In a more recent work, Liang *et al.* [36] provide sputter yield values for three distinct fuzz layers with varying thicknesses and porosities under Ne bombardment. They report a sputter yield decrease of down to 20% of the flat surface sputter yield, in good agreement with the data presented in Ref. [24]. Contrary to our work, however, they point out that the yield decrease is greater for thicker fuzz layers rather than more porous structures, especially when layers of different thicknesses have similar porosities. Yet, their sputter yields were recorded dynamically during plasma exposure until total erosion of the entire fuzz layer, and only the yield minima of these data series were reported. Despite this underlying difference to our investigations for static targets, the overall qualitative agreement on sputter yield reduction persists. Yang *et al.* [49] report simulated yield reductions ranging from 0.05 to 0.15. While this is lower than our results, also the investigated energies do not match exactly. Their data were taken for energies below 500 eV and their fuzz model is a different one with relatively thinner filaments in comparison to the size of the simulation cell. At the same volume filling, this could potentially lead to more redeposition as the thinner filaments allow for more even spacing and higher chances of being in the line of sight of a sputtered atom. Again, they report findings as a function of layer thickness, which is a parameter we did not vary in our study. At higher energies (2 keV Ar), the data of Yang *et al.* [50] also agree quantitatively with ours, considering that they present sputter yields at even lower porosities.

D. Comparison to nanocolumnar tungsten

The near-universal behavior observed in Fig. 7 suggests that the porosity-induced suppression of sputtering can be captured by a simple scaling relation once the rough-surface sputter yield is known. To assess the applicability of this scaling beyond the fuzz structures considered here, we next confront our model with independent experimental data for other porous tungsten systems. Specifically, we apply the porosity-dependent scaling derived above to nanocolumnar tungsten and compare the resulting predictions to experimental sputter yield measurements reported by Lopez-Cazalilla *et al.* [14], as shown in Fig. 8.

In their work, Lopez-Cazalilla *et al.* [14] studied the sputtering of nanocolumnar tungsten (NCW) both experimentally and numerically. Their samples showed a surface coverage of 58%, which corresponds to the volume filling due to the columnar nature of the specimens. Moreover, they were characterized by atomic force microscopy (AFM), among others. Because of the finite tip size, the AFM cannot resolve the space between the nanocolumns. The authors then carried out 3D sputtering simulations also for this rough surface envelope. Therefore, Y_r is available for this case as well as an experimentally measured sputter yield at a given, well-defined porosity. The experimentally applied fluences are also low enough to prevent significant erosion, thus enabling a meaningful comparison to our static simulation study. We reprint

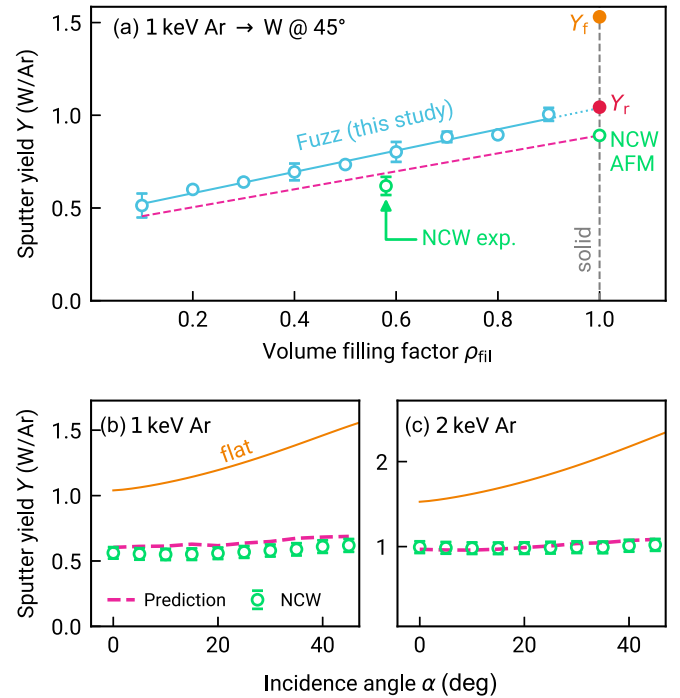


FIG. 8. Comparison of the findings of this work to data for nanocolumnar tungsten (NCW) by Lopez-Cazalilla *et al.* [14]. (a) Application of the porosity dependent fit function for the fit parameters from Fig. 7 (dashed pink line) to the NCW data (green circles). (b) Incidence angle dependent sputter yields for NCW under 1 keV Ar bombardment, both as per our model prediction (pink, dashed) as well as experimentally measured by Lopez-Cazalilla *et al.* [14] (green). Flat surface yields (orange) given for reference. (c) Same as in (b) for 2 keV Ar.

these data from Lopez-Cazalilla *et al.* [14] and contrast them with our model predictions in Fig. 8. Figure 8(a) illustrates the porosity-dependent scaling to nano-columnar tungsten under 1 keV Ar bombardment: The starting point for $\rho_{fil} = 1$ is given by the simulated data for the NCW surface envelope as resolved by the AFM (empty green circle). From there the linear porosity dependence follows by recovering the slope from the universal normalized slope shown in Fig. 7. The prediction by this approach is given by the dashed pink line. It agrees within error bars with the experimentally measured value from Ref. [14]. For comparison, we also show the sputter yields for flat, rough and porous fuzzy structures from Fig. 4(a) in Fig. 8(a). We show the experimental NCW sputter yields from Ref. [14] over incidence angle for 1 keV and 2 keV in Figs. 8(b) and 8(c). We limit the presentation to the angle range up to 45° where the assumption of a constant m/Y_r is justified (cf. Fig. 7). Our model predictions are again given by the dashed pink line and match well with the experimental data (green circles). This good agreement and experimental validation to other porous model systems hints towards a universal applicability of our findings.

Finally, experimental validations of this otherwise purely computational study could provide beneficial support for our model. Measuring the sputter yield of W fuzz is not straightforward, however, and quantitative, direct comparison to existing literature tends to fall short because some

parameters do not match between fuzz experiments and our study (fuzz layer thickness, energy, fluence-dependent morphology changes). Moreover, many of the reported sputter yields were obtained from simulations themselves and experimental data remains scarce; see also the corresponding paragraph above. Typical approaches rely on plasma exposure in linear plasma devices, where fluences are high enough to facilitate erosion of the nanostructure (e.g., as in Ref. [36]), or rely on techniques that do not survive the conditions necessary for fuzz growth (such as a quartz crystal microbalance [27]). This challenge could potentially be solved using a quartz microbalance to catch sputtered ejecta (as demonstrated, e.g., in Refs. [4,51]) in combination with samples that can be grown in a controlled fashion. Nanowire networks could provide exactly this: they have been reported to be produced by electrodeposition of tracks etched in polymers via ion irradiation [52]. In this approach, a highly interconnected network of filaments is formed, similarly to fuzz structures. One big advantage is the high degree of control: Both the filament thickness as well as the porosity can be varied in a wide range of parameters, thus potentially enabling a complementary, systematic experimental study.

V. SUMMARY AND CONCLUSION

We simulated the sputter yields of porous tungsten fuzz structures under Ar and D ion impingement at various ion energies, incidence angles and porosities using three-dimensional BCA simulations. Our results reveal a linear decrease of the sputter yield as a function of porosity, starting from the rough-surface yield Y_r rather than the flat-surface yield as a representative quantity for the zero-porosity case. When expressed relative to this rough-surface yield, the slope of the linear porosity dependence is found to be nearly constant across projectile species and ion energies for a wide range of incidence angles up to 45° . This demonstrates that porosity acts as a suitable parameter for sputtering, complementary to the well-established geometric effects of surface roughness, and provides a simple scaling framework for describing sputter yield suppression in porous tungsten systems. The applicability of this framework beyond the simulated fuzz structures is further supported by its consistency with experimentally reported sputter yields for (differently porous) nanocolumnar tungsten.

As a further step towards application in material science and design, especially in the field of nuclear fusion

research where sputtering of W fuzz critically affects reactor component lifetimes, additional aspects beyond the present well-controlled model system must be considered: The simulations presented here assume static surface morphologies, whereas at sufficiently high ion energies and fluences, erosion, and redeposition processes will dynamically modify the surface geometry. The fuzz layer thickness was kept constant, although experimental data suggest that it may influence sputtering behavior in more realistic specimens, particularly when porosity itself varies with depth. Moreover, the sheath potential is influenced by the surface morphology and thus, the ion incidence angles will be affected as well and not be constant anymore. All these factors will have to be accounted for when transferring these results to erosion estimations for plasma-facing components in nuclear fusion devices.

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DATA AVAILABILITY

Data supporting this study are openly available [53]. The repository includes sputter yield data for the entire parameter space covered, an interactive JUPYTER notebook for convenient exploration of the data set, an exemplary SDTrimSP-3D input file as well as the code to generate Figs. 2–8.

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