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Low energy sputtering of Mo surfaces

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ABSTRACT

Surfaces of materials subject to irradiation will be affected by sputtering, which can be a beneficial effect, like in the coating industry where a material is sputtered and redeposited on to another material to coat it. However, in most cases sputtering is an unwanted side-effect, for instance in nuclear fusion reactors, where the wall material will be degraded. This effect needs to be understood in order to be able to predict its consequences. To understand the sputtering, on an atomistic level, we have thoroughly investigated molybdenum surface sputtering by computational means. Molybdenum was chosen as detailed experimental studies have been carried out on it and it is one candidate material for the diagnostic mirrors in ITER, facing the plasma. In this study, we thoroughly investigate the molybdenum samples of different surface orientations, and their response to low energy argon plasma irradiation, by molecular dynamics simulations. We find both a surface orientation and ion energy specific sputtering yield of the samples, and a very good agreement with the experiments available in the literature. A few different setups were investigated to observe differences as well as to understand the key features affecting the sputtering events. The different simulation setups revealed the optimal one to represent the experimental conditions as well as the mechanisms behind the observed discrepancies between different modelling setups.

1. Introduction

The harsh environment in fusion test reactors and proposed fusion power plants will not only degrade the wall and structural materials, but also affect the material surfaces. Surface sputtering is a known phenomenon, and is widely used for coating, where the coating material is sputtered by energetic ions and then redeposited on to another material. In the case of fusion devices, like tokamaks and stellarators, surface sputtering is an issue as the sputtered atoms can both be redeposited on another place in the reactor and cause problems as well as cool down the plasma. Many studies on the sputtering phenomena have been carried out on various materials already over half a decade ago, mainly though on polycrystalline surfaces [1,2]. In order to be able to predict the exact sputtering of surfaces, atomistic insights of the phenomena and the effects of surface orientation are needed.

In addition to wall materials getting sputtered, the diagnostic devices needed for the reactor to work properly, both optical and laser-based [3,4], will get sputtered. This shield, or so-called diagnostics mirror, will be affected by the constant radiation present and the possible deposition of sputtered wall material on these mirrors will affect the operation of the whole reactor, as the diagnostics will not work properly. Single crystalline materials have been found to be good at maintaining the optical reflectivity during sputtering [5–7]. In order for the mirrors to work correctly, the mirrors need to be cleaned, as contamination of the mirror will decrease the operational lifetime. It has been found, for instance, that there is a significant tungsten contamination on diagnostic mirrors in operational tokamaks [8]. To be able to continue using the mirrors, plasma cleaning of the surface is suggested, to decrease the need for a complete replacement [9]. The cleaning is done via low energy argon irradiation. Another factor to optimize the mirror lifetime is to choose a material and surface orientation that has a low sputtering yield, as it has been found that different surface orientations will yield different results, both experimentally and computationally [10–13].

Different surface orientations of molybdenum have been experimentally exposed to low energy, 60 eV, argon irradiation

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[14]. The total weight loss was measured for three surface orientations, the (100), the (110) and the (111) surfaces, under the same conditions. It was found that the (100) surface showed the highest weight loss and the (110) surface the lowest weight loss. Therefore, to utilize Mo as mirror material, the (110) surface is the best choice, as it can withstand most cleaning procedures before the need of complete replacement. A few simulations were carried out in the same manuscript, and a qualitative agreement was observed, however, a quantitative agreement was not obtained. Neither were any of the mechanisms of the sputtering investigated nor the surface modifications studied. Additionally, the investigated temperature was different from the experimental one.

In this article, we investigate four different low-index surface orientations of single crystal molybdenum and subject them to argon irradiation. Different energies, between 30 eV and 200 eV, were studied to see the onset of sputtering and to observe the mechanisms leading to it. These were carried out both to explain the huge discrepancy observed earlier between simulations and experiments, and to explain the mechanisms not previously studied. Additionally, few different methodologies were used to obtain all the details to understand the sputtering yield and the sputtering event itself. Both single and cumulative simulations were carried out to see possible effects of previous surface modification. Furthermore, both atomistically perfect and atomistically rough surfaces were subject to the same procedure, to get a deeper insight in the phenomena.

2. Methods

The sputtering simulations were carried out with the classical molecular dynamics code PARCAS [15,16], with an adaptive time-step [17]. The interactions between Mo atoms were described by the interatomic potential by Ackland and Thetford [18], with the Ziegler-Biersack-Littmark (ZBL) repulsive potential implemented by Salonen [19]. The Ar−Ar and Ar−Mo interactions were described by the DMol potential [20]. The simulations were carried out at 550 K, comparable with previous experiments. Different energies were investigated, from 30 eV up to 200 eV for single impact (40 eV−100 eV for cumulative). All simulations were carried out in a setup where the incoming ions were perpendicular to the surface, according to previous experiments on similar systems. The incoming ion was chosen to hit the surface at a random place every time.

Two different setups were carried out: single ion sputtering and cumulative sputtering. In the single ion sputtering investigation, each incoming ion was hitting a pristine surface. In the cumulative sputtering simulations, the pre-existing damage from the previous events and possible Ar contamination were included. The simulation cells contained roughly 2 000 atoms in the single recoil event and roughly 6 000 atoms in the cumulative irradiation simulations. Four different surface orientations were investigated, the (100), (110), (111) and (112) surfaces. The simulation cell in the (100) setup was 10 unitcells (UC) in all directions and in the other setups 7 UCs in the [110] direction, 12 UCs in the [111] direction and 4 UCs in the [112] direction, for the single impact simulations. For the cumulative simulations, the cell was three times deeper. In addition to study pristine surfaces, atomistically rough surfaces were investigated. These rough surfaces were obtained by removing every second topmost atomic row on the surfaces. Snapshots of these surfaces can be seen in Fig. 1. The coordination of atoms in different layers, including the second nearest neighbour shell, is shown in Table 1. The layer numbering in this table starts from the top going towards the bulk. These rough surface simulations were carried out to see the effect of non-perfect surfaces on the sputtering yield, as in experiments some deviations from atomistically perfect surfaces are seen. Both single and cumulative irradiation were carried out on the rough surface.

For all energies and surfaces in the single ion sputtering simulations, a total of 40 000 incoming ions were simulated. The surface was first thermalized and then 1 000 ions interacted with that surface, always a pristine one. After the 1 000 incoming ions, a new surface was thermalized with a different seed and irradiated again 1 000 times. This was done 40 times to obtain the statistics. For the cumulative sputtering event, four surfaces of each orientation were thermalized and irradiated by 20 000 ions, to obtain statistics.

The single ion sputtering simulations were simulated for 10 ps each. All atoms that were over the cutoff of the potential above the surface were considered sputtered or reflected. In these simulations the bottom layers of atoms were fixed and a few layers above the fixed atoms were thermally controlled by a Berendsen thermostat [21], with a time constant of 200 fs. In the cumulative sputtering simulations, a similar layered structure on the simulation cell was used, although much thicker one to obtain the complete evolution. The cumulative sputtering simulations were carried out in two phases. First, a 5 ps simulation where only a few bottom layers were thermally controlled was carried out. Secondly, a 5 ps long simulation, where all mobile atoms were thermally controlled, was carried out, to get rid of any extra temperature, that could build up over the 20 000 recoil events. In the cumulative simulations, the atoms that were over the cutoff of the potential above the initial surface was deleted from the simulation cell, as they would be sputtered/reflected.

To investigate the surface modification probabilities we analyzed the coordination number of each atom, and compared with the perfect crystal sample with the correct surface orientation. We looked at the number of atoms within the second nearest neighbour shell of all atoms, with the cutoff in the middle between the second and third nearest neighbour shell. A sputtering and deposition event as well as a surface reconstruction will appear in this analysis as a different set of coordination numbers for the cell. If there are any differences, we counted this as a modified surface. The deposited energy was calculated as the ion energy minus the kinetic energy of the ion after the impact.

3. Results

3.1. Single ion sputtering

Results for single ions hitting a pristine smooth and rough surface can be found in Fig. 2 (a) and (b), respectively. The relative standard error of the mean of the different thermalizations is below 6% for sputtering yields above 0.01 and below 2.5% for sputtering yields above 0.05. From the figures the relative huge difference at low energies is not visible, as the sputtering yield is quite low. A zoom-in of the low energy sputtering is shown in Fig. 3(a) and (b), for the smooth and rough surface, respectively. In particular the onset can be more clearly seen from these zoomed-in figures.

Looking at the sputtering yield as a function of energy we can observe for the smooth surface a very similar behaviour for the (100), (111) and (112) surfaces, at low energies. The sputtering yield increases and at around 50 eV the (100) surface starts to show a highest yield, the (111) surface the medium and the (112) surface the lowest of these three. The (110) surface show almost no sputtering in this energy range. The sputtering yield will then increase the most for the (110) surface, and after around 120 eV it shows the second highest sputtering yield, slightly below the (100) surface. A surface orientation dependent onset energy for sputtering of the smooth surface can be observed, which is about 35 eV for all surface except the (110) which has an onset energy of around 60 eV. Looking at the results for the atomistically rough surface, a

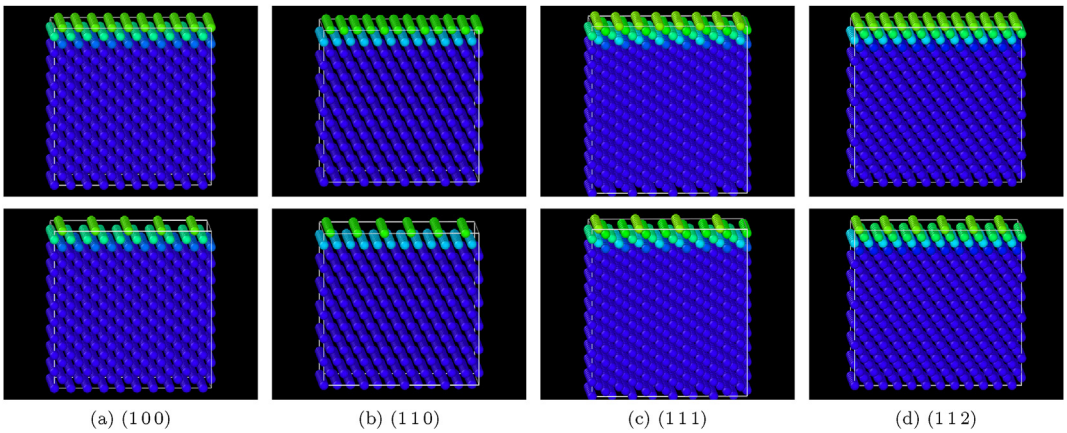

Fig. 1. The atomistically smooth and rough surfaces for the different surface orientations. Upper row represents the smooth surfaces and the lower row the atomistically rough surfaces. The color coding is according to the height of the atoms, to highlight the exact structure of the surface. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

Table 1
Coordination of atoms in the different layers for the investigated smooth and rough surfaces. Numbering starts from the topmost layer going down towards bulk. The number given is the coordination number, multiple numbers appear where depending on place there are several different ones in the same layer, and "Bulk" means this layer already have a perfect environment.

	Smooth				Rough			
	(100)	(110)	(111)	(112)	(100)	(110)	(111)	(112)
1st	9	10	7	8	7	6	7	6
2nd	13	Bulk	10	12	11	12	8/9	10
3rd	Bulk		13	Bulk	13/Bulk	Bulk	11/12	13
4th			Bulk		Bulk		13/Bulk	Bulk
5th							Bulk	

completely different trend can be seen. All surfaces show a very similar sputtering yield at low energies, with the same onset energy of around 35 eV. The sputtering yield is lower for the (100) and higher for the (110) orientations, compared to that of the smooth setup. The differences between different orientations are minute until high energies. At the highest energies, above 150 eV, the results are very similar to those of the smooth surface.

The general trends seen for single impact simulations: 1) The two different setups (smooth and rough) result in different sputtering yields for the same surface; 2) The order of the different surfaces are different in the different modelling setups; 3) The order of sputtering yield of different surface orientations also depends on the ion energy; 4) For the smooth surface it is clear that there is an onset energy, surface dependent, when sputtering starts to occur; 5) The atomistically rough surface show less surface orientation dependence compared to the smooth surface.

3.2. Cumulative sputtering

To investigate a more experimental like setup, cumulative irradiation of the different surface orientations was carried out. The results for the cumulative ion irradiation simulations can be found in Fig. 4(a) and (b), for the smooth and rough surface, respectively. From the figures it is immediately clear that the results are almost identical in both setups. The cumulative simulations show a more similar sputtering yield of all different orientations, however, a clear separation is still seen. No crossovers, as seen for the single impact simulations were seen. The (100) surface shows the highest sputtering yield, followed by the (111) surface. The lowest sputtering yield was observed for the (110) surface, and the (112) surface showed a bit higher sputtering yield. These qualitative results are very close to those observed experimentally under similar conditions, discussed below. As no difference was seen between the different starting points, like for the single impact simulations, but a different absolute result compared to both single impact setups, we can conclude that there is some surface roughness present during the whole simulation run. This is further backed up by looking at the sputtering as a function of incoming ion count, which

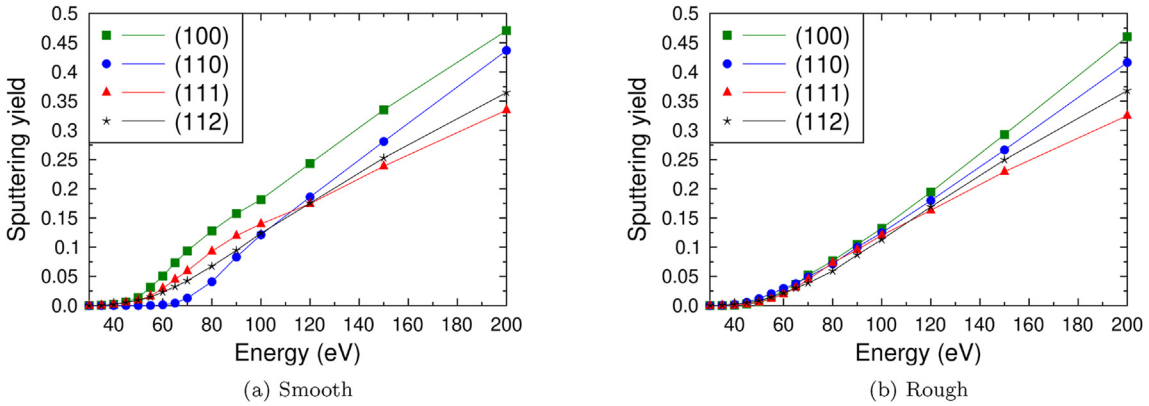

Fig. 2. Sputtering yield for the different surfaces as a function of energy for single impact simulations. (a) is the perfectly smooth surface and (b) the atomistically rough surface.

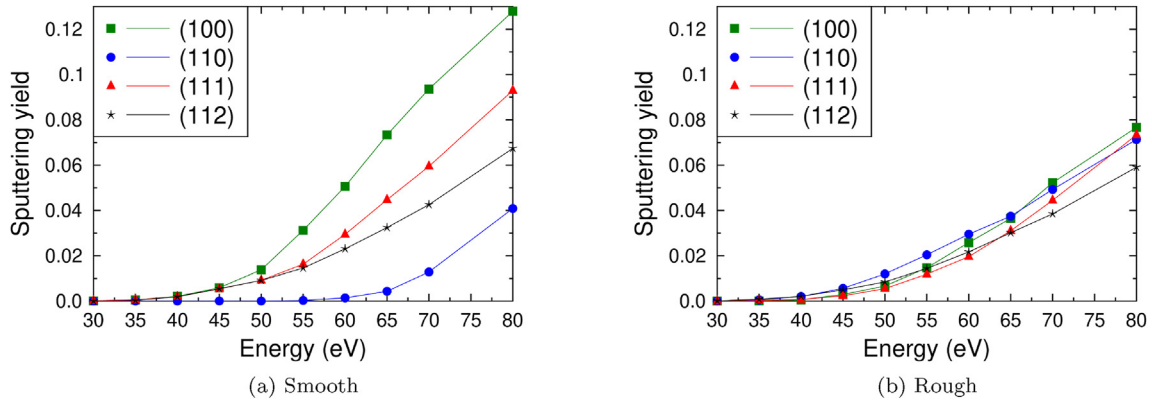

Fig. 3. A zoom-in at the lower energies of Fig. 2 for both setups.

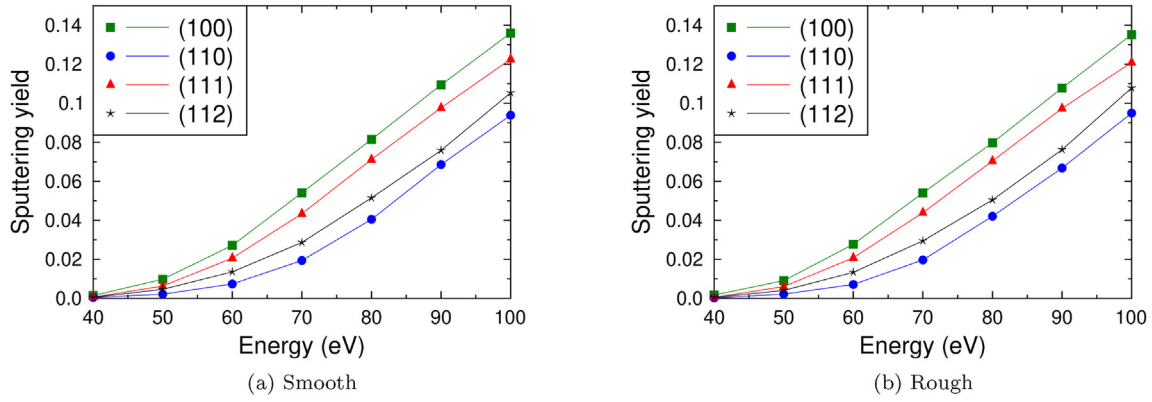

Fig. 4. Sputtering yield for the different surfaces as a function of energy for cumulative impact simulations. (a) is the perfectly smooth surface and (b) the atomistically rough surface.

showed a linear response, so no detectable onset. The lack of onset suggests that the surface modification is achieved quite quickly and thereafter the surface is kept in a non-pristine configuration.

3.3. Deposited energy

To investigate possible differences in energy transfer to different surface orientations, we analyzed the energy transferred from the incoming ion to the surface. The energy transferred divided by the incoming ion energy is shown as a function of ion energy in Fig. 5(a) and (b), for both single impact setups, respectively. We can observe some differences between the different surfaces, however, even though the relative difference can be quite large, the real difference is only on the level of $\sim$ 2 eV between the (111) and the (110) surfaces for the smooth surface. For the smooth surface, all four orientations show the same increasing trend in deposited energy. For the rough surface, a small deviation is seen for the (110) surface, where the increase as a function of incoming ion energy is less steep, related to the reflection yield, shown later, for this surface.

3.4. Surface modification

To investigate the phenomena more closely and mechanisms behind the sputtering events, we studied the possible surface modifications after the single ion impact event. Both the smooth and the rough surfaces were subject to this analysis. It was observed that none of the smooth surfaces did reorient during the thermalization, neither did the (100) nor the (111) rough surfaces. The rough (110) and (112) surfaces did in between 2 and 10 of the 40 relaxations show some kind of reorientation. These cases are excluded from the surface modification analysis.

In Figs. 6 and 7 the different mechanisms leading to a surface modification is plotted, for all surface orientations and both setups, respectively. Their sum is the total probability for some kind of surface modification. The different mechanisms are divided in to the four categories:

- *Only Reflection*
  No sputtering event is happening.
  The argon ion is reflected.
- *Only Deposition*
  No sputtering event is happening.
  The argon ion is deposited on the surface.
- *Sputtering-Deposition*
  Molybdenum sputtering is happening.
  The argon ion is deposited on the surface.
- *Sputtering-Reflection*
  Molybdenum sputtering is happening.
  The argon ion is reflected.

Looking at the overall trend, for both setups, it can be seen that there is a surface dependent modification probability. The most drastic difference is seen for the (111) surface in the smooth setup and the (110) and (112) surfaces in the rough setup. The modification probability is increasing with energy, as both the sputtering and Ar deposition is increasing as well as the surface atom

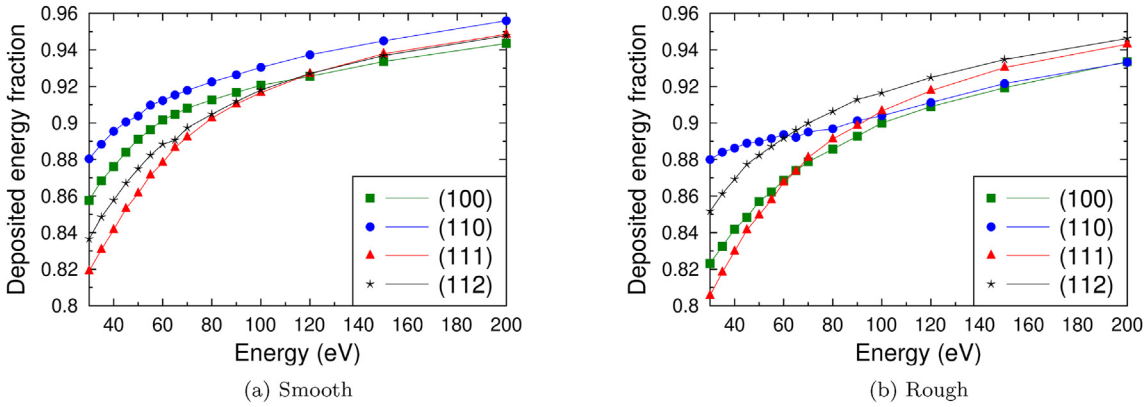

Fig. 5. Deposited energy fraction as a function of incoming ion energy for the different surfaces. (a) is the perfectly smooth surface and (b) the atomistically rough surface.

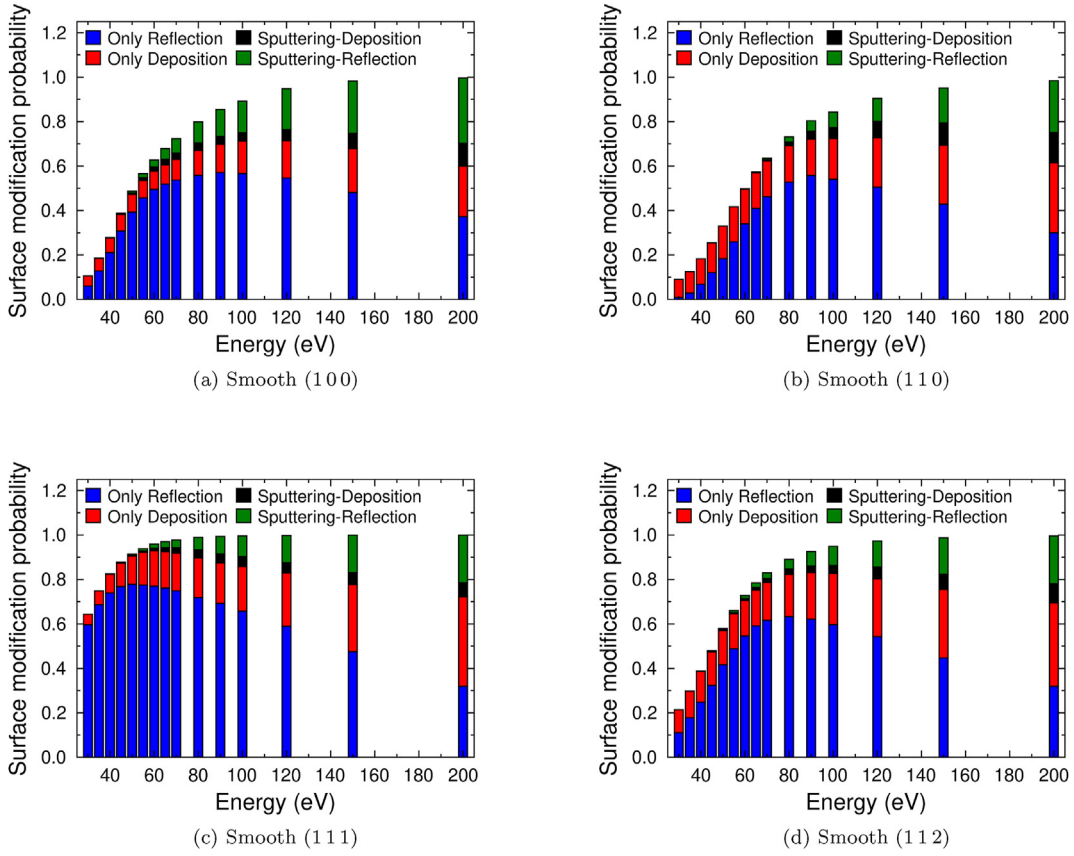

Fig. 6. The different mechanisms leading to a surface modification for the smooth surfaces.

reconfiguration already seen at low energies easily can happen at these energies. At low energies, the largest contribution to surface modification is due to atom rearrangement on the surfaces, followed by argon deposition. As the energy increases, surface modification by sputtering in combination with either deposition or reflection is increasing. This trend is seen for both smooth and rough surfaces, except for the smooth (110) surface, where deposition is the main contributing factor up to a bit higher energies.

3.5. Reflection yield

The reflection yield for single ions hitting a pristine smooth and rough surface can be found in Fig. 8(a) and (b), respectively. From the graphs we can see a high reflection yield at low energies, which almost linearly goes down with increasing ion energy. For both setups we can see that the (100) has the highest reflection yield, whereas the other surfaces have quite similar ones, with some exception mainly for the rough surface at the lowest and highest energies.

4. Discussion

In the Results section a huge difference in sputtering yield was seen between the smooth and rough starting point in the single impact simulations. In addition, it was observed that the cumulative irradiation did not show such a difference as well as the

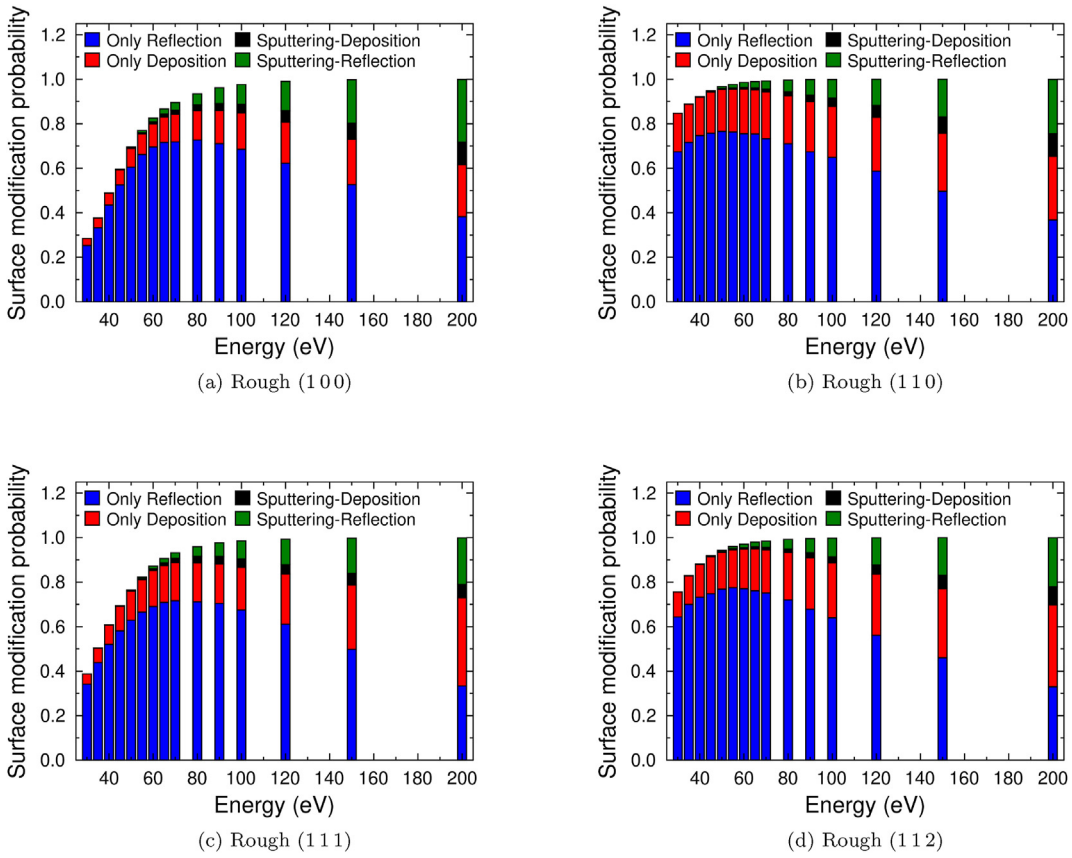

Fig. 7. The different mechanisms leading to a surface modification for the rough surfaces.

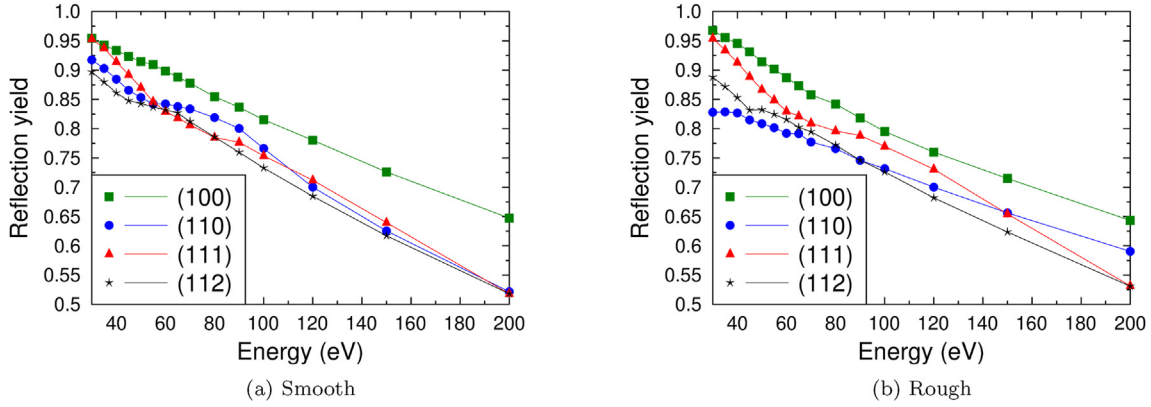

Fig. 8. Reflection yield for the different surfaces as a function of energy. (a) for the perfectly smooth surface and (b) the atomistically rough surface.

cumulative setup did not agree with neither of the single impact setups. To understand the huge discrepancies between the two setups in single ion impacts and their difference to cumulative irradiation, several possible factors were looked at. We looked at possible difference in; 1) reflection yield; 2) deposited energy; 3) surface modification probability; all three described below.

1. We can observe that the (100) surface has the highest reflection yield of argon, in both setups, and also the highest sputtering yield. However, the other surfaces show quite similar reflection yields, with some variation, even though they show differences in sputtering yield. This shows that there is not a direct correlation between the reflection yield and sputtering yield.

2. The deposited energy analyzis showed that there are some differences in the energy deposited to surfaces of different orientations. For the smooth surface, the (110) surface will absorb the most energy, and the (111) the least. For the rough surface, the same holds true for low energies, with some variation at higher energies. Again, there is not a clear relation between the deposited energy and the sputtering yield. Neither does the (100) surface with a high reflection yield show the least of deposited energy.

3. The surface modification analysis revealed that even at the very low ion energies (few tens of eV), there are modifications happening to the surface, even though the sputtering is minimal. For the perfectly smooth surface, the (111) surface had already at

30 eV a 2/3 probability for surface modification, which was mainly attributed to one of the topmost atoms moving to a nearby surface position. The other surfaces, showed a much smaller probability for modification, however, still 10% at 30 eV and already 50% at $\sim$ 60 eV. The rough surfaces had even higher probabilities for changes already at lower energies, which is attributed to one of the topmost atoms in the rows moving to the atoms places where the deleted atoms were located. The movement of surface atoms due to energy transfer was seen to be the dominating factor for surface modification, followed by deposition of argon, especially at lower energies. Only the smooth (110) surface had the deposition as the main contributing factor at low energies, explained by the close packed surface not allowing atoms to move easily. For the rough surfaces, it has already been noted that thermal energy present during relaxation, was in some cases enough to modify the (110) and (112) surfaces. This explains why already a small amount of energy added will result in a very high modification probability for the (110) and (112) surfaces.

Looking at the results of these three factors to try to explain the differences between the single ion setups and the cumulative setup, as well as the non-existing difference between the two different cumulative setups, we can conclude that the differences in reflection yield and in deposited energy are not responsible for the differences in sputtering yield, as no clear correlation is seen. Neither will these differences explain the non-existing difference between the smooth and rough cumulative setups. The one factor that can explain both differences is the surface modification probabilities of the different orientated surfaces. At low energy, even though very little sputtering is happening, there is a high probability for surface modification. The main mechanisms leading to the surface modification at low energies is atom rearrangement, followed by deposition of argon. This, in addition to the completely different sputtering yield of the single ion on smooth surface and on rough surface, can explain the discrepancy between single impacts and cumulative impacts, as well as the very similar results for both starting points for the cumulative irradiation simulations.

Looking at the differences between the sputtering yield at low energies of smooth and rough surfaces in single impact setups, we can see that the (112) surface shows similar results, the (110) surface an increase in sputtering yield, the (111) surface a slight decrease in sputtering yield and the (100) surface a drastic decrease in sputtering yield. For the different orientations of smooth surfaces we can observe differences both in the coordination of the surface atoms and in the mechanisms leading to surface modification probability. For the rough surfaces, on the other hand, the coordination is closer and the mechanisms behind surface modification are more similar for all surface orientations. This can explain on a general level why all the rough surfaces show quite similar results at low energies. Focusing on the difference between the smooth and the rough surface of the same orientation. The increase in sputtering yield of the rough (110) surface can be explained by the smooth (110) surface being the most stable (also most close-packed) surface and the rough (110) surface showing the highest probability for modification. The coordination of the surface atoms are also going from most coordinated to least coordinated. The (111) smooth surface has a high probability at low energies to be modified, and the rough (111) has a slightly lower probability and indeed shows a slightly lower sputtering yield. The (111) surface neither show a huge change in coordination of the topmost atoms. The other two surfaces are not as well described by this approach. Both the decrease in coordination and increase in surface modification probability of the (100) and the (112) surfaces, would predict a higher sputtering yield, which is not the case. This shows that there is in addition to the before-mentioned factors also a surface geometry factor.

Previous experiments by Litnovsky et al. [14] showed a surface orientation dependent sputtering yield during a plasma cleaning procedure setup. The target was biased to -65 V and the plasma potential of the argon was -5 V, leading to an ion energy of 60 eV, more details in Refs. [14,22]. It was found that the (100) surface had the highest sputtering yield, the (111) surface a sputtering yield a bit lower and the (110) surface the lowest sputtering. In the same study some preliminary simulation results at a different temperature showed the same trend, however, a huge discrepancy in the relative and absolute differences between simulations and experimental results was seen [14]. The results, both experimental and computational, are gathered in the Table 2 for 60 eV argon irradiation. In the same table the results from our two setups under two different conditions are shown for the same energy of 60 eV. We can immediately observe that the previously used 300 K instead of 550 K do not affect the sputtering yield in single impact setup, as a very similar result is seen. The rough surface will drastically affect the sputtering in the single impact simulations, where both the magnitude of sputtering and the order of different surface orientations are changed, compared to the smooth surface. Neither of the single impact simulations show a good agreement with the experimental results, indicating the need for a better methodology to describe the phenomenon. Looking at the cumulative simulations, both setups yielded the same results, as well as an decent agreement with the experimental results. The relative difference between surfaces are much closer to experimental results and the absolute values are also much closer. So, with these cumulative simulations we can obtain a good qualitative match. However, looking at the results for cumulative irradiation at 90 eV, we can observe almost perfect agreement with the absolute values, also shown in the Table 2. This offset seen between simulations and experiments is most likely due to fitting of the interatomic potential. The single impact simulations, not shown in the table, will not yield an as good agreement at any investigated energy. With these results we can observe that to get a good insight in the sputtering yields, we need to conduct cumulative irradiation simulations. However, the initial surface morphology, when the features are small like in experiments of very flat surfaces, will not drastically affect the end results.

5. Conclusions

We have in this article thoroughly investigated the sputtering of molybdenum surfaces, by computational means. We focused on molybdenum, as it has been experimentally studied in the interesting energy region. However, the surface orientations dependent sputtering yield has not been subject to thorough investigation, and the mechanisms behind the dependence not determined. We could observe huge discrepancy between different simulations setups, both on a qualitative and quantitative level. We showed that the cumulative irradiation setup will yield a very good qualitative agreement as well as a good quantitative agreement by adjusting the ion energy. The main reason why single impact simulations yielded different results as well as results not comparable with experiments was the lack of surface roughness. It was observed that even though very little sputtering happened, in many cases there was a high probability for surface modification, that will affect the sputtering yield of the modified surface. The main mechanism of surface modification at low energy was atom rearrangement due to energy deposition, followed by argon deposition. At higher energies sputtering became an important factor, in addition to the other two. We have shown that the best surface orientation with least sputtering during a plasma cleaning procedure is the (110) surface orientation of Mo mirrors. This is also true for possible higher cleaning energies, than the 60 eV used in present

Table 2
Sputtering yield, in units of sputtered atoms per incoming ion, for the different surface orientations for 60 eV argon irradiation at 550K. *Investigated temperature in this study was 300K. ☉Cumulative simulation of the smooth surface with 90 eV argon irradiation. Both previous experimental results and simulation results, Ref. [14], are compared with the simulated ones obtained in this manuscript. The values in parenthesis are the normalized sputtering yields to the (100) surface in the corresponding setup.

	Exp. [14].	Simul.* [14]	Sing. Smooth	Sing. Rough	Cumul. Smooth	Cumul. Rough	Cumul. Smooth☉
(100)	0.12 (1.00)	0.046 (1.00)	0.051 (1.00)	0.026 (1.00)	0.027 (1.00)	0.028 (1.00)	0.11 (1.00)
(110)	0.08 (0.67)	0.0005 (0.01)	0.0014 (0.03)	0.030 (1.15)	0.0074 (0.27)	0.0071 (0.25)	0.069 (0.63)
(111)	0.10 (0.83)	0.027 (0.59)	0.029 (0.57)	0.020 (0.77)	0.021 (0.78)	0.021 (0.75)	0.098 (0.89)
(112)	–	–	0.023 (0.45)	0.022 (0.85)	0.014 (0.52)	0.013 (0.46)	0.076 (0.69)

investigations.

Data availability

The raw/processed data required to reproduce these findings cannot be shared at this time due to technical or time limitations.

CRediT authorship contribution statement

F. Granberg: Methodology, Investigation, Formal analysis, Writing - original draft, Visualization. **A. Litnovsky:** Conceptualization, Writing - review & editing, Supervision. **K. Nordlund:** Conceptualization, Writing - review & editing, Project administration, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jnucmat.2020.152274.

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