EFFECT OF INCREASING SURFACE ROUGHNESS ON SPUTTERING AND REFLECTION

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In this work, the SDTrimSP-2D code was used for numerical simulation of the interaction of ions with a 2D periodical structure as idealized test system to investigate the influence of surface roughness on sputtering. Sputtering yield and reflection coefficient have been studied as a function of the size of the pitch grating structure. Simulations show that the most important changes in ion-surface interactions occur when the structure size gets approximately equal to the size of the collisional cascade..

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INTRODUCTION

The sputtering of surface atoms by ion bombardment is a well-known process [1], which is utilized by many plasma technological applications. Most experiments are performed with a polished and smooth surface; the simulations assumed also that the surface is perfectly plane. Up to now, the influence of surface roughness on sputtering is not understood well, because there was no suitable model, which was able to provide a comprehensive description. Only few attempts had been made in the past. Ruzic has modified the TRIM.SP code to study the sputtering of the surface with fractal geometry [2]. Kuestner, Eckstein and co-authors had considered the rough surface as an aggregate of simple surfaces at inclined angles [3]. Later, the SDTrimSP-2D code [4] has been developed to simulate interaction of ions with the 2-D non-planar surfaces. It is a powerful tool for the study of surface morphology effects. The validation of the code has been performed exposing a Si pitch grating with typical dimensions of 200…250 nm to 6 keV Ar ion beam [5, 6].

In this work 6 keV Ar ion projectiles are bombarding a Si pitch grating with a periodic 2D structure of varying size representing surface roughness. This rather idealized system has been used for numerical investigation of the sputtering yield and reflection coefficient as a function of the size of the surface roughness. The characteristic size of the surface morphology is varied in the range of 1…100 nm. Previous studies [5, 6] have validated the code for this particular target-projectile combination and it was confirmed that such structure exhibits all the effects expected for rough surface: local increase of sputtering due to inclined incidence of ions, contribution from sputtering by reflected projectiles, strong influence of the redeposition, etc.

1. METHODS

The simulations have been performed by the SDTrimSP-2D code [4]. The surface is shaped in two dimensions (vertical and lateral) and extended in the third direction. The cross-section of the surface is shown in Fig. 1,a; one can see that the typical dimension h characterizes width and height of the structure.

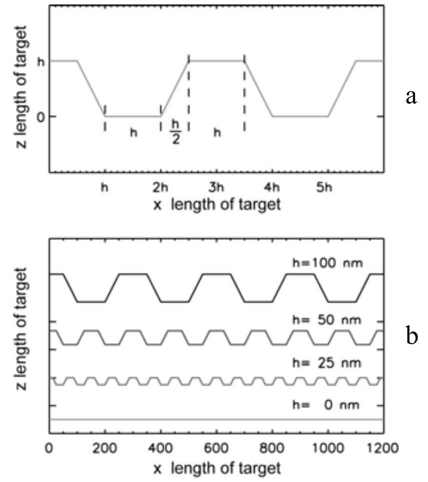

Fig. 1. Cross-section of the Si surface with 2-D structure: a – typical sizes of the structure in units of h; b – structure scaled according to different h values

The simulations have been run in static mode, i.e. projectiles and collisional cascades do not change the structure and elemental composition of the irradiated surface. Each simulation was run with a particular value of the typical dimension h, varied between 1 and 100 nm. While the typical size h is changed, the shape of the structure is preserved; Fig. 1,b shows the size of cross-sections of the structure for different h values.

As results, one can obtain the dependence of sputtering yield and reflection coefficient on the typical roughness size h. Moreover, code diagnostics delivers the partial sputter yields from different parts of the surface: left, right, top and bottom parts of the structure. Therefore, one can analyze the contributions of different surface parts to the total sputtering yield and reflection coefficient.

2. RESULTS AND DISCUSSION

Fig. 2 shows typical trajectories of projectiles and recoils, forming a collisional cascade for an impact at normal incidence. The absolute maximum of depth profiles is 30 nm and the absolute maximum of lateral spreads, R, is 16 nm for all calculated trajectories. The average of the maxima of depth profiles for all cascades is 16.5 nm and the average of all maxima of lateral spreads, R, is

10.2 nm. These two values were calculated from the point of the impact of projectile to the depth position where one has the maximum number of intermediate points of trajectories. While the typical size h of the structure is increasing, the mean size R of the collisional cascade remains the same (see Fig. 2). The influence of one cascade is more local if the size h increased. Fig. 3 shows the dependence of sputtering yield and reflection coefficient on typical structure size h.

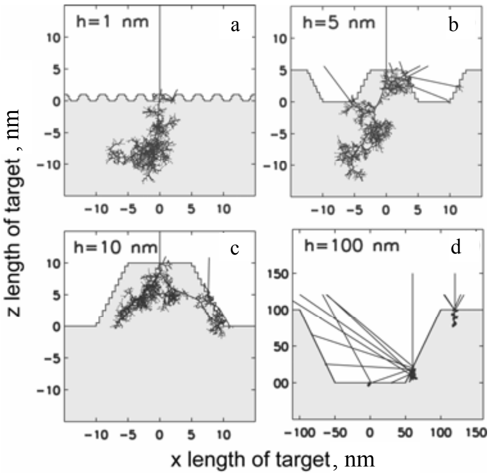

Fig. 2. Trajectories of projectile and recoils during the development of the collisional cascade:
a – h=1 nm; b – h=5 nm; c – h=10 nm; d – h=100 nm

When R>>h, the collisional cascade develops under the bottom surface of the structure, as one can see in Fig. 2,a. One should expect that this surface behaves as a planar one with regard to sputtering and reflection. The number of atoms reaching the surface is only slightly increased in comparison to the case of a planar surface. The effect of inclined surfaces is small. Furthermore, the mean free path of the projectile is 0.27 nm. The influence of target geometry in this case is negligible. Therefore, geometrical effects should have rather small influence on sputtering and reflection. This is confirmed by the simulation, which indicates that the sputtering yield of a planar surface differs only marginally from the rough one (Y_{planar}=1.4 and Y_{rough}=1.5). Simulations show that the sputtering yield and the reflection coefficient grow only slightly, when h<1 nm (see Fig. 3).

At R≈h, the situation becomes different. Here, the size of the collisional cascade and the structure are similar. The cascade spreads over approximately one structure period, as one can see in Fig. 2,b and c. The number of recoils, which reach the surface at the inclined side of the structure, increases. They may leave the surface as sputtered atoms and, if re-deposition is avoided, these atoms contribute to the overall sputtering yield. This is comparable with the effect of bombardment at an inclined incident angle in the planar case.

The strongest growth of the sputtering yield and reflection coefficient occurs, until the typical structure size does no longer exceed the size of the collisional cascade (mostly for 1 nm<h<10 nm). However, different parts of the surface behave different in terms of sputtering and reflection. Fig. 3 shows the partial sputtering yields and reflection coefficients for top, bottom and inclined surfaces. Sputtering is possible for two cases: either a projectile reaches the particular surface or an event occurs on this particular surface due to particles originating from projectiles impacting at different locations. The simulation shows that the yields for these two cases are not equal and one can extract additional information on the development of collisional cascades on rough surfaces.

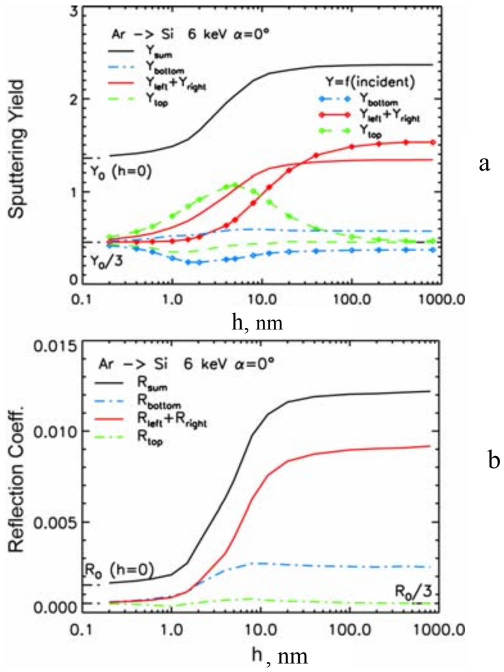

Fig. 3. Sputtering yield as a function of typical size h of the structure. The partial values of the parameters have been obtained according to the location, from which the atom leaves the structure; the lines marked as "incident" in the legend show the sputtering yield according to the location, where the projectile enters the surface (a). Reflection coefficient as a function of typical size h of the structure; the partial values of the parameters have been obtained according to the location, from which the atom leaves the structure (b)

Projectiles bombarding the top of the structure produce the highest partial sputtering yields (see Fig. 3 in the range of structure size h of 1 nm<h<10 nm). In contrast, there are much less atoms sputtered from this location. Collisional cascades develop due to bombardment of the top surface, which produces recoils. These leave the surface by reaching side and bottom structures. The sputtering yield produced by direct bombardment of the sides is lower than that produced indirectly from atoms leaving through the side structure. Extra sputtering events are produced by collisional cascades initiated on other surfaces (obviously, the top one). Similar behavior is seen on the bottom of the structure. Summarizing, one can conclude that the collisional cascades are initiated mostly on the top of the structure and their development can produce sputtered atoms on the sides. The same effect is less pronounced if cascades from the sides are considered. Finally, on the bottom surface the collisional cascades mainly go deep into the structure material and additional sputtering is produced by recoils originating from collisional cascades initiated on other surfaces.At large structure sizes, when R<<h, the collisional cascade is much

smaller than the structure; a typical example is shown in Fig. 2,d. Now, the interaction of ions with the structure can be well described in a 1-D approximation, i.e. one can calculate sputtering yield and reflection coefficient assuming that projectiles interact with aggregates of the inclined surfaces, as it has been performed by Kuestner et al. [3]. However, the redeposition has not been taken into account in this 1-D approximation. The analysis of the data presented in Fig. 3 shows that the contribution from the top surface to the sputtering is strongly reduced.

The reflection coefficient has a similar dependency as the sputtering yield (see Fig. 3); the inclined surfaces produce more reflected projectiles due to the effective incident angle and to multiple reflections. One example of possible trajectories is shown in Fig. 2,d. The reflection coefficient from the top surface remains constant, while the structure size is growing. This is explained by the fact that most projectiles are obviously scattered from the top surface through single reflection events. In contrast, projectiles incident on side surfaces are reflected towards the other surfaces of the structure. Therefore, there are projectiles, which experience multiple scattering before finally leaving the surface. While the structure size is increasing, one can observe that the last reflection of the scattered projectiles occurs mostly at the side surface. Some of the scattered projectiles leave the structure reflected from the bottom of the structure. This explains why the reflection coefficient from the bottom location is growing with structure size h.

CONCLUSIONS

In this work, the SDTrimSP-2D code was used to investigate the interaction of ions with a rough surface. We used an idealized representation, namely a 2D periodical structure as test system to clarify the basic physics trends. Such a 2D periodic Si pitch grating has been exposed to an ion flux of 6 keV Ar and the sputtering yield and reflection coefficient have been studied as a function of the size of the pitch grating structure. It has been shown that the bombardment of the surface at normal angle of incidence (relatively to the macroscopic plane) results in increases of both the sputtering yield and reflection coefficient with increasing structure size. The largest increase of the sputtering yield is observed in the range between 1 and 10 nm, which corresponds to the typical size of collisional cascades, initiated by the 6 keV Ar projectiles. Therefore, if the roughness size is larger than the typical size of the collisional cascade, one gets the highest possible sputtering yield. Another benefit of large surface roughness is the reproducibility of sputtering yields or deposition rates, if the deposition utilizes sputtering (like in magnetron sputter deposition).

REFERENCES

1. R. Behrisch, W. Eckstein (ed). *Sputtering by Particle Bombardment. Experiments and Computer Calculations from Threshold to MeV Energies.* Berlin, Springer, 2007.
2. D. Ruzic. The effects of surface roughness characterized by fractal geometry on sputtering // *Nucl. Instrum. Meth.* 1990, v. B47, p. 118-125.
3. M. Kuestner, W. Eckstein, E. Hechtl, and J. Roth. Angular dependence of the sputtering yield of rough beryllium surfaces // *J. Nucl. Mater.* 1999, v. 265, p. 22-27.
4. A. Mutzke, R. Schneider. *SDTrimSP-2D: Simulation of Particles Bombarding on a Two Dimensional Target Version 1.0.* IPP Report 12/4. Garching, Max-Planck-Institute
5. I. Bizyukov, A. Mutzke, R. Schneider, and J. Davis. Evolution of the 2D surface structure of a silicon pitch grating under argon ion bombardment: Experiment and modeling. // *Nucl. Instr. and Meth.* 2010, v. B268, p. 2631-2638.
6. I. Bizyukov, A. Mutzke, M. Mayer, H. Langhuth, K. Krieger, R. Schneider. Macroscopic parameters of the interaction of an Ar^+ ion beam with a Si pitch grating // *Nucl. Instr. and Meth.* 2012, v. B278, p. 4-7.

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ВЛИЯНИЕ ШЕРОХОВАТОСТИ ПОВЕРХНОСТИ НА РАСПЫЛЕНИЕ И ОТРАЖЕНИЕ

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Код SDTrimSP-2D использовался для моделирования взаимодействия ионов с двухмерной поверхностью, которая взята в качестве идеализированной тестовой системы для исследования влияния шероховатости. Коэффициенты распыления и отражения изучались как функции характерного размера структуры дифракционной решетки. Моделирование показало, что наиболее важные изменения во взаимодействии ионов с поверхностью происходят тогда, когда размер структуры приблизительно равен размеру столкновительного каскада.

ВПЛИВ ШОРСТКОСТІ ПОВЕРХНІ НА РОЗПИЛЕННЯ ТА ВІДБИТТЯ

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Код SDTrimSP-2D використовувався для моделювання взаємодії іонів з двомірною поверхнею, яка обрана у якості ідеалізованої тестової системи для дослідження впливу шорсткості. Коефіцієнти розпилення і відбиття вивчалися як функції характерного розміру структури дифракційної решітки. Моделювання показало, що найбільш важливі зміни у взаємодії іонів з поверхнею відбуваються тоді, коли розмір структури приблизно дорівнює розміру каскаду зіткнень.