The influence of target surface morphology on the sputter deposition flux

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Abstract. The effect of the target surface morphology on the sputter deposition flux and the energy flux is investigated by comparing solid targets to pressed powder targets. A significant, material dependent difference of the effective sputter yield between both target types is noticed. This difference is explained by combining two effects: a local increase of the elemental sputter yield and the redeposition of sputtered atoms onto the target. Both effects strongly depend on the target surface morphology. The experimental trends are reproduced by Monte Carlo simulations. This allows a description of the angular distribution of the sputtered atoms which is an important parameter to define the particle flux and the energy distribution of the atoms arriving on the substrate. Using the previously developed particle trajectory code SIMTRA, the latter is demonstrated for the studied materials (Al, Ag, Cu, and Ti).

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1. Introduction

Modelling the growth of thin films is a challenging endeavour that requires a good understanding of several processes and the parameters that drive them. The material flux towards the substrate, and the energy distribution of the arriving atoms play a key role[1]. For magnetron sputter deposition this translates to the sputter yield and the angular distribution profile. The first determines the amount of atoms that will enter the gas phase and the second describes the direction in which the sputtered atoms are ejected from the target.

In theory, the sputter yield of a material is defined as the number of atoms that are sputtered per incoming ion. For an atomically flat surface this is a well defined quantity. However, when a real target with a specific surface morphology is used, it is recommended to distinguish between the 'elemental sputter yield' and the 'effective sputter yield' of the target. The effective sputter yield in that case is defined as the number of atoms that leave the target per incoming ion. This value can deviate from the elemental sputter yield due to the target surface morphology [2, 3, 4, 5]. The effect is twofold and is depicted in figure 1, which schematically represents a not atomically flat surface. First of all, due to the fact that a real surface is composed of hills and valleys, the ions will impinge the target surface under an angle θ rather than under normal incidence. This leads to a local increase of the elemental sputter yield [6, 7, 8]. Secondly, atoms that are being sputtered from a rough surface have a probability to get redeposited onto the target due to the geometry of the surface, which results in a lower effective sputter yield. Hence, the global change in the effective sputter yield will be determined by the dominating effect.

The angular distribution of atoms ejected from a target which is bombarded by energetic ions under normal incidence is generally a cosine-type distribution[6, 9]. The orientation of the hills and valleys will however also influence the shape of this profile as the inclined planes will promote the ejection of atoms along the local surface normal, rather than the target normal. This can result in typical heart-shaped or under-cosine profiles which have been observed experimentally[10, 11, 12].

In this work the influence of the target morphology is investigated by measuring the effective sputter yield of four different materials (Cu, Al, Ti and Ag), using both solid targets as well as cold isostatically pressed powder targets. The observed discrepancy in the sputter yield of each material, depending on the kind of target that is used, can be understood and explained by the observed differences in surface morphology. A combination of SRIM[13] simulations and an in-house developped Monte Carlo (MC) code is used in order to quantify the deviations of the effective sputter yields. The MC code furthermore allows to construct the global angular distribution of the ejected atoms, which in turn is used as input for the previously developped particle trajectory code SIMTRA[14, 15]. These latter simulations show the influence of the angular distribution on the deposition rate and the energy flux towards a substrate during sputter deposition.

2. Experimental details

All experiments were carried out in a stainless steel vacuum chamber. A turbomolecular pump, backed up by a rotary pump was used to pump down the chamber to a base pressure of 10^{-4} Pa. The solid targets were 99.99% pure Cu, Al, Ti and Ag targets from Kurt J. Lesker with a diameter of 52 mm and a thickness of 3 mm. The pressed powder targets were obtained by pressing 99% pure Cu, 99.5% pure Al, 99.99% pure Ti and 99.99% pure Ag into stainless steel rings with an inner and outer diameter of resp. 46 and 52 mm and a thickness of 2 mm. The maximum grain size of the powder atoms was 50 μ m for the Cu and Al (Goodfellow), 45 μ m for the Ag (Goodfellow) and 44 μ m for the Ti (Alfa Aesar). These pressed powder targets were then mounted onto a 1 mm thick copper plate with a diameter of 52 mm, resulting in a pressed powder target with the same dimensions as the solid targets. All targets were mounted onto an unbalanced magnetron powered by a Huttinger DC power supply and sputtered for several hours in a pure Ar atmosphere of 0.4 Pa at constant discharge voltage. These experiments were repeated for each target material for different discharge voltages. The mass of the targets before and after sputtering was determined by a microbalance with a resolution of 1 mg. From the mass difference, the effective sputter yields were determined (see section 3.1). In order to check whether material loss occurred due to evaporation or mechanical fall off of the powder, the targets were also weighed before mounting them into the chamber and again after several hours of pumping. No difference in mass was observed, which evidences that evaporation and mechanical fall off can be neglected.

The surface morphology of the targets was measured with an optical profilometer (WYKO NT3300). Before sputtering, each target was scanned over three randomly selected sample areas of 242.1 by 184.2 μ m with a resolution of 328.95 nm in both X and Y direction. The same measurements were again carried out on each target inside the racetrack after sputtering.

3. Results and discussion

The yield measurements and the target surface analysis are described in sections 3.1 and 3.2. Section 3.3 describes how the effective sputter yield can be calculated from the elemental sputter yield. It is shown that two parameters are needed in order to do this: the yield amplification factor α and the atom redeposition probability factor P_{λ} . The calculation of these factors is described in sections 3.3.1 and 3.3.2 respectively. Next, in section 3.3.3, these two factors are combined to reproduce the measured effective sputter yields. Finally, the angular distributions of sputtered atoms are calculated and used to simulate the deposition flux. These results can be found in the sections 3.4 and 3.5.

3.1. Sputter yield measurements

The effective sputter yield of all targets was determined from the mass difference Δm before and after several hours of sputtering at a constant discharge voltage. As discussed in [16, 17], the effective sputter yield Y_{eff} can be retrieved from this mass difference using the following equation:

$$Y_{eff} = \frac{\Delta m \cdot N_A}{M} \cdot \left(\frac{\sum_t I_t}{e \cdot (1 + \gamma_{isee})}\right)^{-1} \tag{1}$$

where N_A is Avogadro's constant, M the molar mass (g/mol) of the material, I_t (C/s) the discharge current at time t, e the elementary charge (C) and γ_{isee} the ion induced secondary electron emission yield[18, 19].

Figure 2 shows the measured sputter yields of different materials obtained by sputtering from the powder and solid targets as described in section 2. The difference between the effective sputter yields of the powder targets and those of the solid ones is quite remarkable. Furthermore this appears to be material dependent. While on average there is a decrease of 16% and 24% from solid to powder target for Ag and Cu

resp., there is an average increase of 48% for Al. No significant change in sputter yield observed for the Ti targets.

3.2. Target surface analysis

The data file of each optical measurement is a matrix containing the measured height of each data point. From this matrix a sub matrix of 100 by 100 μ m was selected for further analysis.

First, a mesh of the XY-plane is created using a Delaunay triangulation. Each element of the sub matrix is then assigned to the corresponding triangle vertex, resulting in a set of N_{Δ} triangles describing the sample area. Of each triangle Δ_i the normal is determined. The polar angle θ_i between the target normal and the triangle normal defines the local angle of incidence of the incoming ions.

In order to adequately describe the surface morphology a parameter is needed that, unlike the average roughness, not only takes into account the height of each measured point, but also the orientation of the surface triangles as this will determine the redeposition of atoms. In that respect, each surface can be described by calculating the fraction of triangle normals that intersect with another triangle of that surface. This fraction is zero for all solid targets and ranges up to 15% for the powder targets.

3.3. Calculating the effective sputter yield

The effective sputter yield Y_{eff} of a surface S, composed of N_{Δ} triangles Δ_i can be calculated from the elemental sputter yield Y_0 :

$$Y_{eff} = f_c(E, S) \cdot Y_0 \tag{2}$$

where $f_c(E, S)$ is defined as the correction factor for the surface S that is being bombarded by ions with an energy E. This correction factor is given by:

$$f_c(E,S) = \frac{1}{N_\Delta} \cdot \sum_{i=1}^{N_\Delta} \alpha_i(E,\theta_i) P_\lambda(\Delta_i)$$
(3)

The yield amplification factor $\alpha_i(E, \theta_i)$ describes the change in the elemental sputter yield due to an off normal angle of incidence, while $P_{\lambda}(\Delta_i)$ is defined as the probability that an atom which is ejected from Δ_i will leave the surface without being redeposited.

In order to calculate the exact value of $f_c(E, S)$ for a given surface, the yield amplification factor $\alpha_i(E)$ and the probability factors $P_{\lambda}(\Delta_i)$ must be calculated for each triangle of that surface. The first, which describes the angular dependence of the sputter yield, can be done by using SRIM[13], while for the latter a Monte Carlo code was developped to calculate atom redeposition onto the target surface. 3.3.1. Angular dependence of the sputter yield The software package SRIM[13] allows the user to calculate the sputter yield for an atomically flat surface of a given material that is being bombarded with energetic ions under a specific angle θ . These simulations were carried out for Cu, Al, Ti and Ag as target material. The angle of incidence was varied from 0 to 85 degrees with an interval of 5 degrees. Figure 3 shows the relative sputter yield amplification factor $\alpha(E)$ a a function of the angle of incidence for the different target materials.

The simulations show that the sputter yield initially increases as the angle of incidence increases. This can be explained by the fact that the collision cascade is developed closer to target surface, hence enabling more atoms to be sputtered[20]. Furthermore, the relative increase in yield is material dependent. While the yields of Al and Ti increase by a maximum factor of 4.5 and 3.42 respectively, the maximum increase for Cu and Ag is merely a factor of 1.34 and 1.17. As the actual sputter yield is determined by the dynamics and the development of the collision cascade in the target, this increase will be influenced by a number of different factors such atomic mass, energy transfer factor, surface binding energy etc.[6, 7, 20]. At higher angles of incidence ($\geq 70^{\circ}$) the relative sputter yield decreases again as more ions are getting reflected by the surface.

3.3.2. Redeposition of atoms onto the target surface The developed MC code calculates the flight path of an atom across a surface file as described in paragraph 3.2. This is done by randomly selecting a point P(x, y, z) on the surface from which the atom will be ejected. Next, the polar and azimuthal ejection angles θ and ϕ are randomly chosen from an angular distribution function given by the formula [21]:

$$\frac{\mathrm{d}^2 Y}{\mathrm{d}\Omega^2} = \frac{\|\cos\theta\|}{\pi} \left(1 - \frac{1}{4} \sqrt{\frac{E_{th}}{E}} \left(\cos\theta_i \cdot \gamma\left(\theta\right) + \frac{2}{3} \pi \sin\theta_i \cdot \sin\theta \cdot \cos\phi \right) \right)$$
(4)

Where E_{th} is the threshold energy for sputtering, E is the energy of the impinging ion, θ_i the angle of incidence and $\gamma(\theta)$ a logarithmic function of $\sin \theta$.

As the flight path of the atom is determined by the ejection point P and the ejection angles θ and ϕ , it can be calculated if the flight path intersects with the surface and hence the atom is redeposited. These calculations are repeated for N_{sim} atoms and to each atom j a value $\delta_j^{\Delta_i}$ is assigned, where the index Δ_i denotes the triangle from which it is ejected. The value of $\delta_j^{\Delta_i}$ is either 1, meaning the atom leaves the surface or 0 meaning it gets redeposited onto the surface. The probability $P_{\lambda}(S)$ that an atom ejected from a surface S will actually leave that surface can then calculated by:

$$P_{\lambda}(S) = \frac{1}{N_{sim}} \sum_{j=1}^{N_{sim}} \delta_j^{\Delta_i}$$
(5)

The amount of atoms that are redeposited is determined by the morphology of the entire surface, so it is necessarry to take into account as many triangles as possible. The minimum number of atoms that have to be simulated in order to obtain a subset If $P_{\lambda}(S)$ is the probability for an atom to leave the surface without being redeposited, then $1 - P_{\lambda}(S)$ gives the fraction of atoms that are redeposited onto the target. These values were calculated for all measured surfaces, and can be seen in figure 4, where the redeposition fraction $1 - P_{\lambda}(S)$ is plotted as a function of the fraction of intersecting normals for each specific surface. The relatively high degree of scattering around the origin is due to the fact that when no surface normals are intersecting, a small amount of redeposition can still occur due to the local orientation of the surface triangles.

While the redeposition fraction increases linearly in the region that was investigated here, it should be noted that this linear relationship will not hold over the entire interval [0,1]. Indeed, it is impossible to obtain a redeposition fraction of 1 as this will be limited by the fact that as long as the polar angle of the local triangle normal is smaller than 90°, atoms have a non-zero probability of getting sputtered in the direction along the target normal and hence won't get redeposited. This implies that as the fraction of intersecting triangle normals increases, the increase of the redeposition fraction will slow down and asymptotically reach a maximum value. Furthermore, this maximum redeposition value will be energy and material dependent as the exact shape of the angular distribution becomes more important with an increasing fraction of intersecting triangle normals.

In order to evaluate the redeposition fraction for each element and target one must average out over all measured surfaces of each separate target. These values can be found in figure 5. This shows that redeposition is limited to only 2 to 4% in the case of the solid targets, regardless of the target material, while for the powder targets this fraction increases up to 24%. Furthermore for the powder targets, redeposition of Al (15%) is significantly lower than for Cu, Ti and Ag ($\pm 23\%$). This again can be understood by taking into account the average fraction of intersecting surface normals, as this ranges from 1% to 9% in the case of Al, while for Cu, Ti and Ag the values range from 10% to 15%.

3.3.3. Combining SRIM with MC code In order to calculate the correction factor $f_c(E, S)$, the results from SRIM and the MC code must be correctly combined. According to (3) the correction factor can be obtained by calculating $P_{\lambda}(\Delta_i)$ for each triangle and then multiplying it with the corresponding amplification factor α_i .

 $P_{\lambda}(\Delta_i)$ can be calculated in the same way as $P_{\lambda}(S)$ using (5) except now all atoms must be ejected from the same triangle, so the index Δ_i has to remain fixed. Figure 6 shows some calculated values of $P_{\lambda}(\Delta_i)$ as a function of N_{sim} for several Δ_i of a pressed titanium powder target. It is clear that for each triangle Δ_i at least 5,000 atoms must be simulated before $P_{\lambda}(\Delta_i)$ converges. Taking this into account, together with the fact that at least 25,000 triangles (see paragraph 3.3.2) have to be sampled, the total number of atoms that have to be simulated for one surface is 125 million.

Alternatively, it might be more instructive to swiftly scan a larger number of triangles, rather than to accurately calculate every individual $P_{\lambda}(\Delta_i)$ for a select number of triangles. In that case the sample size will be determined by the convergence of $f_c(E, S)$ rather than the convergence of each individual term $\alpha_i(E, \theta_i)P_{\lambda}(\Delta_i)$. The expression for $f_c(E, S)$ is then:

$$f_c(E,S) = \frac{1}{N_{sim}} \sum_{k=1}^{N_{sim}} \alpha_i(E,\theta_i) \delta_k^{\Delta_i}$$
(6)

Indeed, when N_{sim} is large enough and approaches $N_{\Delta}N'$ (whith N' a constant), (6) becomes:

$$\lim_{N_{sim}\to N_{\Delta}N'} f_c(E,S) = \frac{1}{N_{\Delta}N'} \sum_{k=1}^{N_{\Delta}N'} \alpha_i(E,\theta_i) \delta_k^{\Delta_i}$$
$$= \frac{1}{N_{\Delta}N'} \sum_{i=1}^{N_{\Delta}} \sum_{j=1}^{N'} \alpha_i(E,\theta_i) \delta_j^{\Delta_i}$$
$$= \frac{1}{N_{\Delta}} \sum_{i=1}^{N_{\Delta}} \alpha_i(E,\theta_i) \frac{1}{N'} \sum_{j=1}^{N'} \delta_j^{\Delta_i}$$
$$= \frac{1}{N_{\Delta}} \sum_{i=1}^{N} \alpha_i(E,\theta_i) P_{\lambda}(\Delta_i)$$
(7)

which is the same as (3), the exact value of $f_c(E, S)$.

Figure 7 shows $f_c(E, S)$ for a sputtered Ag powder target and an unsputtered solid Ag target as a function of the number of simulated atoms. It is clear that with (6) a sample size of 100,000 atoms is sufficient to obtain a stable value, which means an average gain in calculation time of 3 orders.

For each of the investigated elements, $f_c(E, S)$ was calculated for two different energies. These energies were chosen in such a way that the corresponding sputter yields were available for both the solid as the powder targets. This in order to minimize the error due to extrapolation. Furthermore, the assumption was made that the mean ion energy is 80% of the discharge voltage[20, 22, 23]. The calculated correction factors for each material and target type can be found in table 1.

The trends of the measured sputter yields in figure 2 can now be understood by the interpretation of these correction factors. In the case of Cu and Ag, atom redeposition dominates over the yield amplification, as the correction factors are smaller than one. This effect is even more pronounced in the case of the powder targets, hence lower sputter yields are obtained from the powder targets. For Al on the other hand, which has a correction factor larger than 1, yield amplification is the dominating effect. This is again more pronounced in the case of the powder targets, leading to a much higher effective sputter yield. The sputter yield of Ti hardly changes as its correction factors are close to 1.

element	E_{ion} (eV)	f_c^{sol}	f_c^{pow}
Cu	360	0.9939	0.8469
Cu	400	0.9970	0.8580
Al	304	1.1124	1.4470
Al	336	1.1082	1.4372
Ti	240	0.9892	0.9724
Ti	320	1.0004	1.0160
Ag	320	0.9773	0.8077
Ag	400	0.9836	0.8265

Table 1. Correction factors $f_c(E, S)$ for different surfaces (solid and pressed powder) and different ion energies.

It is now possible to correlate the sputter yields of the powder targets to those of the solid targets by dividing each of them with the corresponding correction factors:

$$\frac{Y^{pow}}{f_c^{pow}} = \frac{Y^{sol}}{f_c^{sol}} \tag{8}$$

where f_c^{sol} and f_c^{pow} are the correction factors for a solid and a powder target resp. This is plotted in figure 8 where the linear fit gives a coefficient of 1.05 ± 0.06 , illustrating that the simulations are in good agreement with the experimental data.

3.4. Angular distribution of sputtered atoms

From the results of the previous sections, it can be concluded that the combination of SRIM and the developped MC code adequately describes the amount of sputtered atoms that enter the gas phase by taking into account the surface morphology. However, in order to get a good description of the deposition flux at the substrate, detailed information on the nascent angular distribution of the sputtered atoms is required.

This information can also be obtained from the output of the MC code by analysing the angles under which the atoms are emitted. As an example, figure 9 shows the angular distributions obtained for several different Cu surfaces (similar distributions were found for the other materials).

The extreme heart shape of the distributions of the not atomically flat surfaces can be understood by taking into account the inclined triangles that constitute these surfaces. Inclined triangles will promote the ejection of atoms along the local triangle normal, hence the probability for an atom to be emitted along the surface normal decreases. This is illustrated in figure 10, where the fraction of atoms that are emitted under an angle θ between -15° and 15° is plotted as a function of the mean polar angle of the triangle normals for the different surfaces. It is clear that as the triangles become more inclined, less atoms will be emitted under a small angle. Furthermore, this is a pure geometrical effect, as the decrease is the same regardless of the material. It should be noted that these local angular distributions are only valid for the measured sample areas of 100 x 100 μ m. In order to obtain the global angular distribution of the entire target, the macroscopic shape of the racetrack has to be accounted for. This is done by rotating the local angular distribution at each point of the racetrack over the angle between the tangent line at that specific point and the target normal. This is illustrated in figure 11. This figure also shows the angles below which particles are redeposited inside the racetrack, hence these are not taken into account for the calculation of the global angular distribution. Depending on the depth of the racetrack this fraction ranges from less that 1% (0.5 mm) to 15% (2.5 mm).

The probability $P(\theta)$ that an atom is ejected from the target under an angle θ is then given by:

$$P(\theta) = \int w_f(r) P_r(\theta) dr \tag{9}$$

with $P_r(\theta)$ the local probability at point r and w_f a weighing factor that takes into account that the number of particles that are sputtered from r depends on the depth of the racetrack at that specific point, i.e. the local angular distribution from a point that lies deep inside the racetrack should have a higher contribution to the global angular distribution than the one from a point which lies higher in the racetrack. These weighing factors $w_f(r)$ can be written as:

$$w_f(r) = \frac{f(r)}{2\pi \int f(r)rdr} \tag{10}$$

where f(r) denotes the depth of the racetrack at r. This was measured with an optical profilometer. In order to investigate the influence of the racetrack depth, the function f(r) was rescaled to different depths, retaining the orginal measured shape.

Figures 12 and 13 resp. show the global angular distributions for a Cu solid and powder target as a function of the racetrack depth, obtained with the method described above (similar distributions were obtained for the other materials). Two observations are made. First of all, there is still a distinct difference between the powder targets and the solid targets. Due to the specific surface morphology of the powder targets, more material is sputtered under large angles. Secondly, as the the target becomes more eroded, the heart shaped angular distribution evolves towards a cosine distribution. This is the case for both solid as powder targets, albeit more slowly for the latter. This implies that both the microscopic morphology of the target surface as well as the macroscopic shape of the racetrack have a significant influence on the nascent angular distribution of the sputtered particles.

It can be noted that in the case of rotatable magnetrons [24, 25, 26], no racetrack is formed as the target is uniformly eroded. Hence the 'age' of a rotatable target should have no influence on the angular distribution, which would then only be determined by the morphology of the target surface.

3.5. Deposition flux

To investigate the influence of the angular distribution on the the deposition rate and the energy flux towards a substrate, the software package SIMTRA[14, 15] was used. The global angular distributions obtained in the previous section were fitted and used to calculate the energy and number of atoms arriving on a substrate located 10 cm above the target surface in an argon atmosphere of 0.5 Pa.

Figures 14 and 15 show that the heart shape of the angular distributions causes a decreases in both the number of sputtered atoms that arrive at the surface as well as their average energy. This implies that the nascent energy distribution is not only altered by the interaction between the sputtered atoms and the working gas[15], but also by the morphology of the target surface. Depending on the specific shape of the angular distribution, the energy flux at substrate due to the sputtered atoms can vary with almost 20%. As discussed in [1, 27, 28, 29], the energy per arriving adatom plays a crucial role in the growth mode of the deposited film. Hence, the surface morphology and 'age' of the target can have a significant influence on the properties of the deposited films.

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4. Conclusion

In this work the relationship between the target surface morphology, the effective sputter yield and the angular distribution of sputtered atoms is investigated. The sputter yields of four different metals were experimentally determined by sputtering from solid targets as well as pressed powder targets. The differences between the sputter yields obtained for the different targets could be understood by analysing the target surface morphology. The roughness of the powder targets enhances two effects. First of all, there is an increase in the local elemental sputter yield due to a non normal angle of incidence. Secondly, this also promotes the redeposition of sputtered atoms onto the target. Depending on the dominating effect, the sputter yield obtained from a 'rough' target can be either higher or lower than the sputter yield obtained from a 'smoother' target. Using optical profilometry measurements as input for SRIM and a developped MC code, these two effects were quantified and the changes in the sputter yields could be reproduced.

The local angular distributions obtained from the MC code are extremely undercosine or heart-shaped and can be explained by the orientation of the local surface normals. To obtain the global angular distribution for a specific target, the macroscopic shape of the racetrack has to be taken into account. It is shown that the angular distribution changes drastically as the target becomes more eroded.

These results show that the target surface morphology has a significant influence on both the effective sputter yield and the nascent angular distribution. As these determine the deposition flux towards a substrate during thin film growth, the surface morphology should be taken into account especially when simulations of the sputter process are compared or employed to explain sputter experiments.

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References

- [1] S. Mahieu and D. Depla. Journal of Physics D: Applied Physics, 42(5), 2009.
- [2] M. Kustner, W. Eckstein, V. Dose, and J. Roth. Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 145(3), 1998.
- [3] M. A. Makeev and A. L. Barabasi. Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 222(3-4), 2004.
- [4] M. A. Makeev and A. L. Barabasi. Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 222(3-4), 2004.
- [5] Qiangmin Wei, Michaela Eddy, Kun-Dar Li, and Lumin Wang. Journal of Physics D-Applied Physics, 42(16), 2009.
- [6] P. Sigmund. *Physical Review*, 184(2), 1969.
- [7] W. Eckstein. Sputtering yields, volume 110 of Topics in Applied Physics. Springer-Verlag Berlin, Berlin, 2007.
- [8] Y. Yamamura. Radiation Effects and Defects in Solids, 80(3-4), 1984.
- [9] R. Behrisch. Sputtering by particle bombardment I. Physical sputtering of single-element solids. Springer-Verlag, 1981.
- [10] M. Horkel, K. Van Aeken, C. Eisenmenger-Sittner, D. Depla, S. Mahieu, and W. P. Leroy. Journal of Physics D-Applied Physics, 43(7), 2010.
- [11] R. Ramos, G. Cunge, M. Touzeau, and N. Sadeghi. Journal of Physics D-Applied Physics, 41(15), -2008—.
- [12] A. Goehlich, D. Gillmann, and H. F. Dobele. Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 179(3), 2001.
- [13] J. F. Ziegler, J. P. Biersack, and U. Littmark. 1985.
- [14] K. Van Aeken, S. Mahieu, and D. Depla. Journal of Physics D-Applied Physics, 41(20), 2008.
- [15] D. Depla and W.P. Leroy.
- [16] F. Boydens, W. Leroy, R. Persoons, and D. Depla. Physica Status Solidi a-Applications and Materials Science, 209(3), 2012.
- [17] M. Saraiva, V. Georgieva, S. Mahieu, K. Van Aeken, A. Bogaerts, and D. Depla. Journal of Applied Physics, 107(3), 2010.
- [18] D. Depla, G. Buyle, J. Haemers, and R. De Gryse. Surface & Coatings Technology, 200(14-15), 2006.
- [19] D. Depla, S. Heirwegh, S. Mahieu, J. Haemers, and R. De Gryse. Journal of Applied Physics, 101(1), 2007.
- [20] D. Depla and S. Mahieu. Reactive Sputter Deposition, volume 109 of Springer Series in Materials Science. Springer, New York, 2008.
- [21] Z. L. Zhang and L. Zhang. Radiation Effects and Defects in Solids, 159(5), 2004.
- [22] M. J. Goeckner, J. A. Goree, and T. E. Sheridan. *Ieee Transactions on Plasma Science*, 19(2), 1991.
- [23] D. Czekaj, B. Goranchev, E. K. Hollmann, V. A. Volpyas, and A. G. Zaytsev. Vacuum, 42(1-2), 1991.
- [24] W. P. Leroy, S. Konstantinidis, S. Mahieu, R. Snyders, and D. Depla. Journal of Physics D-Applied Physics, 44(11):7.

- [25] W. P. Leroy, S. Mahieu, D. Depla, and A. P. Ehiasarian. Journal of Vacuum Science & Technology A, 28(1):108–111, 2010.
- [26] R. De Gryse, J. Haemers, W. P. Leroy, and D. Depla. Thin Solid Films, 520(18):5833-5845, 2012.
- [27] H. Kersten, H. Deutsch, H. Steffen, G. M. W. Kroesen, and R. Hippler. Vacuum, 63(3):385–431, 2001.
- [28] J. A. Thornton. Journal of Vacuum Science & Technology a-Vacuum Surfaces and Films, 4(6):3059–3065, 1986.
- [29] S. Mahieu, K. Van Aeken, and D. Depla. Journal of Applied Physics, 104(11):7, 2008.

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Figure 1. Schematic representation of a rough surface and its influence on the sputter yield. An ion strikes the surface under an angle θ . The small dashed line is the local surface normal. Particles that are sputtered below the large dashed line will get redeposited onto the target surface.



Figure 2. Measured sputter yields for the different materials at several discharge voltages.



Figure 3. Relative sputter yields of different elements as a function of the angle of incidence according to SRIM.



Figure 4. The redeposition fraction 1 - $P_{\lambda}(S)$ for all surfaces as a function of the fraction of intersecting normals.



Figure 5. Average redeposition fractions for the different elements and targets.



Figure 6. $P_{\lambda}(\Delta_i)$ as a function of N_{sim} for seven randomly selected Δ_i 's.



Figure 7. Correction factors $f_c(E, S)$ as a function of the number of simulated atoms for an unsputtered solid Ag surface (top) and a sputtered Ag powder surface (bottom).



Figure 8. Corrected effective sputter yields obtained from a solid target as a function of those from a powder target (see (8)).



Figure 9. Simulated angular distributions for different Cu sample areas. The cosine distribution is added as a reference.



Figure 10. Fraction of atoms sputtered under a polar angle $-15^{\circ} < \theta < 15^{\circ}$ as a function of the mean polar angle of triangle normals.



Figure 11. Illustration of the rotated local angular distribution at certain points inside the racetrack. The dashed lines show the maximum emission angles from those points. Sputtered particles leaving the target below these lines are redeposited inside the racetrack.



Figure 12. Global angular distribution of a Cu powder target for different racetrack depths.



Figure 13. Global angular distribution of a Cu powder target for different racetrack depths.



Figure 14. Relative number of arriving atoms and energy as a function of the fraction of atoms sputtered under a polar angle $-15^{\circ} < \theta < 15^{\circ}$ for different Cu angular distributions.



Figure 15. Relative energy per arriving atom (left) and relative number of arriving atoms (right) as a function of the fraction of atoms sputtered under a polar angle $-15^{\circ} < \theta < 15^{\circ}$ for different angular distributions of all elements.