Ion beam sputtering of Ti: Influence of process parameters on angular and energy distribution of sputtered and backscattered particles

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Abstract

In the present study, the influence of ion energy and geometrical parameters onto the angular and energy distribution of secondary particles for sputtering a Ti target with Ar ions is investigated. The angular distribution of the particle flux of the sputtered Ti atoms was determined by the collection method, i.e. by growing Ti films and measuring their thickness. The formal description of the particle flux can be realized by dividing it into an isotropic and an anisotropic part. The experimental data show that increasing the ion energy or decreasing the ion incidence angle lead to an increase of the isotropic part, which is in good agreement with basic sputtering theory. The energy distribution of the secondary ions was measured using an energy-selective mass spectrometer. The energy distribution of the sputtered target ions shows a maximum at an energy between 10 eV and 20 eV followed by a decay proportional to E^{-n} , which is in principle in accordance with Thompson's theory, followed by a high energetic tail. When the sum of incidence angle and emission angle is increased, the high-energetic tail expands to higher energies and an additional peak due to direct sputtering events may occur. In the case of backscattered primary Ar ions, a maximum at an energy between 5 eV and 10 eV appears and, depending on the scattering geometry, an additional broad peak at a higher energy due to direct scattering events is observed. The center energy of the additional structure shifts systematically to higher energies with decreasing scattering angle or increasing ion energy. The experimental results are compared to calculations based on simple elastic two-particle-interaction theory and to simulations done with the Monte Carlo code SDTrimSP. Both confirm in principle the experimental findings.

Keywords: Ion beam sputtering; Titanium; Angular distribution; Energy distribution

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26 **1. Introduction**

27 The basic principle of the physical vapor deposition (PVD) technique is to deposit material onto a
28 substrate by condensation of atoms or clusters that have been vaporized or sputtered from the solid or
29 liquid phase. When the target material is sputtered by the bombardment with energetic ions, ion beam
30 parameters (ion energy or ion species) and the incidence angle have a strong influence on angular and
31 energy distribution of sputtered target particles and backscattered primary particles and, therefore, on
32 the thin film properties. In the case of the ion beam sputter deposition (IBSD) technique, the ion
33 source and the target are spatially separated, allowing the manipulation of the sputtering parameters
34 over a wide range. Thus, the IBSD is a versatile tool for tailoring thin film properties.

35 A widely recognized theory for the description of the sputtering process is the linear cascade theory
36 [1]. The fundamental assumption of this theory is that the impinging ions cause a linear cascade of
37 binary collisions leading to an isotropic distribution of recoil atoms. From this theory, Thompson
38 derived his widely-used formula for the angular and energy distribution of the sputtered atoms for an
39 amorphous target [1]. Goehlich et al. performed a series of investigations [2, 3, 4, 5, 6] of the influence
40 of ion energy and geometrical parameters on the energy distribution of the sputtered particles,
41 exemplary, for sputtering of Al, Ti or W by Ar or Xe ion bombardment. Their investigations showed
42 that Thompson's formula is in good agreement with the experimental findings in case of ions at
43 normal incidence and for ion energies in the range of several keV. But the energy distribution showed
44 deviations from Thompson's formula in the case of oblique incidence and sub keV energies due to
45 anisotropy effects, i.e. direct sputtering or scattering events [2]. Stepanova et al. derived a criterion for
46 a minimum ion energy, which is needed in order to fulfill the isotropy approximation, i.e. Thompson's
47 formula [7]. The minimum energy depends on the mass ratio between the impinging ions and the
48 target atoms, the surface binding energy, and the mean energy of the sputtered target atoms.

49 Supposing a typical value of the surface binding energy of 5 eV and the mean energy of the sputtered
50 target atoms to be 15 eV, the minimum energy for the bombardment of a Ti-target by Ar ions is about
51 1.7 keV. Therefore, ion energies below 1.7 keV should lead to significant deviations from the isotropic

distribution of recoil atoms. These deviations from the ideal case of the linear cascade regime are in good agreement with our findings regarding the sputtering of Ti.

The investigations by Goehlich et al. are restricted to the properties of the sputtered target particles but neglect the properties of the backscattered primary particles. However, the backscattered primary particles have a strong influence on the properties of thin films grown by ion beam sputter deposition [8, 9, 10]. There are some works that are focusing on the measurement of the energy distribution of the secondary Ar and Ti particles for sputtering of Ti with Ar ions, but they are limited in the choice of the incidence and emission angle [11, 12, 13].

Recently, we have reported about the systematic investigation of secondary particle and thin film properties of the ion beam sputter deposition process of Si [14], Ge [8, 15] and Ag [9, 10, 14, 16]. Here we present experimental angular and energy distribution of sputtered and backscattered particles in the ion beam sputter process of Ti bombarded with Ar ions. The experimental data are compared and discussed with calculation results based on simple elastic two-particle-interaction theory and with simulation results done with the Monte Carlo code SDTrimSP [17].

2. Experimental

A schematic geometry sketch of the experimental setup inside the vacuum chamber is shown in Fig. 1. The setup consists of a broad-beam ion source, a target holder and an energy-selective mass spectrometer (ESMS).

The in house developed broad-beam ion source is of RF-type with a three grid multiaperture extraction system [18]. Ar was used as sputter gas with a gas flow rate of 3.5 sccm. The RF-power was set to 70 W, which resulted in a total ion beam current of about 10 mA. The current density of the ion beam at the target position was measured with a faraday cup and can be described by a symmetric two-dimensional Gaussian. The maximum current density and the corresponding full width at half maximum (FWHM) were $1.8 \mu\text{A}/\text{mm}^2$ and 5 mm, $6.3 \mu\text{A}/\text{mm}^2$ and 26 mm, and $4.8 \mu\text{A}/\text{mm}^2$ and 36 mm for set ion energies of 0.5 keV, 1.0 keV, and 1.5 keV, respectively.

The target was polycrystalline Ti (diameter 10 cm, thickness 3 mm, purity 99.99%).

The energy-selective mass spectrometer (ESMS) Balzers Quadstar PPM 422 was used to measure the energy distribution of sputtered or backscattered ions. The ESMS operates in the mass range from 1 amu up to 512 amu and in the energy range from 0 eV up to 500 eV with a resolution of 1 amu and 0.5 eV, respectively. The ESMS was mounted on a CF-flange at the chamber wall and protrudes 200 mm inside the chamber. The acceptance angle of the used ESMS setup decreases with increasing ion energy [19]. The influence of the energy dependent acceptance angle is not corrected for but is assumed to be small, because the agreement between the overall shape of the measured and simulated energy distributions is very good.

Ion source and target are mounted on rotary tables on identical rotation axes such that different combinations of ion incidence angle α and polar emission angle β can be realized. Caused by the dimension of the ion source and the ESMS, the minimal detectable emission angle was 60°, 30° or 0° for primary ion incidence angles of 0°, 30° or 60° respectively. The energy distribution of sputtered (Ti) and backscattered (Ar) ions was measured at emission angles in steps of 10° for primary ion energies of 0.5 keV, 1.0 keV and 1.5 keV, and incidence angles of 0°, 30° and 60°.

Additionally, a semicircular substrate holder was placed inside the chamber [8, 9] in order to collect the sputtered Ti for the determination of the angular distribution and the flux of the sputtered particles. The distance from target to ion source and target to substrate holder was 15 cm while the distance from target to ESMS was 25 cm.

Therefore, Ti films were deposited on polished p-type <100> Si substrates (size 12 x 12 mm²) using the same process parameters as for the ESMS measurements. The films were characterized concerning their film thickness using profilometry. The measured thickness was divided by the deposition time to determine the angular distribution of the sputtered titanium particle flux. Since the total flux of Ar ions that impinges on the Ti target depends on the set ion energy and incidence angle, each angular distribution of the sputtered titanium particle flux is divided by the total flux of impinging Ar ions in order to achieve a higher degree of comparability. Nevertheless the term particle flux is used in the following although actually the particles flux per incident Ar ion is presented.

The base pressure of the vacuum chamber was $2 \cdot 10^{-6}$ mbar and the working pressure was $4 \cdot 10^{-5}$ mbar.

Ti is known to be highly reactive, especially, with oxygen. Even though the presence of oxygen cannot

be excluded completely, we saw that its influence is very small. An (partial) oxidation of the target would result in a creation of sputtered oxygen particles or molecules containing Ti and O. However, we could only detect an extremely small signal in the ESMS measurements (six orders of magnitude smaller than that of Ti ions) related to oxygen ions or ionized molecules. An oxidation of the growing films would lead to a change of the mass and atomic density of the deposited Ti layers and therefore affect the determined angular distribution of the sputtered particles. At the given working pressure these effects are small as we could show for selected samples by Rutherford backscattering spectrometry measurements. The oxygen content is less than 5%.

3. Simulations and calculations

In addition to the measurements, energy distributions were simulated using the Monte Carlo simulation code SDTrimSP version 5.00 [17] which is widely used for simulations of sputtering phenomena in amorphous or polycrystalline materials. SDTRIM.SP is based on the binary collision approximation, i.e. it assumes that collisions between atoms can be approximated by elastic binary collision described by an interaction potential. Additionally, it is assumed that the energy loss to electrons can be handled separately as an inelastic energy loss. The code determines the path of the primary particle and of the recoils inside the target by using the asymptotes of the calculated real trajectories. It is assumed that the target is amorphous and the distance between two collisions is handled by a mean free path length.

For each presented simulation the number of primary ions was set to 10^8 . The Kr-C potential was used, as it describes ion-solid interactions sufficiently well over a wide energy range [20]. The surface binding energies of the Ti and Ar atoms were set to 4.84 eV and 0 eV, respectively. The inelastic energy loss model was an equipartition of the Lindhard-Scharff [21] and the Oen-Robinson-model [22]. The simulation target was assumed to consist of 90 at.% Ti particles and 10 at.% Ar particles. The composite $\text{Ti}_{0.9}\text{Ar}_{0.1}$ target considers primary Ar particles that are implanted into the target. This assumption is justified by experimental findings that revealed contributions by direct Ar-Ar backscattering [10, 14, 15, 16]. All other simulation parameters were taken from the database of SDTrimSP or from the list of experimental parameters.

The most common approach for the description of the sputtering process in the considered energy range up to some keV is the deposition of momentum and energy through linear cascades. However, target atoms can also be sputtered by a single collision with an incident ion. Such direct sputtering events can be identified in experimental as well as in simulated energy distributions [10, 14, 15, 16]. Similarly, direct scattering events can occur.

A simplified way of describing the direct interaction between two particles is to make use of the conservation of energy and momentum in an elastic collision. Assuming an incoming primary particle 1 with energy E_{10} ($=E_{ion}$) impinging on a target particle 2 at rest (i.e. $E_{20} = 0$ eV), the energy of particle 1 (E_{11}) and particle 2 (E_{21}) after the collision can be calculated by:

$$E_{11} = E_{10} \left(\frac{m_1 \cos(\gamma) \pm \sqrt{m_2^2 - m_1^2 \sin^2(\gamma)}}{m_1 + m_2} \right)^2 \quad (1)$$

$$E_{21} = \frac{4m_1m_2}{(m_1 + m_2)^2} E_{10} \cos^2(\gamma) \quad (2)$$

Here γ ($\gamma = 180^\circ - \alpha - \beta$) denotes the scattering angle. m_1 and m_2 are the mass of particle 1 and particle 2, respectively. For $m_1 < m_2$ only the plus sign in Eq. (1) is valid [23].

In Tab. 1 calculated energies according to Eq. (1) and Eq. (2) for direct sputtering/scattering events between an incoming Ar ion ($m_1 = 39.95$ amu) and a Ti target atom ($m_2 = 47.87$ amu) (Ar-Ti) or an implanted Ar particle (Ar-Ar) are given. When considering the interaction between a primary Ar ion and an implanted Ar particle, Eq. (1) and Eq. (2) become identical ($m_1 = m_2$). This means that in the case of an Ar-Ar collision it cannot be distinguished between backscattered Ar particle 1 and sputtered Ar particle 2 in the experimental energy distribution, as they appear at the same energetic position for a given scattering angle γ . On the contrary, in the case of the simulated energy distribution, it is possible to follow the trajectories of all particles and therefore it can be differentiated between the backscattered and the sputtered Ar particles.

4. Results and discussion

4.1. Angular distribution of sputtered Ti particles

In Fig. 2 the experimental particle flux distribution of sputtered Ti particles is shown for several combinations of ion energy E_{ion} and ion incidence angle α . The data set for an ion energy of 1.0 keV

and incidence angle of 30° serves here as reference, i.e the particle flux for each parameter set is normalized to the maximum particle flux of this referential set. The corresponding maximum deposition rate lies at 0.63 nm/min at an emission angle of 40° .

For all parameter sets, the Ti particle flux increases with increasing ion incidence angle and increasing ion energy, because the total sputter yield increases. The shape of all particle flux distributions can be described by the superposition of two cosine functions, dividing the particle flux into an isotropic ($\Phi_{iso}(\beta)$) and an anisotropic part ($\Phi_{aniso}(\beta)$). The data were fitted by

$$\Phi(\beta) = \Phi_{iso}(\beta) + \Phi_{aniso}(\beta) = \Phi_{iso,0} \cdot \cos(\beta) + \Phi_{aniso,0} \cdot \cos^m(\beta - \beta^*) \quad (3)$$

Here $\Phi_{iso,0}$ and $\Phi_{aniso,0}$ are the maximum values of the isotropic and anisotropic components, β^* is the emission angle related to the tilt of the anisotropic component, and m is the exponent of the cosine of the anisotropic part describing the degree of anisotropy. The isotropic part represents the part of the particle flux that is emitted in accordance with Thompson's formula. Tab. 2 summarizes the best-fit parameters for the experimental angular particle flux distributions.

The data were also fitted by using the anisotropic part from Eq. 3 only. Tab. 3 summarizes the corresponding best-fit parameters. Fitting with Eq. (3) leads to a reduced mean square error (MSE) of about $1 \cdot 10^{-3}$ while fitting with the anisotropic part of Eq. (3) only leads to a reduced MSE of about 1. Consequently, the superposition of an isotropic and an anisotropic part describes the measured particle flux in more appropriate manner than an anisotropic distribution alone. One major drawback of the used fitting formula described in Eq. (3) is the relatively high number of fitting parameters. This leads to a high standard error for example for the factor m of about 1.

Fig. 2 and Tab. 2 show that increasing the ion energy or decreasing the ion incidence angle leads to a preference of the isotropic part. This behavior can be explained by a better developed linear collision cascade, because higher ion energy or smaller ion incidence angle lead to a deposition of the ion energy deeper into the target. Therefore, the average number of collisions of primary particles and recoils is increased. As a consequence, the recoils have a higher probability to perform enough collisions along their way to the surface so that their collision cascades become fully developed, which results in an isotropic distribution of the sputtered target particles. This should hold, especially, for normally incident ions.

Similarly shaped particle flux distributions were also reported in [24, 25]. Roosendaal et al. [26] investigated the influence of the sputtering parameters onto the angular and energy distribution of sputtered particles analytically. They conclude that anisotropy effects are enforced by lower energies of the impinging particles, larger incidence angles, and higher mass ratios of the projectile particles to the target particles.

However, we would like to point out that other effects, for instance, surface roughness of the target, may also lead to anisotropic contributions to the flux distribution of sputtered particles [27].

4.2. Energy distribution of sputtered Ti particles

Fig. 3 depicts measured energy distributions of sputtered Ti ions. Every measured energy distribution shows a maximum at an energy between 10 eV and 20 eV. Above that, in the range of up to about 50 eV, the shape of the curves follows an E^{-n} decay that is in agreement with Thompson's theory. This holds especially for scattering angles $\gamma > 90^\circ$, i.e. $\alpha + \beta < 90^\circ$. Above an energy of 50 eV, the E^{-n} decay is followed by a high energetic tail. The slope of the high energetic tail becomes less steep with increasing emission angle. This high energetic tail is tentatively assigned to deviations from the ideal case of isotropic recoil cascades. Goehlich et al. [2] observed a similar effect during the sputtering of Ti with Ar ions at ion energies of 300 eV and 500 eV with increasing emission angle, which they described as a broadening of the energy distribution. They assigned this effect to anisotropies in the particle flux caused by the conservation of momentum of the impinging particles along the collision cascade.

The measured energy distributions in Fig. 3 (b, d, f) show that the shape of the energy distribution mainly depends on the choice of the scattering angle γ ($\gamma = 180^\circ - (\alpha + \beta)$), almost independent from the choice of specific values of α and β .

For an incidence angle of $\alpha = 60^\circ$, and emission angles of $\beta = 60^\circ$ and $\beta = 70^\circ$, the measured energy distribution shows an additional feature that can be assigned to direct sputtering events, because the energetic position of this additional feature is in good agreement with the energy calculated by Eq. (2) given in Tab. 1.

The simulated energy distributions in Fig. 4 reproduce the experimental findings well, i.e. the characteristic features related to the direct sputtering event and the decreasing inclination of the energetic tail with increasing emission angle. In contrast to the experimental data, the simulated distribution already shows contributions by direct sputtering for an incidence angle of $\alpha = 60^\circ$ and an emission angle $\beta = 50^\circ$. In the experiment this feature seems to be hidden by noise.

In Refs. 15 and 16 we presented the energy distribution of sputtered Ge and Ag particles under the bombardment of Ar and Xe ions. In the case of sputtered Ag particles under Ar ion bombardment [16] the same characteristic decreasing inclination of the high energy tail with increasing emission angle was observed. The same holds for the bombardment of Ge [15] although the energy distribution of the sputtered Ge ions is less influenced by the choice of the scattering angle.

An obvious difference between the energy distributions in [15] and [16] in comparison to the energy distributions of the sputtered Ti ions in Fig. 3 is the fact that the high energetic tail is more pronounced in case of the sputtered Ti atoms. A possible explanation for this observation is that the ratio between the mass of the impinging Ar ions ($m_1 = 39.95$ amu) and the Ti target atoms ($m_2 = 47.87$ amu) favors a higher maximum transferrable energy (see Eq. (2) with $\gamma = 0^\circ$) of about 99% of the initial energy of the Ar ions than in the case of Ge ($m_2 = 72.61$ amu) with 92 % and Ag target atoms ($m_2 = 107.61$ amu) with 79%.

4.3. Energy distribution of scattered Ar particles

Fig. 5 depicts the measured energy distribution of backscattered Ar ions. The experimental data show a maximum at an energy below 10 eV followed by a sudden signal drop and an additional broad structure at higher energies. The additional structure is assigned to direct Ar-Ar scattering because its energetic position is in good agreement with the calculated energy according to Eq. (1) But this additional structure seems to be broadened towards higher energies. According to Tab. 1 the energy of a primary Ar ion, that is backscattered under a given scattering angle γ by a Ti particle, is always higher than the energy of an Ar ion, that is backscattered by an Ar particle. The reason for this lies in the higher atomic mass of Ti in comparison to that of Ar. Therefore, it is very likely that the additional

structure is a superposition of contributions by Ar-Ar and Ar-Ti scattering that is dominated by the former.

Fig. 6 shows simulated energy distributions of Ar particles that are sputtered from a $\text{Ti}_{0.9}\text{Ar}_{0.1}$ -Target. The simulated energy distributions clearly show the contribution by direct sputtering of Ar particles. The energetic position of this feature is in good agreement with the experimental findings in Fig. 5 and calculation results according to Eq. (2) (see Tab. 1).

The simulated energy distributions of the backscattered Ar particles in Fig. 7 show an additional feature that can be related to Ar ions that are backscattered from a Ti particle by a single collision (direct scattering). The energetic position of the additional feature is again in good agreement with calculation results according to Eq. (1) (see Tab. 1). It should be noted that the additional feature, which is related to direct Ar-Ar scattering, cannot be seen in Fig. 7 as it seems to be superimposed by the feature of the direct Ar-Ti scattering.

The simulated data (Figs. 6 and 7) lead to the conclusion that the dominating single collision event is the Ar-Ti scattering process. The experimental data seem to contradict this conclusion as they depict the Ar-Ar backscattering to be dominating. This is a strong evidence that a considerable amount of primary Ar ions is implanted into the Ti-Target and that these implanted primary particles take a severe influence on the direct scattering and sputtering process.

In Refs. 15 and 16 we presented measured energy distributions of Ar ions backscattered from a Ge and a Ag target. In both cases, we observed very similar structures related to direct Ar-Ar scattering but the energy distributions also showed distinct structures that can be related to direct Ar-Ag and Ar-Ge scattering. The lacking of these distinct structures for Ar bombardment of Ti (see Figs. 5) is caused by the fact that the mass ratio between Ar and Ti is closer to unity than for Ar and Ag, or Ar and Ge. This leads to an overlap of the structures caused by the direct Ar-Ar and Ar-Ti scattering as their energetic positions converge.

5. Conclusion

We investigated the influence of geometrical parameters and ion energy onto the angular and energy distribution of secondary particles during the ion beam sputtering of Ti by Ar ions. The angular distribution of the sputtered Ti particles can be described by the superposition of an isotropic and an anisotropic part. The isotropic part increases with increasing ion energy and, in case of oblique incidence, with decreasing incidence angle. This dependency is explained by the depth distribution of the deposited energy of the bombarding Ar ions.

For scattering angles $\gamma > 90^\circ$ ($(\alpha + \beta) < 90^\circ$) the measured and simulated energy distribution of the sputtered particles is in good agreement with the Thompson formula. With decreasing scattering angle, the energy distribution shows a pronounced high energetic tail that is shifted towards higher energies. This broadening of the energy distribution is assigned to anisotropy effects.

Especially in the case of the backscattered Ar ions, contributions from direct sputtering and scattering events can be identified for scattering angles $\gamma < 70^\circ$. The position of these peaks is in good agreement with calculations based on simple elastic collision theory.

By comparing the measured and simulated energy distribution, we conclude that during the sputtering process a significant part of the impinging Ar ions is implanted into the Ti-Target. These implanted Ar atoms seem to dominate the direct backscattering of primary Ar ions.

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7. References

- [1] M. W. Thompson, Philos. Mag. **18** (1968) 377.
- [2] A. Goehlich, N. Niemöller, and H. F. Döbele, Phys. Rev. B **62** (2000) 9349.
- [3] A. Goehlich, N. Niemöller, H. F. Döbele, J. Nucl. Mater. **241-243** (1997) 1160.

- [4] A. Goehlich, D. Gillmann, H.F. Döbele, Nucl. Instrum. Methods. Phys. Res., Sect B **164-165** (2000) 834.
- [5] A. Goehlich, N. Niemöller, H. F. Döbele, J. Nucl. Mater. **266-269** (1999) 501.
- [6] A. Goehlich, D. Gillmann, H.F. Döbele, Nucl. Instrum. Methods. Phys. Res., Sect B **179** (2001) 351.
- [7] M. Stepanova, S.K. Dew, Nucl. Instrum. Methods. Phys. Res., Sect B **215** (2004) 357.
- [8] C. Bundesmann, R. Feder, R. Wunderlich, U. Teschner, M. Grundmann, and H. Neumann, Thin Solid Films **589** (2015) 487.
- [9] C. Bundesmann, R. Feder, J.W. Gerlach, and H. Neumann, Thin Solid Films **551** (2014) 46.
- [10] C. Bundesmann, R. Feder, T. Lautenschläger, and H. Neumann, Contrib. Plasma Phys. **55** (2015) 737.
- [11] E. Kusano, T. Kobayashi, N. Kashiwagi, T. Saitoh, S. Saiki, H. Nanto, A. Kinbara, Vacuum **53** (1999) 21.
- [12] J. Bohlmark, M. Lattemann, J.T. Gundmundsson, A.P. Ehasarian, Y. Aranda Gonzalvo, N. Brenning, U. Helmersson, Thin Solid Films **515** (2006) 1522.
- [13] E. Franke, H. Neumann, M. Zeuner, W. Frank, F. Bigl, Surf. Coat. Technol. **97** (1997) 90.
- [14] R. Feder, F. Frost, H. Neumann, C. Bundesmann, and B. Rauschenbach, Nucl. Instrum. Methods Phys. Res., Sect. B **317A** (2013) 137.
- [15] R. Feder, C. Bundesmann, H. Neumann, and B. Rauschenbach, Nucl. Instrum. Methods Phys. Res., Sect. B **334** (2014) 88.
- [16] R. Feder, C. Bundesmann, H. Neumann, and B. Rauschenbach, Nucl. Instrum. Methods Phys. Res., Sect. B **316** (2013) 198.
- [17] A. Mutzke, R. Schneider, W. Eckstein, and R. Dohmen, SDTrimSP: Version 5.00, IPP Report 12/8 (2011).
- [18] M. Zeuner, F. Scholze, B. Dathe, and H. Neumann, Surf. Coat. Technol. **39** (2001) 142.
ghfg
- [19] E.A.G. Hamers, W.G.J.H.M. van Sark, J. Bezemer, W.J. Goedheer, W.F. van der Weg, Int. J. Mass Spectrom. Ion Processes **173** (1998) 91

- [20] W.D. Wilson, L.G. Haggmark, J.P. Biersack, Phys. Rev. B **15** (1977) 2458.
- [21] J. Lindhard, M. Scharff, Phys. Rev. **124** (1961) 128.
- [22] O.S. Oen, M.T. Robinson, Nucl. Instr. Meth. **132** (1976) 647.
- [23] L.J. Brillson, Surfaces and Interfaces of Electronic Materials (Wiley-VCH, Weinheim, 2010).
- [24] H. Oechsner, Appl. Phys. 8 (1975) 185.
- [25] G.K. Wehner, D. Rosenberg, J. Appl. Phys. 31 (1960) 177
- [26] H.E. Roosendaal, J.B. Sanders, Radiat Eff. Defects Solids 52 (1980) 137
- [27] F. Boydens, W.P. Leroy, R. Persoons, D. Depla, Thin Solid Films **531** (2013) 32.

Table 1: Calculated energies according to Eq. (1) and Eq. (2) for the interaction between Ar and Ti particles (Ar - Ti), or between Ar and Ar particles (Ar - Ar). For the sake of convenience, we only present calculated data for the geometrical parameter sets where direct sputtering/scattering events can be identified in the experimental or simulated energy distribution.

E_{i0} [keV]	α [°]	β [°]	Ar - Ti		Ar - Ar
			E_{1l} [eV]	E_{2l} [eV]	$E_{1l} = E_{2l}$ [eV]
0.5	30	50	27	-	-
		60	45	0	0
		70	76	15	15
		80	122	58	58
1.0	30	50	54	-	-
		60	90	0	0
		70	152	30	30
		80	244	116	117
1.5	30	50	81	-	-
		60	135	0	0
		70	228	45	45
		80	366	174	175
1.0	0	60	22	-	-
		70	33	-	-
		80	54	-	-
1.0	60	40	152	30	30
		50	244	116	117
		60	265	248	250
		70	506	410	413

Table 2: Best-fit parameters according to Eq. (3) for the experimental particle flux distributions in Fig. 2.

E_{ion} [keV]	α [°]	$\Phi_{iso,0}$ [arb. u.]	$\Phi_{aniso,0}$ [arb. u.]	$\Phi_{iso,0}/\Phi_{aniso,0}$	m	β^* [°]
0.5	30	0.18	0.44	0.4	5.0	49
1.0	30	0.67	0.54	1.2	3.8	51
1.5	30	0.99	0.48	2.1	5.3	53
1.0	0	0.47	0.21	2.2	5.6	54
1.0	60	0.83	0.68	1.2	5,9	41

Table 3: Best-fit parameters when applying the anisotropic part from Eq. (3) only for the experimental particle flux distributions in Fig. 2.

E_{ion} [keV]	α [°]	$\Phi_{aniso,0}$ [arb. u.]	m	β^* [°]
0.5	30	0.52	2.9	39
1.0	30	1.0	1.8	30
1.5	30	1.2	1.7	24
1.0	0	0.55	3.1	36
1.0	60	1.3	1.7	15

Figure 1

Figure 1: Sketch of the experimental setup.

Figure 2

Figure 2: Experimental (symbols) und fitted (lines) Ti particle flux distributions for the Ar ion bombardment of a polycrystalline Ti-Target. Panels (a,c,e) illustrate the influence of the ion energy ($E_{ion} = 0.5 \text{ keV}, 1.0 \text{ keV}, 1.5 \text{ keV}$) at a fixed ion incidence angle ($\alpha = 30^\circ$), panels (b,d,f) illustrate the influence if the ion incidence angle ($\alpha = 0^\circ, 30^\circ, 60^\circ$) at a fixed ion energy ($E_{ion} = 1.0 \text{ keV}$). The experimental data are normalized to the maximum of the particle flux at an ion energy of 1.0 keV and an incidence angle of 30° . The red line refers to the fitting function $\Phi(\beta)$ in Eq. 3 with the parameters in Table 2. The blue lines show the isotropic ($\Phi_{iso}(\beta)$) and the anisotropic part ($\Phi_{aniso}(\beta)$) of this fitting function. The green line refers to the fitting function $\Phi_{aniso}(\beta)$ in Eq. 3 without the use of the isotropic part with the parameters in Table 3.

Figure 3

Figure 3: Measured energy distributions of Ti ions sputtered from a polycrystalline Ti-target for selected emission angles β . Panels (a,c,e) illustrate the influence of the ion energy ($E_{ion} = 0.5 \text{ keV}, 1.0 \text{ keV}, 1.5 \text{ keV}$) at a fixed ion incidence angle ($\alpha = 30^\circ$), panels (b,d,f) illustrate the influence if the ion incidence angle ($\alpha = 0^\circ, 30^\circ, 60^\circ$) at a fixed ion energy ($E_{ion} = 1.0 \text{ keV}$). The arrows mark the energetic position of the additional feature that is caused by direct sputtering events.

Figure 4

Figure 4: Simulated energy distributions of Ti particles sputtered from a $\text{Ti}_{0.9}\text{Ar}_{0.1}$ target for selected emission angles β . Panels (a,c,e) illustrate the influence of the ion energy ($E_{ion} = 0.5 \text{ keV}$, 1.0 keV , 1.5 keV) at a fixed ion incidence angle ($\alpha = 30^\circ$), panels (b,d,f) illustrate the influence if the ion incidence angle ($\alpha = 0^\circ$, 30° , 60°) at a fixed ion energy ($E_{ion} = 1.0 \text{ keV}$). The arrows mark the energetic position of the additional feature that is caused by direct sputtering events.

Figure 5

Figure 5: Measured energy distributions of Ar ions backscattered from a polycrystalline Ti-target for selected emission angles β . Panels (a,c,e) illustrate the influence of the ion energy ($E_{ion} = 0.5 \text{ keV}$, 1.0 keV , 1.5 keV) at a fixed ion incidence angle ($\alpha = 30^\circ$), panels (b,d,f) illustrate the influence if the ion incidence angle ($\alpha = 0^\circ$, 30° , 60°) at a fixed ion energy ($E_{ion} = 1.0 \text{ keV}$). The arrows mark the energetic position of the additional feature that is caused by direct scattering events.

Figure 6

Figure 6: Simulated energy distributions of Ar particles sputtered from a $\text{Ti}_{0.9}\text{Ar}_{0.1}$ -target for selected emission angles β . Panels (a,c,e) illustrate the influence of the ion energy ($E_{ion} = 0.5 \text{ keV}$, 1.0 keV , 1.5 keV) at a fixed ion incidence angle ($\alpha = 30^\circ$), panels (b,d,f) illustrate the influence if the ion incidence angle ($\alpha = 0^\circ$, 30° , 60°) at a fixed ion energy ($E_{ion} = 1.0 \text{ keV}$). The arrows mark the energetic position of the additional feature that is caused by direct sputtering events.

Figure 7

Figure 7: Simulated energy distributions of Ar particles backscattered from a $\text{Ti}_{0.9}\text{Ar}_{0.1}$ -target for selected emission angles β . Panels (a,c,e) illustrate the influence of the ion energy ($E_{ion} = 0.5 \text{ keV}$, 1.0 keV , 1.5 keV) at a fixed ion incidence angle ($\alpha = 30^\circ$), panels (b,d,f) illustrate the influence if the ion incidence angle ($\alpha = 0^\circ$, 30° , 60°) at a fixed ion energy ($E_{ion} = 1.0 \text{ keV}$). The arrows mark the energetic position of the additional feature that is caused by direct scattering events.

Figure 1

Figure 2

Figure 3

(a)

Figure 4

Figure 5

Figure 6

Figure 7