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Fluence dependent changes of surface morphology and sputtering yield of iron: Comparison of experiments with SDTrimSP-2D

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ABSTRACT

The influence of surface morphology modifications on the sputtering yield of thin Fe films by monoenergetic Ar ions is studied by using a highly sensitive quartz crystal microbalance (QCM) technique. The morphology changes are induced by prolonged sputtering up to a total Ar fluence of $8 \times 10^{21}\ m^{-2}$. Atomic force microscopy (AFM) measurements are performed to analyse the sample topography before and after irradiation and to determine surface roughness parameters. Numerical modelling with the codes SDTrimSP and SDTrimSP-2D are performed for comparison. Our investigations show that by using the local distribution of projectile impact angles, as derived from AFM measurements, as well as the elemental composition of the samples as an input to the codes SDTrimSP and SDTrimSP-2D the agreement between experiment and simulations is substantially improved.

1. Introduction

Ion induced sputtering is one of the most important topics of ion-surface interaction and has a wide variety of practical applications, like surface cleaning, etching, thin-layer deposition or surface analytic techniques. Sputtering also plays a major role in erosion of wall material in nuclear fusion devices [1] or in space weathering by solar wind ion impact observed on lunar or planetary surfaces [2,3]. Plasma facing components (PFC) in a fusion device are constantly eroded by ion and neutral particle bombardment, which limits their lifetime. For a future fusion power plant tungsten is foreseen as material for PFCs and tungsten containing steels, like EUROFER are considered as possible alternatives for recessed area PFCs in the reactor vessel [4]. Experiments with Fe-W films (with 1.5 at% W), which is assumed to be a model system for EUROFER (nominally 0.33 at% W), showed a significant reduction of the erosion rate during low energy ion bombardment [5]. The reduced erosion rate was explained by preferential sputtering of Fe, causing a W surface enrichment. However modifications of the surface structure due to erosion were measured in addition [6], which also influence the sputtering behaviour. In order to separate the effect of surface enrichment of high Z materials from the effect of surface structural modifications, we set out to conduct sputtering experiments with pure Fe sample films and investigated the effect of surface morphology changes on the sputtering yield due to prolonged ion erosion.

Theoretical descriptions (e.g. [7]) and simulations (e.g. [8]) of sputtering often only consider perfectly flat surfaces. However, this is an idealization, and while it is possible to create reasonably flat films for some materials, this assumption will often lead to discrepancies with the actual experimental conditions. Fig. 1 shows a sketch of how the roughness of a surface may affect the sputtering process. It shows a projectile ion hitting the surface under a nominal angle of 0 degrees, which would mean normal incidence for a perfectly flat surface. However, due to the rough surface condition the local angle of incidence θ is different, with its value being strongly dependent on the exact point of incidence. Beside surface sputtering also projectile reflection may occur. Sputtered target atoms are assumed to follow a cosine distribution with its maximum in the direction of the local surface normal. Experiments have shown, that the sputtering yield as a function of local impact angle Y (θ) follows more a $\cos^y(\theta)$ distribution,

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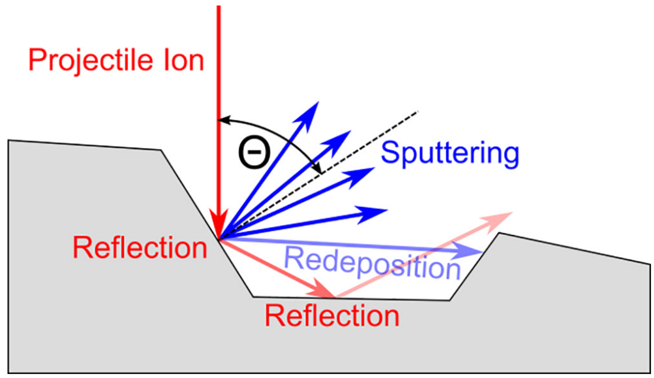

Fig. 1. Sputtering of a rough surface. A projectile ion, which is represented by the red arrow, hits a surface under nominal normal incidence. However due to the surface structure the local angle of incidence θ differs from 0 degree and thus affects the sputtering yield. Some of the sputtered atoms cannot escape the surface and get redeposited, while multiple reflections of the projectile ion may lead to further erosion of the surface (after [10]).

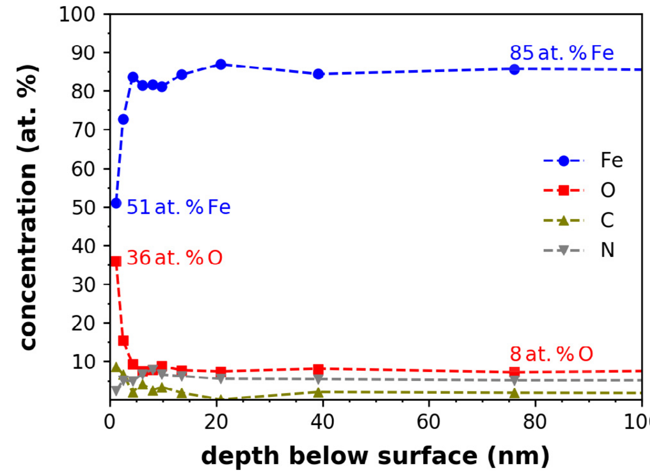

Fig. 2. The XPS analysis of the Fe-film as function of depth shows a significant oxide layer on top of the sample.

where y is frequently greater than 1 [9]. As is indicated in Fig. 1, not all of the sputtered atoms are able to escape the surface. Some of them may hit other parts of the rough surface and could be deposited there. Additionally, the projectile is reflected with a certain probability and may hit the surface a second time. The energy of the reflected projectile is lower than the incident energy, but might still be high enough to lead to further sputtering. These sputtered particles are then again partly redeposited (omitted in Fig. 1 for clarity) and with a given probability further reflection may occur.

Evidently, a theoretical description of the sputtering of rough surfaces becomes quite complex. Küstner et al. achieved remarkable results using STM images as an input and a simple model to describe redeposition effects ([10,11]). However, more detailed modelling of this situation is necessary to take into account effects such as shadowing (especially for flat ion incidence some parts of the surface will not be accessible to the ions) and the change in angular and energy distributions, where Fig. 1 already indicates large changes compared to a flat surface. For this reason, we have used the recently developed SDTrimSP-2D code [12,13] to take the actual surface structure into account in the sputtering simulations and compare the results of the simulations to our experimental data.

2. Experimental approach

The measurements have been performed using a highly sensitive quartz crystal microbalance (QCM) developed at TU Wien and described in more detail in [14,15]. This setup is an ideal tool to measure small mass changes and allows in-situ investigation of a dynamic erosion behaviour [6,16]. Our investigations concentrated on mono-energetic Ar ions of 500 eV hitting on an Fe-coated QCM sample. Ar might be used as seeding gas in fusion reactors like ITER, to avoid local overheating of the PFCs by radiative cooling [17]. Additionally Ar - > Fe sputtering yields are significantly higher than D – > Fe sputtering yields, making Ar^+ projectiles ideally suited for our experiments.

Typically 400 nm thin Fe films were deposited onto polished quartz crystals, by using a magnetron sputter deposition apparatus at IPP Garching, Germany. As the QCM technique only allows the measurement of the total mass change of the quartz and the presence of an oxide layer on the Fe film was assumed, one of the Fe films was analysed by X-Ray Photoelectron Spectroscopy (XPS). Sputter depth profiling via Ar-ion sputtering in combination with XPS was used to obtain the quantitative elementary analysis as a function of depth. This measurements were conducted on a custom SPECS XPS system with a monochromatized Al K-alpha source (μFocus 350) and a wide-angle lens hemispherical analyser (WAL 150).

XPS results are given in Fig. 2 and show a high concentration of O at the surface indicating a native oxide layer as expected. Long term sputtering shows that the Fe concentration only reaches 85% in the bulk of the film and substantial concentrations of O, N and C are still detected in the XP spectra. We will show below, that for the simulations it is essential to take the actual elemental composition into account.

The evolution of the sputtering behaviour of the Fe model films under Ar ion bombardment was then investigated at the specific angle of incidence of $\alpha = 60$ degree and in dependence of the bombarding ion fluence (results are shown in Section 4). Measurements were performed at an Ar ion flux of $\approx 5 \times 10^{16}\,\mathrm{m^{-2}\,s^{-1}}$ and at an Ar base pressure of 1×10^{-7} mbar.

AFM images of the Fe-coated quartz crystal samples were taken before and after prolonged irradiation (see Fig. 3a and b). On the initial surface, nano-scale structures are visible (Fig. 3a) that significantly change during the ion bombardment. For example after application of a total Ar fluence of $8 \times 10^{21}\,\mathrm{m^{-2}}$ under an angle of incidence of 60 degree a structure strongly aligned with the incoming projectile direction becomes visible (Fig. 3b).

3. Modelling with SDTrimSP

SDTrimSP is a Monte Carlo code that allows the simulation of ions hitting a solid target based on the binary collision approximation (BCA) [8]. It represents a dynamic enhancement of the widely used “static” TRIM code [19] and the dynamic code TRIDYN [20,21]. In the dynamic mode composition and thickness changes of the sputter target are included, while in the static mode these changes are suppressed. In addition the code allows parallel computing, which reduces computing time. SDTrimSP results perform very well for calculating sputtering yields especially compared to the SRIM code [22,23]. The target in a SDTrimSP calculation is set up one-dimensionally, where several discrete layers of different compositions can be defined. This means that only depth-dependent aspects of the target's change due to particle bombardment can be taken into account.

The two-dimensional expansion SDTrimSP-2D developed at the Max Planck Institute for Plasma Physics (IPP) allows implementing a surface structure into an SDTrimSP simulation [12]. This is realized by expanding the geometrical description from layers to a grid, where the cell modification is calculated from the material transport following the collision cascades. Surface cells can grow and shrink based on the transport of target atoms and thus a change in the surface morphology can be simulated. First results presented in [24] confirmed the validity of the model and reproduce experimental observations precisely.

The surface topography of our Fe films as deduced from the AFM