Macroscopic parameters of the interaction of an Ar^+ ion beam with a Si pitch grating

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Abstract

A Si pitch grating has been exposed to a 6 keV Ar^+ ion beam at normal angle of incidence as well as at angles of 35° both parallel and perpendicular to the structure. Sputtering of the grating has been observed experimentally by Rutherford back-scattering; the bombardment has been simulated by the SDTrimSP-2D code. The numerical simulations show reasonable agreement with experimental results. A pronounced anisotropy effect has been observed comparing the sputtering of the grating parallel and perpendicular to the structure.

Keywords: SDTrimSP-2D, sputtering, reflection, roughness, ion-surface interactions.

PACs numbers: [reserved for the case if needed]

1. Introduction

Interaction of energetic ions with a surface leads to removal of target atoms from the surface and the respective effect is called sputtering [1], [2]. The sputtering yield has been measured for a large number of projectile-target combinations and a wide range of projectile energies [1] [3]. It has been shown that results of experiments can be well reproduced by existing numerical codes based on the binary collision approximation, as long as chemical effects (chemical erosion) don't play a role. This confirms that presently the sputtering process is well understood and existing physical models can adequately describe it [3].

Most of the presently existing numerical codes are capable to treat only 1D surfaces, where the concentration of implanted species is varied along the depth. The TRIDYN code can be considered as a good example of such a model [4]. It has been recently rewritten in a more organized way and renamed to SDTrimSP [5]. This version of the code has a clear modular structure and allows easy extensions by attaching more modules. The SDTrimSP code may be used to overcome the 1D limitation of the approach by extending the grid of the existing model into the second and third lateral dimensions. Following this approach, one may hope to obtain a predictive code, which is useful for the system with arbitrary choice of target morphology, elemental composition of target and incident flux; the code would be then extremely useful for engineering in the field of the surface science.

The currently existing extension of the SDTrimSP code, which is able to simulate bombardment of the 2D surface (for example, a diffraction lattice), has been titled SDTrimSP-2D [6]. Recent investigations have been aimed on experimental validation of the 2D version of the code by comparing the surface cross-section profiles obtained by scanning electron microscope and by simulation [7], [8]. In these experiments a diffraction lattice with a period of 500 nm and a height of 200 nm has been used. The investigations have used volatile (argon) and non-volatile (carbon) ions. It has been shown that the code was able to follow the evolution of the surface morphology, when the pitch grating structure has been exposed to ion flux at normal angle of incidence and at inclined angles of incidence (both parallel and perpendicular to the structure orientation).

While the results of the code have been confirmed on the micro-scale, the investigations have left unclear one very important question: whether the code is able to follow the macroscopic parameters of ion-surface interactions? The aim of the present work is to address this question. We expose the Si pitch grating structure to a 6 keV Ar^+ beam at normal angle of incidence as well as at angles of 35° both parallel and perpendicular to the structure. The macroscopic areal density of Si atoms has been measured *in-situ* as a function of the incident Ar^+ fluence by means of Rutherford back-scattering spectroscopy and the obtained experimental data are compared to the results of simulations in order to validate the SDTrimSP-2D code.

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2. Experimental

The experiments were performed using the Dual-Beam Experiment facility at IPP Garching [9]. The Si pitch grating was exposed to a 6 keV Ar^+ ion beam, which has been generated by a Duoplasmatron ion beam system. The ion beam was mass-separated by a 60° bending magnet and focused on the surface of the grating with a 3 mm ion beam spot. The sample holder can be rotated, so the angle of incidence can be changed from 0 to 35°. The sample can be installed on the target holder in such a way that inclined bombardment can be performed perpendicular or parallel to the grating structure. The pitch grating and respective angles of incidence are shown in Figure 1.

The Si pitch grating sample has been taken from the same set of samples as the ones used in [7] and [8]. Its period is 500 nm and the height is 200 nm, the deviation from these values has been measured by scanning electron microscope and is within 5-20 nm. The structure has been created on top of a Si wafer, covered with a Ta interlayer, which has been introduced for labeling purposes. The cross-section of the pitch grating is shown in Figure 2.

Sputtering of the pitch grating was observed by means of Rutherford backscattering spectroscopy at the Tandem accelerator at IPP Garching [10]. A 2 MeV ^{4}He beam at normal incidence was used. The RBS detector was a solid-state detector with an energy resolution of 15 keV and a solid angle of about 1.58 msr at a scattering angle $\theta = 165°$. The sample was oriented in such a way that the grating structure was parallel to the exit beam. At this geometry correlation effects, such as incidence through a valley and exit through a hilltop, do not play a role.

The experimental procedure was as follows: After a first IBA analysis of the virgin sample the surface was sputtered by bombardment with the Ar beam. After this sputtering step the sample was analyzed again by the MeV He beam followed by another sputtering step. In the DBE installation sputtering and subsequent IBA can be performed in the same setup without breaking the vacuum.

Computer simulations of IBA spectra were performed using the code SIMNRA 6.50 [10]. Spectra of the grating structure are calculated by using a linear superposition of sub-spectra, as described in [11]. SIMNRA 6.50 allows to use arbitrary layer thickness distribution functions supplied by input file. Correlation effects, such as incidence through a valley and exit through a hilltop or multiple surface crossings, are neglected. This is a reasonable approximation for the sample orientation used in the experiments, see above.

The morphology of the grating steps was investigated additionally by the HELIOS device of the IPP. This is a scanning electron microscope (SEM) with focused ion beam (FIB), type Nanolab 600/FEI. Here, the focused ion beam was used to produce cross-sections of the surface layer followed by tilting the sample and investigation of the cross section by means of SEM.

3. Computer simulations

The simulations have been performed by the SDTrimSP-2D code [6]. 6 keV Ar^+ ions have been launched towards the surface consisting of Si atoms, which is shaped in two dimensions (vertical and lateral) and extended in third dimension. It can be run in static or dynamic mode (SD) on sequential or parallel systems (SP). SDTrimSP-2D uses a 2-D mesh to represent the surface morphology, the first dimension is the direction perpendicular to the macroscopic surface plane, and the second is in a direction parallel to that plane. This representation is sufficient to simulate the ion bombardment of surfaces with 2D micro-structure extended into the 3rd dimension. It shares the same physical model of ion-surface interactions with other codes of the TRIM family. However, the resolution of a second dimension requires a 2-D domain with separate cells.

The code follows the density changes in the target material due to projectile and recoil particles coming to rest after a complete slowing-down at the end of their trajectories. In SDTrimSP/TRIDYN, this is done by a 1-D relaxation of the cells. Each trajectory creates a mass flux in the cells it passes. These fluxes can act as sink or source terms for the particle densities. To ensure particle conservation within the numerical setup, which uses a 1D grid of cells in which each cell has a constant volume density according to the material, volume changes of the 1D cells (expansion or contraction perpendicular to the surface) are used to represent changes to the number of particles in a cell. In SDTrimSP-2D, this procedure has been extended to 2D, subject to the requirement that all volume changes applied are divergence free. This reflects particle conservation in the projectile-target system expressed by volume changes. For each cell, the resulting mass fluxes (representing the transfer of particles into or out of the cell) are taken to be anisotropic by introducing the anisotropy coefficient (K_{anis}) of the volume relaxation. This anisotropy coefficient defines the ratio of horizontal volume changes (representing horizontal mass fluxes parallel to the surface) and perpendicular volume changes (representing mass fluxes in vertical direction). The horizontal transport (parallel to the surface) is usually set smaller than the vertical one, because swelling or shrinking are primarily observed experimentally in the vertical direction.

In the simulations presented here an anisotropy coefficient of 0.5 was used. The horizontal transport (parallel to the surface) is usually set smaller than the vertical one, because swelling or shrinking is primarily observed experimentally in the vertical direction. This anisotropy coefficient was calibrated in previous work [7]. Thus, the cells at the surface exposed to incident ions can change in two directions. The volume of cells without sides bordering on the surface is kept fixed. The relaxation process is done in several iterations until the divergence of the mass fluxes (transfer of particles between cells) becomes zero and steady-state conditions without internal tension are obtained. From this steady-state, divergence-free solution the volume changes are applied. In addition, splitting and annihilation of cells was introduced in SDTrimSP-2D, according to a maximum and minimum number of atoms, to be able to represent creation of holes or strong deposition.

Since the surface is a periodic structure in the lateral direction, periodic boundary conditions in this direction are used.

4. Results and discussion

The pitch grating has been exposed at three different angles of incidence. These are somewhat different from the ones used in [7] because of limitations in angular rotation at the Dual Beam Experiment in Garching. The comparisons of the experimentally measured areal densities of Si atoms with the results of simulation are shown in Figure 3. All three cases show the same tendency for sputtering of the Si structure: it decreases monotonically with increasing fluence. The only difference being obvious here is the slope, which indicates different erosion rates. Since the structure height is rather limited, at higher fluences Si removal may strip the Ta layer. Therefore, one can observe the flat part of the calculated curves, see Figure 3 (b) and (c). In the experiments, the bombardment has been stopped as soon as the Rutherford backscattering analysis indicated no remaining Si on top of the Ta layer.

One can notice the influence of 2D anisotropic structure on Si sputtering. The Si removal occurs faster, when the pitch grating is bombarded at inclined angle parallel to the structure. As a result, the Ta layer has been revealed at a lower fluence, when the surface is exposed to Ar^+ ion beam parallel to the structure. At inclined angle perpendicular to the structure, the Si removal is suppressed by the stronger redeposition of the sputtered Si atoms on the walls of the structure. The stronger redeposition rate for the case of perpendicular bombardment has been confirmed in previous work [7], where the local sputtering and redeposition have been investigated.

Si removal is slowest at normal angle of incidence, because redeposition on the walls is supplemented with lower sputtering yield. Although some local incidence events may occur at rather high angle of incidence, the average angle of incidence is lower than that for case of inclined incidence.

Comparing experimental data and simulation, one can observe qualitative agreement. On the experimental side there are two sources for quantitative disagreement: measurement of the fluence and measurement of the Si areal density. The experimental data for the amount of Si should be accurate within about 5%, which is typical for RBS measurements. Although Si is difficult to be seen directly because it is on top of a high Ta background, the shift of the high-energy edge of the Ta peak towards lower energies is a very sensitive measure of the amount of Si on top. Therefore, the main source of disagreement is probably the error of the fluence measurement.

A 2-dimensional surface exhibits a much more complicated dynamics of ion-surface interactions. A plane surface does not change its structure under ion bombardment. The morphology of a structured surface, however, is modified by the sputtering process. In turn, the modified surface changes the sputtering yield and re-deposition fraction. Therefore, a 2D structured surface exposed to ion flux is a system with back-coupling which is a principal difference from a plane surface.

The calculated evolution of the surface sputtering yield and reflection coefficient as a function of fluence is shown in Figure 4. The common tendencies are a peak in the sputtering yield at a fluence of $(250\text{-}300)\times10^{15}\ \mathrm{cm}^{-2}$ and decrease of the sputtering yield when Si is almost vanished. Simultaneously, the reflection coefficient rises since it is higher for Ta than for Si. However, the peak sputtering yield is highest for the case of parallel bombardment and is lowest for the case of normal incidence, the case of perpendicular bombardment is in between. The respective peaks in the reflection coefficient are arranged in the same way. This can be explained by the relation between sputtering and redeposition: the redeposition is lower for normal angle of incidence and for inclined bombardment parallel to the structure, while sputtering is generally higher for cases of inclined bombardment.

The anisotropy effect (i.e. the difference between inclined bombardments parallel and perpendicular to the structure) is clearly evident in the behavior of the sputtering yield. The bombardment parallel to the structure produces a higher sputtering yield, but it rises stronger and after reaching its peak value falls faster. In contrast, bombardment perpendicular to the structure rises up slower and remains almost steady-state in the range from 250×10^{15} cm^{-2} to 600×10^{15} cm^{-2}. At fluences above 600×10^{15} cm^{-2} the sputtering yield decreases strongly. However, for the case of perpendicular bombardment the fall occurs slower. The lower sputtering yield for perpendicular bombardment is everywhere explained by stronger contribution of redeposition processes.

5. Conclusions

Si pitch gratings have been exposed to a 6 keV Ar^+ ion beam at three different angles of incidence: normal angle of incidence as well as at angles of 35° both parallel and perpendicular to the pitch structure. The removal of Si atoms as a function of fluence has been measured by Rutherford backscattering *in-situ* and the obtained results have been compared to numerical simulations by the SDTrimSP-2D code. The comparison has confirmed that SDTrimSP-2D code is capable to reproduce the macroscale erosion of the 2D structured surface. Additional macroscopic data have been obtained by simulations only. Both, simulation and experiment has revealed an anisotropy effect, when the sputtering at inclined angle parallel to the structure differs from the perpendicular one. This investigation supplements work [7], where the SDTrimSP-2D code has shown to be capable to follow the nanoscale evolution of 2D structures. However, due to the experimental uncertainty in fluence at the particular location a full quantative validation was not possible.

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List of Figure Captions

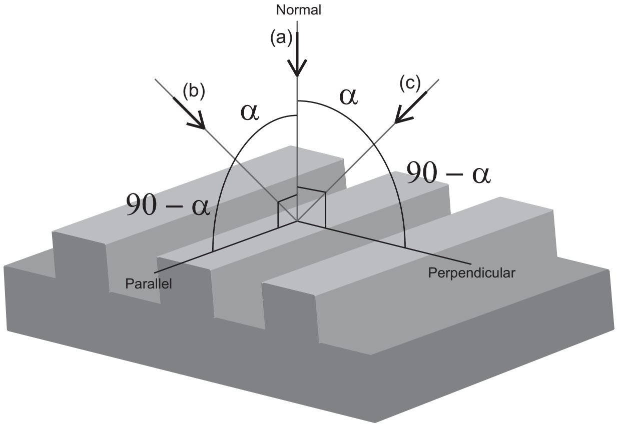

Figure 1. The directions of the ion beam relative to the pitch grating structure: (a) – normal angle of incidence, (b) – incidence at an angle of 35° parallel to the structure and (c) – incidence at an angle of 35° perpendicular to the structure.

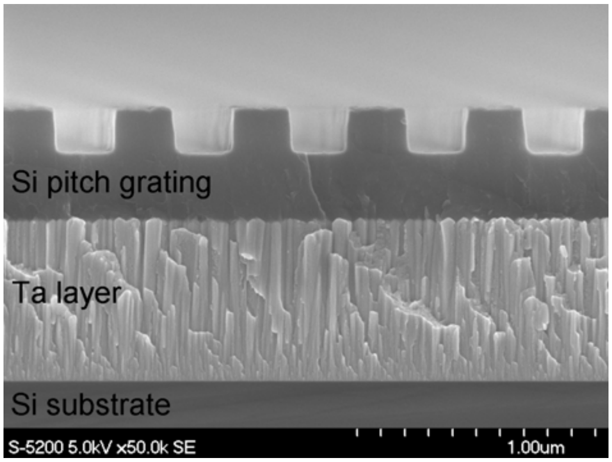

Figure 2. The cross-section of the Si pitch grating obtained by scanning electron microscopy.

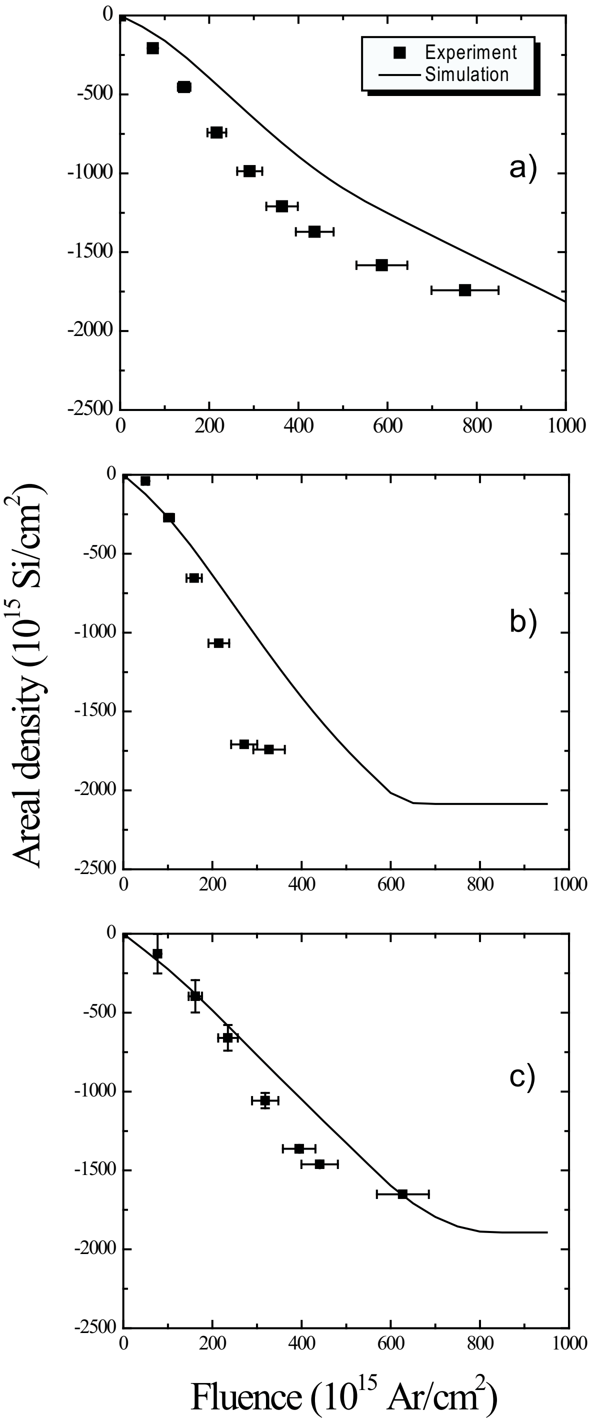

Figure 3. Comparison of the experimentally measured and numerically simulated decrease of the Si areal density as a function of fluence. (a) – normal angle of incidence, (b) – incidence at an angle of 35° parallel to the structure and (c) – incidence at an angle of 35° perpendicular to the structure.

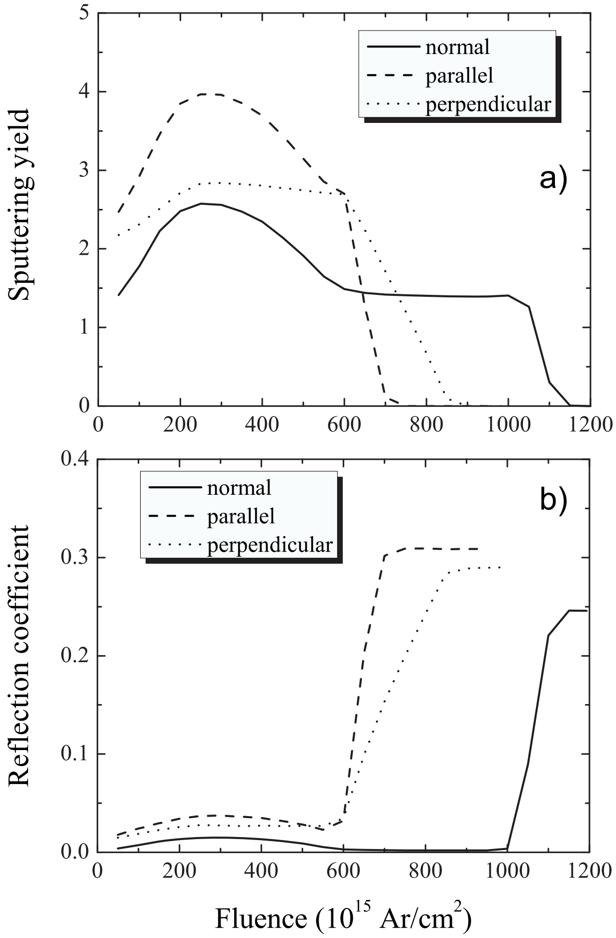

Figure 4. Total sputtering yield (a) and reflection coefficient (b) as a function of fluence obtained by numerical simulation for the three cases of incidence.