Bombardment of a Si pitch grating by C^+ ions at an inclined incident angle parallel to the structure

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Abstract

In this work, the bombardment of a nano-scale Si pitch grating with 6 kV C^+ ions at an angle of incidence of 42° parallel to the structure is investigated both experimentally and by simulations with the SDTrimSP-2D code. The study focuses on the relation between the nano- and macro-scale parameters of ion-surface interactions. The macro-scale parameters are the sputter yields of Si and C atoms and the areal density of the C atoms deposited on the surface; the nano-scale parameter is the 2D profile of the structure. The nano-scale surface profile was obtained experimentally by scanning electron microscopy of specimen cross-sections. The comparison between experiment and simulation reveals good agreement on both macro- and nano-scales.

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1 Introduction

The inner wall of the vacuum vessel of the International Tokamak Experimental Reactor (ITER) will be exposed to high fluxes of energetic ions and neutrals [1, 2, 3] and it is expected that the recycling flux bombarding all surfaces will be seeded by carbon (C) atoms and ions. C ions are accelerated by the sheath potential towards the in-vessel surface and may reach energies of up to several keV [4]. This leads to both sputtering of surface by energetic particles and C ion implantation.

While physical processes governing sputtering are well understood in terms of yields and distributions, the influence of surface morphology on sputtering and deposition is still a question of active research. For example, sputtering and deposition on a rough W surface exposed to C and C+D ion fluxes occurs differently as compared to the same processes on a smooth surface [5, 6]. The simulations in this work have been performed using the SDTrimSP-2D code [7, 9]. This code is a 2D version of the binary collision approximation (BCA) based Monte-Carlo code SDTrimSP [8]. It allows numerical studies of morphology changes in 2D and it delivers nano-scale information about ion-surface interactions.

In this work, a Si pitch grating, representing a 2D surface, is exposed to 6 keV C ions at an angle of incidence α=42° parallel to the structure. The ion surface interactions are studied at both macro- and nano-scale experimentally and by numerical simulations. The nano-scale surface structure is examined with scanning electron microscopy (SEM). These experimental results are compared with simulations providing a comprehensive validation of the code.

Since SDTrimSP-2D provides macro- and nano-scale information, the code allows us to study the relation between local nano-scale processes, like surface modification, redeposition, etc, and global characteristics, like sputtering yield and the areal density of the implanted particles.

The current validation study is an extension of our previous work [9], which focused on the recycling ion species, Ar^+. The choice of material is dictated by the fact that this was the only choice available for a cheap and realistic model system to test and validate the SDTrimSP-2D code. This validated code then can be used for the study of fusion oriented ion-surface interactions, like in [5] and [6].

Non-recycling ions, such as carbon, present an added complication, and are the subject of the current study.

2 Experimental techniques

The design of the Si pitch grating specimen is shown in Fig. 1. The nano-structured specimen is fabricated on a Si wafer with an intermediate Ta layer with a thickness of 650 nm. The Ta layer is used as a reference marker for ion beam analysis and SEM observations, allowing quantitative measurements of the Si erosion. The period of the structure is 500 nm (250 nm for pits and 250 nm for grates); the height of the grates is 200 nm. The actual grating dimensions deviate from the nominal values by 5-20 nm, which imposes a lower limit for the agreement between experimental results and calculations.

To examine the nano-scale evolution of the surface, the Si specimens were irradiated in the UTIAS dual-beam mass-separated ion accelerator [10] with a beam of 6 keV C^+ ions. The major reason for this work is the validation of the 2D binary collision code. The C-Kr potential used in the code to describe the interaction between the projectiles/recoils and target atoms is a valid approximation for the chosen energy of 6 keV extending down to values of ≈ 50eV, where the binary-collision approximation breaks down.

The angle of incidence was fixed to be parallel to the grating structure with an angle of 42°. The experimental geometry is shown schematically in Fig.2. The fluence was derived from a measurement of the ion beam current and the beam spot area. The ion beam current was ≈1 μA over a beam spot with typical diameter of 4-5 mm, such that the average flux was $\approx 0.5\times10^{18}$ $m^{-2}s^{-1}$. For the experiment, at tilted angles the average fluence was $\sim 60\times10^{20}$ m^{-2}. Since the beam spatial distribution is expected to be approximately Gaussian, strong variations in flux and fluence are expected across the exposed area, particularly towards the periphery of the exposed region. Following the bombardment, the specimens were extracted from the vacuum system and cracked to obtain the cross-sections used for SEM with a high-resolution Hitachi S-5200 Scanning Electron Microscope.

3 Results and discussion

The results of simulations with SDTrimSP-2D are shown in Fig. 3, including the total partial sputtering yields of C and Si, which are defined as the ratio of the number of sputtered C or Si atoms to the number of incident C ions. The evolution of the Si pitch grating profile exposed to an C ion flux is examined by the code at both macro- and nano-scales. This allows a better understanding of the mechanisms for the sputtering yield by nano-scale processes changing the surface structure. Particles leaving the system in z-direction are stopped at the top of the domain. In the other direction the system is periodic. The data for the simulation specifying the materials (like binding energies) has been taken from the standard tables existing in SDTRIMSP based on [11].

At the beginning (with a fluence of $<25\times10^{20}$ m^{-2}), the process of C implantation into the Si surface dominates. During this process, the Si sputtering yield is decreasing from 1 to ≈0.72, while the C areal density is rapidly increasing from 0 to $\approx 12\times10^{20}$ m^{-2}. The increase of the C concentration in the surface layer leads to a strong increase of the C sputtering yield, because at this stage it strongly depends on the availability of C atoms on the surface. As has been shown in [12], the formation of a mixed material decreases the sputtering of the surface because the concentration of target atoms is decreased. Using this argument, one can understand that the formation of the mixed C-Si surface is an important process in this fluence range, and it represents an important difference between bombardment with recycling and non-recycling ion species.

Another important process at a fluence of $<25\times10^{20}$ m^{-2} is the formation of inclined surfaces. The concentration of implanted C atoms is lower for such surfaces, while the angle of incidence is higher. Both of these factors increase the Si sputtering yield compared to horizontal surfaces. The erosion of Si from these surfaces is the primary contribution to the total sputtering yield of Si atoms from the structure.

In the fluence range of $25\text{-}75\times10^{20}$ m^{-2}, the system is sustained in a dynamical steady-state. The macroscopic parameters remain relatively stable: the Si sputtering yield is stable around a value of ≈0.72, the areal density of C atoms on the surface is slowly increasing and the C sputter yield varies in the range of 0.8-0.9. The main changes on the surface occur in the structure of the profile. The inclined surfaces remain at nearly a constant slope, but the width of the structure decreases. This effect is very similar to what we have found in previous work [9] and is a direct consequence of the morphological change of the surface. At the beginning, the top and the bottom of the pitch grating behave the same. Then, the sputtering introduces changes on the top by smoothing the corners and increasing the steepness of the structure. Due to this, the sputtering increases more and more on the top, whereas the bottom remains essentially flat.

Because the area and the slope of the inclined surfaces remain practically constant, the Si sputtering yield remains constant, since these surfaces are the main contributors. The total area of the horizontal surfaces stays nearly constant as the decrease of the top horizontal part of the structure is compensated by an increase in the bottom part; the height of the structure remains the same. Therefore, total C areal density and C sputtering yield, which are mainly determined by this part of the surface, are nearly unchanged.

At fluences above 75×10^{20} m^{-2}, the structure height begins to decrease with increasing fluence, thus decreasing the area of the inclined surfaces. This, in turn, leads to a decrease of the Si sputtering yield. This process continues until the structure is completely sputtered away. After that (at fluences > 150×10^{20} m^{-2}) the system becomes essentially 1-D and the surface behaves as a planar one.

The areal density of the implanted C in this fluence range (i.e. >75×10^{20} m^{-2}) increases monotonically; however, it does not create a protective C layer. Instead, the concentration of the C in the mixed surface slowly increases with fluence from 30%-40% to almost 90% (see Fig. 3). At the same time, the C sputtering yield stays about constant, with a slight variation around the value of 0.8.

4 Experimental validation

A single specimen was prepared for the SEM analysis; variations observed in the surface modification are a result of the non-uniform (Gaussian) beam profile, such that the ion current density is gradually reduced towards the edges of the irradiated spot. As a result, the central part of the bombarded surface is irradiated with a higher fluence, while edges are less exposed. Thus, fracturing the specimens along the diameter of the beam spot produced a cross-section of the surface with varying ion beam exposure.

SEM images at two locations (i.e. at different radii of the spot), are shown in Fig. 4. The simulated surface profiles are overlaid in red on the SEM images. In the vertical plane, the bottom of the square has been matched to the interface between the Ta layer and the Si grating; in the horizontal plane, the vertical axes of symmetry were aligned. It was found that the experimental profiles were best matched by simulations at fluences of 20×10^{20} m^{-2} and 45×10^{20} m^{-2}, well within the range expected from the beam current measurements in the experiment. One can see that the shape of the SEM cross-sections is well matched by the simulated profiles. The calculations provide an accurate progression of the surface structure, to within the initial accuracy of the pitch grating structure, 5 – 20 nm.

While the experimental ion fluence cannot be determined at individual points within the beam spot area, the fluence calculated in the simulations (45×10^{20} m^{-2}) is consistent with that of the experiment (60×10^{20} m^{-2}) in the central region of the beam spot (SEM image shown in Fig. 4 (b)) and lower towards the edges.

Conclusions

A Si pitch grating was exposed to 6 keV C ion flux incident at the surface with an angle of incidence of 42° and the ion-surface interaction was studied by means of experiment and simulations with SDTrimSP-2D. A good agreement between the simulations and the experiment was obtained comparing the measured and calculated cross-sections of the structure for different fluences; the deviations between model and experiment were within the manufacturing accuracy of the structure (5-20 nm).

The simulation provides improved understanding of the evolution of the parameters describing both macro- and nano- scale processes. One can relate the evolution of the Si and C sputtering yields, as well as the C areal density to the evolution of the Si pitch grating structure

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Figure 1. The structure of the Si pitch grating sample.

Figure 2. Schematic view of the experimental geometry. Ions are incident on the Si pitch grating at an angle of 42° parallel to the structure.

Figure 3. Evolution of macro-scale (total partial sputtering yields and C total areal density) and nano-scale parameters (surface profile) calculated with SDTrimSP-2D.

Figure 4. SEM images of cross-sections of the Si pitch grating after bombardment at an angle of 42° parallel to the structure. Red coloured graphs are the surface profiles simulated by SDTrimSP-2D. All scales are given in nanometers. Different images correspond to different incident fluences. The fluence value has been taken from the results of the simulation: (a) – 20×10^{20} m^{-2}; (b) – 45×10^{20} m^{-2}.

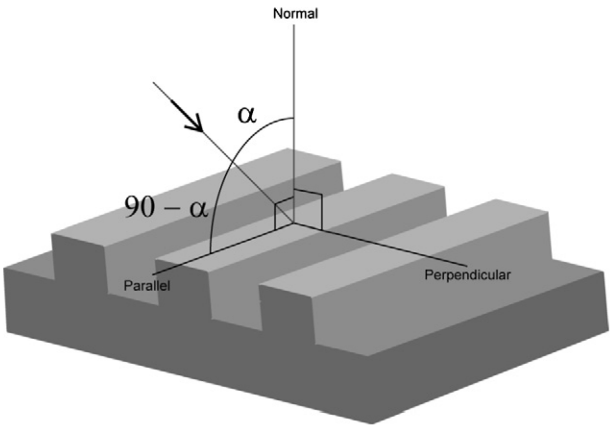

Fig 1

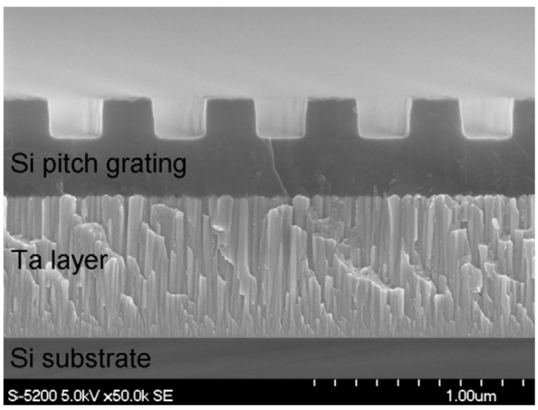

Fig 2

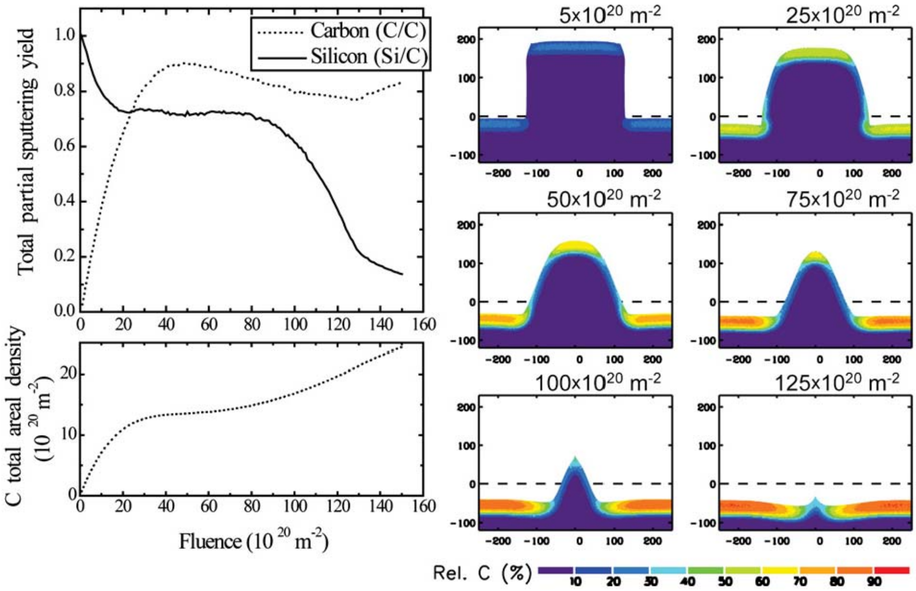
Carbon (C/C)
Silicon (Si/C)
Total partial sputtering yield
C total areal density (10^{20} m^{-2})
Fluence (10^{20} m^{-2})
5×10^{20} m^{-2}
25×10^{20} m^{-2}
50×10^{20} m^{-2}
75×10^{20} m^{-2}
100×10^{20} m^{-2}
125×10^{20} m^{-2}
Rel. C (%)

Fig. 3

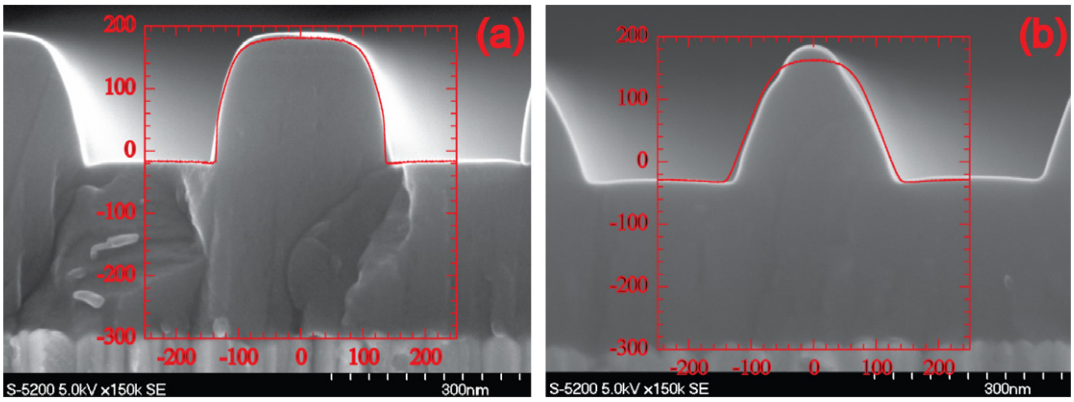
(a)
(b)
S-5200 5.0kV x150k SE
300nm
S-5200 5.0kV x150k SE
300nm

Fig 4

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