Angular Distributions of Sputtered Atoms from Semiconductor Targets at Grazing Ion Beam Incidence Angles

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Abstract. Angular distributions of ion sputtered germanium and silicon atoms are investigated within this work. Experiments are performed for the case of grazing ion incidence angles, where the resulting angular distributions are asymmetrical with respect to the polar angle of the sputtered atoms. The performed experiments are compared to Monte-Carlo simulations from different programs. We show here an improved model for the angular distribution, which has an additional dependence of the ion incidence angle.

Keywords: Sputtering, Germanium, Silicon, Grazing ion incidence, Angular distribution **PACS:** 81.65.Cf, 79.20.Rf

INTRODUCTION

Focused ion beam systems (FIB systems) are used for surface structuring of semiconductors like germanium and silicon [1]. In order to understand the ionetch process effects like sputtering, ion reflection, swelling, etc., have to be well known. As a consequence of sputtering, the redeposition of atoms occurs. Especially in etching of small sized structures, this effect plays an important part. Ion etch simulations consider the redeposition by assuming a symmetrical angular distribution which is described by a cosine of the polar emission angle ϑ to the power of n, where 1 < n < 3 [1]. This assumption is sufficiently accurate for normal incidence ions. But for grazing ion incidence, as it occurs on the sidewalls of the produced structures, the angular distribution is asymmetrical with respect to the target normal. We measured, therefore, the distributions of sputtered germanium and silicon using two different experimental setups. Additionally, we made Monte-Carlo simulations of the sputtering process using different Monte-Carlo programs [2,3,4]. The observed differences between measurements and simulations are discussed. Finally, the improved models for the angular distribution of sputtered atoms are shown in the last chapter.

EXPERIMENTAL SETUP

Two setups were realized for obtaining angular distributions of germanium and silicon:

a) A small piece of a germanium wafer was used as a target for argon ions with a kinetic energy of 20 keV. This setup was placed in a large vacuum chamber of an ion implantation system, which is usually used for tribology research (Fig. 1). The sputtered germanium is collected on a 300 mm silicon wafer with a distance to the target of 20 cm. The implantation angle was varied from 60° to 85° by tilting the germanium target with respect to the ion beam. As the collector sample is a standard silicon wafer, we were able to analyze its surface contamination by a total-reflection x-ray fluorescence system (TXRF). Measuring under total reflection conditions results in a very low detection limit of 1 x 10^{11} at. cm⁻² to 1 x 10^{12} at. cm⁻², depending on the analyzed atom species. The TXRF system Atomika 8300W, which has a spot size of 0.8 cm, was used for this investigation. This setup has, therefore, an angle resolution of about 5°, which is adequate to monitor local inhomogeneities.

b) The setup for the silicon sputtering is realized in a vacuum chamber of a FIB system. As the chamber



FIGURE 1. Experimental setup a) for the Ar⁺:Ge sputtering experiments. The ion incidence angle α was varied from 60° to 85°.

has much smaller dimensions compared to the tribology vacuum chamber in a), the distance between the target and the collector was only 5.5 mm. Gallium ions with kinetic energies of 30 keV were sputtering the silicon atoms with angles of incidence of 70° and 80°. The collector was a piece of a silicon wafer with a 3 µm polymer coating on it. The coating was used for collecting the sputtered silicon atoms, and the silicon wafer at the bottom served for mechanical stability and also as heat sink, since the collectors were analyzed by Rutherford Backscattering Spectroscopy (RBS). The RBS measurements were performed at the University of Minsk (Belarus) with spatial resolutions of 300 µm. This results in an angle resolution of 6°. In difference to a) (Fig. 1) the target and the collector were arranged parallel in b), which has to be considered in the evaluation of the collected material.

Table 1 shows the measured and simulated values for the total sputter yield. The Monte-Carlo simulations were performed with the program MC_Sim [2]. At very high values of the angle of incidence, the measured sputter yield is much lower than expected from the simulation. This was the reason why the angular distributions for the Ar⁺:Ge, 85° experiment were no more measurable due to too low surface concentrations of germanium on the collector wafer.

RESULTS

Experiments for Ar^+ *: Ge*

For the Ar⁺:Ge experiments, 300 mm silicon wafers were used as collectors. The silicon wafers were analyzed spatially resolved by TXRF. From Monte-Carlo simulations it is known that the sputtered atoms have only a few eV of kinetic energy, thus their penetration depth into the collector is only a few nanometers. Analyzing just the collector surface with the TXRF gives us therefore the desired information about the sputtered atoms in a particular direction. Ion implantation dose for all Ar⁺:Ge experiments were on the order of 1×10^{15} cm⁻². This dose was chosen for two reasons: first, a lower dose would lead to crystal orientation effects in the angular distribution [5]. Second, a higher ion doses leads to a notable material removal. Under these conditions ion etching is known to produce local structures and rippling on the target surface [6]. This roughness influences the sputtering and the obtained angular distributions. Fig. 2 shows the measured germanium distribution on the silicon wafer in the ion incidence plane. 9 is the polar angle of the sputtered atoms with respect to the target normal. Backward emission is indicated by negative 9.



FIGURE 2. Angular distribution of sputtered germanium. 20 keV argon ions with an angle of incidence of 75° were used for sputtering. 9 is the polar angle with respect to the target normal. The continuous lines represent Monte-Carlo simulations.

Experiment Parameter	Ar ⁺ :Ge, 60°	Ar ⁺ :Ge, 70°	Ar ⁺ :Ge, 75°	Ar ⁺ :Ge, 80°	Ar ⁺ :Ge, 82.5°	Ar ⁺ :Ge, 85°	Ga⁺:Si, 70°	Ga⁺:Si, 80°
Simulated sputter yield (MC_Sim)	7	8	10	11	10	8	10	11
Experimental sputter yield	10.8	11.4	10.3	11.4	1.3	0.02	13	16

TABLE 1. Experimental and simulated values for the sputter yield for the experiments Ar^+ : Ge and Ga^+ : Si.

In general, the observed distributions show a local maximum at a direction in a right angle to the primary ion incidence beam (15° in Fig. 2). This maximum is related to primary knock-on atoms (PKA).

In addition to the experiments, Monte-Carlo simulations were performed and compared to the experimental values. For the simulations, different Monte-Carlo codes [2,3] were used. In order to be able to consider a realistic angle resolution as in the experiments, the sputtered atoms in the simulation were collected on a virtual plane with a distance according to the experimental setup. In Fig. 2, the Monte-Carlo simulations are depicted by continuous lines. The position of the PKA peak is reproduced well by all simulations, but the magnitude varies. The differences between the simulation codes are primarily due to different treatments of the target surface.

Experiments for Ga⁺:Si

The parallel-aligned target-collector combination was placed in a vacuum chamber of a FIB system. The disadvantage of measuring the collector with RBS, compared to the TXRF, is the high detection limit of about 1×10^{15} cm⁻², which requires a very large amount of sputtered silicon atoms. In consequence, the implantation doses for the experiments were on the order of 1×10^{18} cm⁻², which leads to etching processes of the silicon surface of several micrometers. The created groove influences the angular distribution, as sputtering from the edges additionally occurs. Fig. 3 contains the angular distribution for silicon atoms sputtered with gallium ions with an angle of incidence of 80°.



FIGURE 3. Angular distribution of sputtered silicon. 30 keV gallium ions with an angle of incidence of 80° were used for sputtering. The continuous lines represent Monte-Carlo simulations.

It should be noted that the angular distributions in Fig. 2 and 3 have not been corrected to the different collector-target alignments.

Like already mentioned in the Ar⁺:Ge experiments, the Monte-Carlo simulations reproduce the position of the PKA peak quit well, but the magnitude is overestimated.

ANALYTICAL MODELS

The experimental results in the last chapter can be used to establish analytical models for the angular distributions. Up to now, reduced models assuming a cosine distribution for the angular distributions are used in etch simulations [1]. In order to be able to consider the mentioned PKA peak in the angular distributions, we added another cosine to the model, which depends on the angle of ion incidence:

$$Y_s = b\cos^n(\vartheta) + c\cos^m(\vartheta - (90 - \alpha')).$$
(1)

 Y_S is the angular distribution per solid angle, b, c, n and m are parameters depending on the primary beam and the target material, and

$$\alpha' = \alpha - \delta \tag{2}$$

corresponds to the primary ion beam incidence angle α reduced by δ . δ has a value of 2° for Ar⁺:Ge and 3° for Ga⁺:Si, and originates from the surface refraction due to the surface binding energy [7]. As we used plane collectors in our experiments, Eq. (1) has to be extended by a factor κ [8] to obtain the angular distribution *f*(*9*) measured on the collector:

$$f(\mathcal{G}) = \kappa(\mathcal{G}) \cdot Y_{\mathcal{S}}(\mathcal{G}). \tag{3}$$

For the Ar^+:Ge setup, κ depends on the angle of ion incidence

$$\kappa(\vartheta) = \cos^3(\vartheta - (90^\circ - \alpha)), \qquad (4)$$

whereas for the parallel alignment in the Ga⁺:Si experiment applies:

$$\kappa(\mathcal{G}) = \cos^{3}(\mathcal{G}) \,. \tag{5}$$

The parameters b, c, n, and m were obtained by backward engineering of the experimental results (see Fig. 4).



FIGURE 4. Angular distribution for Ar⁺:Ge, 80°. The analytical model (Eq. (3)) is adapted by minimizing χ^2 .

treatment of the target surface in the Monte-Carlo simulations.

A more precise analytical model is adapted to the experiments. The accordance in the case of $Ar^+:Ge$ is very good, for $Ga^+:Si$ the noisy distribution due to high implantation doses derogates the results.

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TABLE 2. Model parameters	(Eq. (3)) for the e	experiments Ar ⁺ : Ge and Ga ⁺ :Si.
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Experiment	Ar ⁺ :Ge,	Ga⁺:Si,	Ga⁺:Si,				
Parameter	60°	70 °	75°	80 °	82.5 °	70 °	80 °
b	1.2	1.08	0.86	1.02	0.99	0.3	0.28
с	0.06	0.04	0.15	0.01	0.01	0.7	0.73
n	1.73	1.99	1.5	2.20	2.36	1.0	2.0
m	120	60	10	100	100	0.9	2.8
α	58°	68°	73°	78°	80.5°	67°	77°
γ^2	4.10^{-5}	5.10-5	1.10^{-3}	$2 \cdot 10^{-4}$	4.10^{-4}	$2 \cdot 10^{-3}$	6.10-4

Table 2 shows the results for all experimental data. The mean reduced standard deviation χ^2 was calculated for all angular distributions to indicate the agreement of the model to the experimental values. The Ar⁺:Ge experiments could be modeled very well, the obtained model parameters are all in the same range. For Ga⁺:Si the high implantation dose produced additional noise to the angular distributions, which leads to a quite high χ^2 value. Nevertheless, the obtained parameters for the analytical model are nearly the same for both implantation angles

CONCLUSION

Experiments, Monte-Carlo simulations and analytical models for angular distributions of ion sputtered germanium and silicon are reported within this work. For the experiments the collector-technique was used, where a plane sample collects the sputtered material and is investigated afterwards. According to the experiments, Monte-Carlo simulations were performed to compare the results. The PKA peak due to primary knock-on atoms is reproduced in both cases, but with a different magnitude which results from an inaccurate

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