Available online at www.sciencedirect.com

ScienceDirect

Nuclear Instruments and Methods in Physics Research B 266 (2008) 872–876

NIM B
Beam Interactions with Materials & Atoms

www.elsevier.com/locate/nimb

Ion fluence dependence of the Si sputtering yield by noble gas ion bombardment

A. Mutzke [a,*], W. Eckstein [b]

[a] Max-Planck-Institut für Plasmaphysik, EURATOM Association, D-17491 Greifswald, Germany
[b] Max-Planck-Institut für Plasmaphysik, EURATOM Association, D-85748 Garching bei München, Germany

Received 29 October 2007; received in revised form 14 January 2008
Available online 2 February 2008

Abstract

The effect of sputtering yield enhancement by implantation of noble gases into solid silicon is investigated with the Monte Carlo program SDTrimSP. The process of diffusion is incorporated into the program to describe the outgassing of noble gases. The bombardment of Si with He, Ne, Ar, Xe at normal incidence is studied in the energy range from 1 to 500 keV. Good agreement of the calculated results with experimental data is found.

PACS: 34.50; 79.20.R; 02.50.U; 02.60; 81.15.C

Keywords: Atoms scattering; Atoms sputtering; Atom; Molecule; Ion impact; Applications of Monte Carlo method; Numerical methods; Film deposition

1. Introduction

The sputtering yield is often determined experimentally by the weight-change method, where the mass of the removed material is measured by weighing the target before and after bombardment. Due to the limited sensitivity of the balance a large fluence of incident particles has to be applied. This leads to the measurement of a so-called steady state sputtering yield, which may differ from the yield of the pure material due to the implantation of the bombarding species in the target. For nonvolatile species like metal ions this can lead to a completely changed target composition [1] and dramatic effects like oscillations in the sputtering yield with increasing fluence [2]. For noble gas ions the implantation of these species is usually regarded to be small. The influence of the implanted ions on the sputtering yield depends on the ratio of ion mass to target mass, but also on the depth distribution of the implanted atoms and their maximum atomic fraction in the target. Therefore, the sputtering yield should change with fluence until steady state is reached. Blank and Wittmaack [3] have shown this effect for the bombardment of Si with 140 keV Xe. They found an increase of the sputtering yield of about 20% due to the increased scattering of the implanted Xe. They also determined the total implanted Xe by Rutherford scattering but not a depth distribution.

The purpose of this paper is to go a step further to provide information of the depth distribution and maximum atomic fraction of the implanted Xe dependent on the incident energy. Furthermore, the dependence on the incident species or mass ratio is investigated. Computer simulation is applied for these studies.

2. Simulation

The calculations were performed with the Monte Carlo program SDTrimSP [4], which is a new version of TRIM.SP [5,6]. This advanced version has included all aspects of earlier developments, allows the use of different interaction potentials, different integration schemes, time development

---

[*] Corresponding author.
E-mail address: Andreas.Mutzke@ipp.mpg.de (A. Mutzke).

0168-583X/$ - see front matter © 2008 Published by Elsevier B.V.
doi:10.1016/j.nimb.2008.01.053

as well as static and dynamic calculations. SDTrimSP can run on sequential and parallel architectures.

The implantation of gas atoms in the target changes the density as a function of depth and the scattering behaviour inside the solid and has, therefore, an influence on the collision cascade on the depth profile and on sputtering.

The gas atoms are handled in the usual way, but due to their low binding energy (nearly zero for noble gases) they can more easily be sputtered. This leads to the result that the gas concentration near the surface (depth smaller than the mean range of the implanted ions) is lower than in deeper layers.

The effect of outgassing in the former program TRIDYN was realised by the reemission of atoms, namely the removal of atoms from the target without any transport of these atoms through the surface. In this case the knowledge of the maximum atomic fraction of the noble gas content in the solid is required for their removal.

One possibility of gas transport in the solid is diffusion. The diffusion flux, J, through a surface with a diffusion-coefficient, D, is:

$$J = -D \times \frac{\partial c}{\partial x}, \tag{1}$$

where c is gas impurity concentration and x the depth. The time dependent change of the concentration is:

$$\frac{\partial c}{\partial t} = -D \cdot \frac{\partial^2 c}{\partial x^2}. \tag{2}$$

Another alternative is the direct transport of gas driven from the pressure and density, respectively.

The outgasing flux, J, through a surface with a transport coefficient, K, is:

$$J = -K \cdot c \tag{3}$$

and the corresponding time dependence of the concentration:

$$\frac{\partial c}{\partial t} = -K \cdot \frac{\partial c}{\partial x}. \tag{4}$$

A time dependence is simulated by a fluence dependence. At each fluence step a certain amount of gas atoms is moved to the upper layer (in direction to the surface). The amount is dependent on the concentration c of gas atoms (atoms per volume) in the layer and an outgassing coefficient K. This coefficient can be determined by a comparison with experimental data.

3. Results

The best experimentally documented system is the case of Xe bombardment of Si [3]. This example will be discussed below in more detail. At 140 keV, Xe is deposited at larger depths at zero than at increasing Xe fluence due to the larger scattering of Xe compared with Si. The reflection of Xe is negligible, because the particle reflection coefficient is nearly zero at low fluences and increases to the order of 10^{-4} at steady state.

For a better understanding of the influence of the diffusion and/or outgassing process three examples are considered: (1) no diffusion and no outgassing, $D = 0$, $K = 0$, (2) no diffusion, $D = 0$, $K = K_s$ and (3) no outgassing, $D = D_s$, $K = 0$. The coefficients K_s and D_s for Xe

$$K_s\,(\mathrm{Xe}) = 100 \times 10^{24}\ \mathrm{cm}^3/\mathrm{ion}, \tag{5}$$

$$D_s\,(\mathrm{Xe}) = 20 \times 10^{36}\ \mathrm{cm}^4/\mathrm{ion}, \tag{6}$$

were determined by a comparison with experimental steady state data (the reason for the subscript s in K_s and D_s), see Fig. 1. For 140 keV Xe into Si K_s was determined in such a way, that the areal density at steady state is equal to the experimental result. For He, Ne and Ar the determination of K_s was performed according to the equation

$$K_s(x) = K_s\,(\mathrm{Xe}) \cdot \frac{\mathrm{density}\,(x)}{\mathrm{density}\,(\mathrm{Xe})} \tag{7}$$

with x = He, Ne, Ar.

Measurements of the areal densities at steady state at different incident energies justify the procedure of the K_s determination for Xe and Ar; for He and Ne the same procedure is assumed to be correct.

The calculated values for the areal density of the implanted Xe show exactly the same result as in [3], see Fig. 1, for the case of negligible diffusion, $D = 0$ and $K = K_s \neq 0$, whereas, the other two examples do not agree with the experimental findings. This result is expected since the diffusion of Xe in Si is regarded to be small. An interesting point is the occurrence of a maximum in the areal density at a fluence of about 7×10^{16} atoms/cm^2.

The calculated results for the sputtering yield show good agreement with the experimental values [3], see Fig. 2, for the same case of negligible diffusion as in Fig. 1. The increased scattering in the Si target due to the Xe implantation leads to an increase in the sputtering yield of Si with

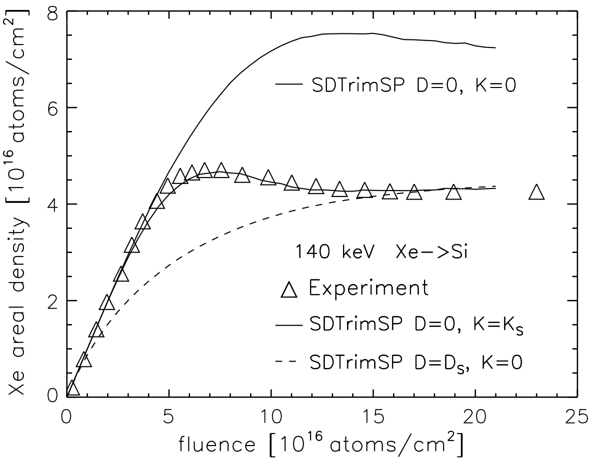

Fig. 1. Calculated areal density of implanted Xe versus the incident fluence compared with experimental data [3]. Si is bombarded with 140 keV Xe at normal incidence.