INFLUENCE OF INTRODUCED ATOMS ON THE COEFFICIENTS OF SPLITTING Si AND SiO$_2$/Si

M.B. Yusupjanova[1], M.N. Raxmatov[1], F.G. Djurabekova[2], D.A. Tashmuhamedova[1]

[1]Department "Instrument-Making", Tashkent State Technical University, st. Universitetskaya, 2, Tashkent, Uzbekistan, ftmet@rambler.ru
[2]Department of Physics, P.O. Box 64, FIN-00014 University of Helsinki, Finland

We have previously obtained epitaxial films of metal silicides by implantation of Ba$^+$, Na$^+$, Co$^+$ ions in Si followed by thermal heating [1, 2]. The process of ion implantation is always accompanied by ion scattering, sputtering and changes in the composition of surface layers. These changes depend on the type of ion and substrate material, on the energy and dose of ions, and on the angle of incidence of ions. These processes in the region of low ion energies (E$_0$ ≤ 5 keV) are currently little studied both experimentally and theoretically. The purpose of this work was to study the effect of embedded Ba atoms on the sputtering coefficient of the silicon surface and to study the effect of ion bombardment on the destruction of a thin oxide film formed on the Si surface.

The bombardment of pure Si and Si with an oxide film was carried out by Ba$^+$, Si$^+$ and Ar$^+$ ions with an energy E$_0$ = 0.5 – 5 keV perpendicular to the surface under vacuum no worse than 10^{-5} Pa. The composition of the surface and near-surface layers was studied by Auger electron spectroscopy (AES). The profiles of the distribution of atoms over the depth were determined by the method of AES in combination with the etching of the surface by Ar$^+$ ions with E$_0$ = 3 keV [3].

Calculations were performed using static models and algorithms developed by T.S.Pugacheva, where a dynamic Monte Carl model CASNEW-D was used [4, 5]. In this model, the change in the concentrations of all components (including the implanted impurity) in each layer of thickness on the order of the interatomic distance is considered.

In Fig. 1 shows the experimental and calculated profiles of the distribution of Ba atoms in Si for Si implanted by Ba$^+$ ions with E$_0$ = 1 keV at doses of D = 5 × 10^{15}, 10^{16} and 8 × 10^{16} cm^{-2} [6]. It can be seen that as the dose increases, the distribution tends to stepwise. The experimental results showed that starting from D = 2 × 10^{16} cm^{-2} with increasing ion dose, the Ba concentration increases slightly only at and near the surface. At high irradiation doses, saturation occurs. In calculations, saturation begins with D = 4 × 10^{16} cm^{-2}, and in the experiment with D = 8 × 10^{16} cm^{-2}. Rough calculations performed according to formula

$$C_{limit} = \frac{1-k_p}{1-k_p+r} \tag{1}$$

Showed that at E$_0$ = 1 keV and r = 0.6, the value of C_{limit} = 0.58 (58 at.%), Which closely corresponds to the exact calculation (C$_{Ba}$ = 52 at.%) And experimental data (C$_{Ba}$ = 49 at.%) . Where r is a dimensionless coefficient whose value lies in the range 0.5-1 and k$_p$ is the reflection coefficient.

In the case of the SiO$_2$/Si system, the cascades of atomic collisions lead to the destruction of the oxide film due to the rupture of Si-O bonds, sputtering, and the transition of some oxygen atoms to the substrate. In the presence of an oxide film on the silicon surface, the energy lost by a fast ion in the surface layer is less than in the absence of a film because of a less efficient energy exchange between atoms of different masses.

Based on computer calculations, it is possible to estimate the effect of the destruction of the oxide film due to the formation of cascades of atomic collisions. The average number of destroyed molecules of SiO$_2$ ($\bar{R}$) per ion is equal to the sum:

$$\bar{R} = Y_0 + F_{O \to Si} + Z_{Si \to O} + I_0 \tag{2}$$

Here, Y$_0$ is the partial atomization coefficient of oxygen, F$_{O \to Si}$ is the number of oxygen atoms transferred from the film to the substrate, Z$_{Si \to O}$ is the number of oxygen substitutions by Si atoms, I$_0$

is the number of knocked out oxygen atoms that formed insertion defects in the film SiO_2. Since the energy of these atoms more than an order of magnitude higher than the energy of thermal motion, they easily migrate to the surface and can be desorbed.
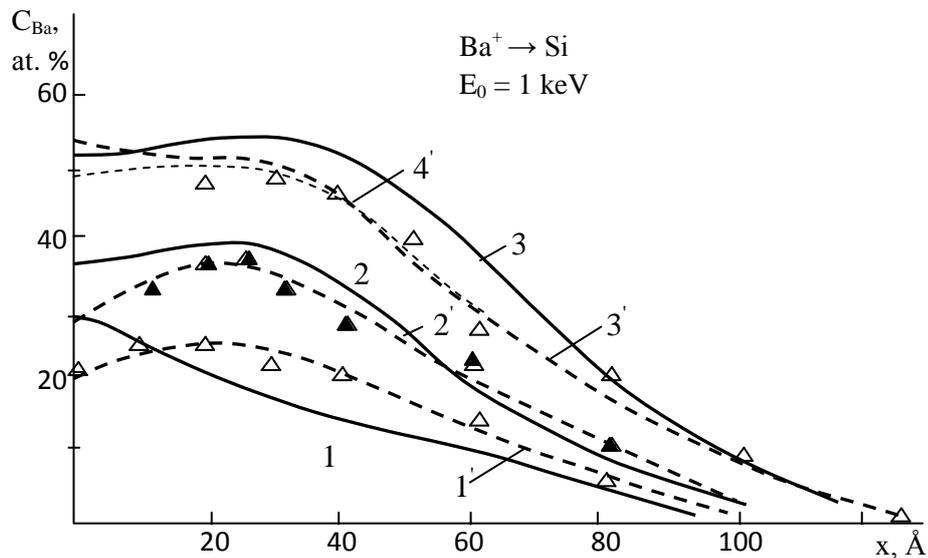

Fig. 1. Calculated (1' – 3') and experimental (1 – 3) dependences of the atomic concentration of Ba in the depth of Si for $E_0 = 1$ keV at doses D, cm^{-2}: 1, 1' – $6 \cdot 10^{15}$, 2, 2' – 10^{16}, 3, 3' – $2 \cdot 10^{16}$, 4' – $8 \cdot 10^{16}$.

The calculations showed that the dependence of the number of destroyed molecules $\overline{R}$ on the ion energy for thin oxide films turns out to be weak in the region $E \geq 1$ keV. The formation of a thermal peak in the cascade zone can lead to thermal decomposition of SiO_2 and desorption of oxygen.

The profiles of the distribution of Ba atoms over the Si depth for Si implanted by Ba ions with $E_0 = 1$ keV at different doses were studied. It is shown that theoretical calculations performed using static models and algorithms are in good agreement with the experimental data.

It is shown that, in the presence of an oxide film on the Si surface, cascades of atomic collisions lead to the destruction of the oxide film due to the rupture of the Si-O bonds, sputtering, and the transition of some of the oxygen atoms to the substrate.

Literature

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