About precipitation of carbon ions on boundary between silicon oxide and silicon during implantation.

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From results of ref. [1] follows, that SIMOX oxide density depends on ion beam energy. The connection of this dependence with the solid state equation is obvious. In ref. [2] the linear connections of density, pressure and refractive index of silicate basalt glasses is shown. Further we simulate experiment [3] and we interpret it.

In the ref. [3] was investigated process of 100 keV carbon ions implantation in a silicon target with thermal and SIMOX oxides at temperature 1030 C. The experiences on an irradiation were carried out by a current 1.5 $\mu A/cm^2$ up to dozes $5*10^{16}$ and $2.5*10^{17}$ cm^{-2}. As a target were chosen commercially accessible (001) SIMOX wafers after two hours in a dry atmosphere at 1000 C. The distribution of the introduced atoms on depth has the brightly expressed correlation with borders between silicon oxides and silicon. The layers of silicon carbide by thickness 40 A, 65 A and 100 A, 360 A for external, internal borders and two dozes of an irradiation accordingly are received.

For an explanation of effect carbon ions precipitation to boundary between silicon oxide and silicon [3] we modify model [4,5].

$$\partial n_a / \partial t = D_a \partial^2 n_a / \partial x^2 - n_a n_v k_{cap} + n_c n_d k_{act} - n_a(x_1 + x_0)/\tau_{1cap} -$$

$$- n_a(x_2 + x_0)/\tau_{2cap} + j_0 \exp(-(R_p - x + x_0)^2 / 2\Delta R_p^2) / \sqrt{2\pi}\, \Delta R_p \quad (1)$$

$$\partial n_c(x,t)/\partial t = n_a n_v k_{cap} - n_c n_d k_{act} \quad (2)$$

$$\partial n_d/\partial t = D_{dv} \partial^2 n_d/\partial x^2 - n_c n_d k_{act} - n_v n_d k_{ann} + j_0 N \sigma_d \Theta(R_p - x + x_0) \quad (3)$$

$$\partial n_v/\partial t = D_{dv} \partial^2 n_v/\partial x^2 - n_a n_v k_{cap} - n_v n_d k_{ann} + j_0 N \sigma_d \Theta(R_p - x + x_0) \quad (4)$$

$$\partial n_1(t)/\partial t = n_a(x_1 + x_0)/\tau_{1cap} \quad (5)$$

$$\partial n_2(t)/\partial t = n_a(x_2 + x_0)/\tau_{2cap} \quad (6)$$

$x_0 = -v_b t$, $N = 5.04*10^{22}$ cm^{-3}, $\sigma_d = 3.52*10^{-16}$ cm^2, $R_p = 2711$ A, $\Delta R_p = 658$ A, $x_1 = 1460$ A, $x_2 = 3060$ A, $j_0 = 1.5$ $\mu A/cm^2$. The values of free parameters of model (D_a, D_{dv}, k_{cap}, k_{act}, k_{ann}, τ_{1cap}, τ_{2cap}) were selected by a method of the least squares so that in the best way to correspond to experimental structures. The results of calculations are given in the table together with Arhenius enthalpys at effective temperature of a substrate.

We suppose two stage precipitation of carbon to the oxygen centres. At the first stage the active carbon ion is trapped by vacancy near boundary. At the second stage there is a precipitate formation with probability P_{pre}. Then we have equation $k_{cap}*N_{pre}*P_{pre}=1/\tau_{cap}$. Assuming $1/P_{pre}=3641$ and

$N_{pre}=4.677*(\rho_{oxi}/2.33)*10^{22}\ cm^{-3}$

we receive the consent in parameters at density internal SIMOX oxide equal to $2.6977\ g/cm^3$ and density of external thermal oxide equal to $1.4595\ g/cm^3$.

Summation of our results with results of ref. [1] gives dependences for SIMOX oxide density ρ from oxygen beam ions implantation energy E as

$\rho(E)=\rho_0(1+(E/E_0)^{2/3})$, (7)

where $\rho_0=1.4595\ g/cm^3$ and $E_0=191.1455$ keV (look figure I). Results of ref. [2] together with ours is possible to be present as

$\rho(n)=\rho_0+(n-n_0)/(dn/d\rho)_0$, (8)

where $n_0=1.2982$, $(dn/d\rho)_0=0.2053\ cm^3/g$ and n – refraction index of SiO_2 . Let's notice, that similar (8) expression take place and for refraction index n_{Si} of porous silicon :

$n_{Si}(\rho_{Si})=2.3324+8.5(dn/d\rho)_0(\rho_{Si}-\rho_0)$.

References

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[3] A. Nejim, P.L. Hemment, J. Stoemenos, NIM PR, v. B120, (1996), pp. 129-132.

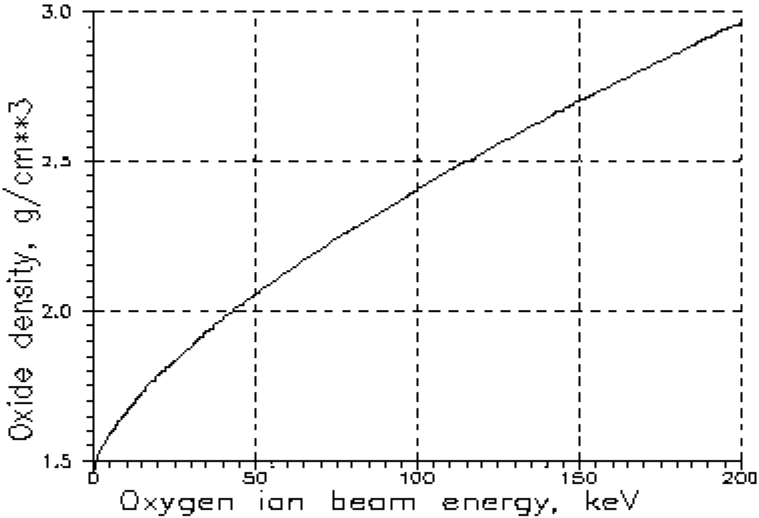
[4] V.A. Starostin , Surface and Coatings Technology , (2002) , vol. 158-159 , pp. 234-237.

[5] P.A. Aleksandrov, E.K. Baranova, V.V. Beloshitsky et. al., Rad. Eff., vol. 88, pp. 249-255, (1986).

Parameter	Value
D_a , 10^{-11} cm^2/s	1.084
D_{dv} , 10^{-11} cm^2/s	0.463
K_{cap} , 10^{-23} cm^3/s	34.848
K_{ann} , 10^{-23} cm^3/s	79.526
K_{act} , 10^{-23} cm^3/s	173.05
τ_{1cap} , s	356.63
τ_{2cap} , s	192.94
H_a , cal/mol	59204
H_{dv} , cal/mol	61405
T_{eff} , K	1304

Table I . Parameters fit results.

Fig. I . SIMOX oxide density (ρ) from oxygen beam ions implantation energy (E) function fit results.


3.0
2.5
2.0
1.5
Oxide density, g/cm**3
0
50
100
150
200
Oxygen ion beam energy, keV