Fundamental Questions of Formation of Thin Buried Layers

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Abstract – In this paper we define dependences for SIMOX oxide density from oxygen ions beam implantation energy. Role of structural phase transitions for ultra thin buried layers formation are discuss.

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

From results of [1] follows, that SIMOX oxide density depends on ion beam energy. The connection of this dependence with the solid-state equation is obvious. In [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 [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 µA/cm² up to dozes 5·10¹⁶ and 2.5·10¹⁷ cm⁻². As a target were chosen commercially (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, 65, 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]:

\[
\frac{dn_1}{dt} = D_1 \partial^2 n_1 / \partial x^2 - n_1 n_2 k_{cap} + n_1 n_2 k_{act} - n_1(n_1 + n_0)\tau_{act} - n_1(n_2 + n_0)\tau_{cap} + f_0 \exp[-(R_p - x + x_0)^2/(2\Delta R_p^2)]/\sqrt{2\pi \Delta R_p^2},
\]

\[
\frac{dn_2}{dt} = D_2 \partial^2 n_2 / \partial x^2 - n_2 n_1 k_{cap} - n_2 n_1 k_{act} + f_0 N_0 \sigma_0 \Theta(R_p - x + x_0),
\]

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\]

where \( n_0 \) = 1.4595 g/cm³; \( E_0 \) = 191.1455 keV (look Fig. 1).

Results of [2] together with ours is possible to be present as

\[
\rho(E) = \rho_0 [1 + (E/E_0)^{2.3}],
\]

where \( \rho_0 = 1.4595 \text{ g/cm}^3 \); \( E_0 = 191.1455 \text{ keV} \) (look Fig. 1).

Table 1. Parameters fit results

<table>
<thead>
<tr>
<th>Parameter Value</th>
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<tbody>
<tr>
<td>( D_{ds} ) 10⁻¹⁰ cm²/s</td>
</tr>
<tr>
<td>( D_{dv} ) 10⁻¹⁰ cm²/s</td>
</tr>
<tr>
<td>( k_{cap} ) 10⁻²³ cm³/s</td>
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<tr>
<td>( k_{act} ) 10⁻²³ cm³/s</td>
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<tr>
<td>( \tau_{max} ) s</td>
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<tr>
<td>( \tau_{max} ) s</td>
</tr>
<tr>
<td>( H_0 ) cal/mol</td>
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<tr>
<td>( H_0 ) cal/mol</td>
</tr>
<tr>
<td>( \mu_0 )</td>
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</tbody>
</table>

We suppose two stage precipitation of carbon to the oxygen centers. 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 \( N_{pre} = 4.677 \times 10^{22} \text{ cm}^{-2} \) we receive the consent in parameters at density internal SIMOX oxide equal to 2.6977 g/cm³ and density of external thermal oxide equal to 1.4595 g/cm³.

Summation of our results with results of [1] gives dependences for SIMOX oxide density \( p \) from oxygen beam ions implantation energy \( E \) as

\[
\rho(E) = \rho_0 [1 + (E/E_0)^{2.3}],
\]

where \( \rho_0 = 1.4595 \text{ g/cm}^3 \); \( E_0 = 191.1455 \text{ keV} \) (look Fig. 1).

Results of [2] together with ours is possible to be present as

\[
\rho(n) = \rho_0 + (n - n_0)/(dn/dp)_0,
\]

where \( n_0 = 1.2982 \); \( (dn/dp)_0 = 0.2053 \text{ cm}^3/\text{g} \); \( n \) is the refraction index of SiO₂.

Notice, that similar (8) expression take place and for refraction index \( n_{Si} \) of porous silicon:

\[
n_{Si}(\rho_{Si}) = 2.3324 + 8.5(dn/dp)_0(\rho_{Si} - \rho_0).
\]
After strong electromagnetic field on porous silicon action, we can change (9) on similar equation:

\[ n_0(\rho_S) = 2.3324 + 7.0(dn/dp)_0(\rho_S - \rho_0). \quad (10) \]

Note, that all formulas for \( n \) are written for the wavelength 6328 Å.

2. Anomalous behavior of hydrogen ions during implantation in beryllium

The investigations have been carried out with samples of pure beryllium of 0.1×1.4×1.4 cm. The samples were placed in a heating cell of the device of the target located in the center of vacuum chamber of the experimental simulating stand and irradiated with hydrogen ions with beam density of current 2.5–3 μA/cm² at 10 keV.

In practice, the whole implanted and captured by vacancies hydrogen remains at the depth up to 0.3 microns. Shown in Fig. 2 are almost similar RBS structures of distribution of hydrogen on depth for a dose 5·10¹⁴ cm⁻² at temperatures of an irradiation 20 and 400°C [6]. In the same figure, their anomalous change (the strong growth of concentration of hydrogen) after an additional irradiation by nitrogen ions with relatively a small doze 1.5·10¹⁴ cm⁻² is shown. For comparison, concentration RBS distributions after ion implantation 10 keV hydrogen in beryllium at 20 and 400°C for dozes 1.7·10¹⁷ and 5·10¹⁴ cm⁻² as presented in [7] are shown in Fig. 3.

Hydrogen depth profiles from [6, 7] was fit by the equation

\[ N_i(x) = N_0\left[(G_1 + G_2) + 0.5(G_3 + G_4)\right], \]

where \( G(x) = \exp[-4(x-x_i)^2/\Gamma^2] \) and parameters values are given in Table 2 for \( E_0 = 10 \) keV H ions (\( R_p = 0.1021, \Delta R_p = 0.0118 \) μm) at 20/400°C beryllium implantation cases (\( j = 2.75 \) μA/cm²).

Unlike depth profiles obtained under other dozes, depth profile at 5·10¹⁷ H/cm² does not vary for 400°C beryllium target implantation case. The attempt is made to understand clearly seen physical analogy between depth profile structure and energy spectrum peaks behavior within the framework of radiation-enhanced diffusion model (see review in [8]).

Assume, that \( E(x) = E_0\left[1 - x/(2R_p)\right] \) and \( N_i(x) \sim \sigma_{upar}(E(x)) \). Increase of hydrogen range twice is caused with orientation effects at ions braking process. Sorted peaks positions are given in Table 3.

The behavior of a resonance in capture cross section of hydrogen by vacancies in beryllium at a doze of implantation 5·10¹⁷ cm⁻² (structural phase transition) seems to us to be similar to that of the first resonance in fission cross section of Cf²⁴⁹ when irradiated strongly polarized neutrons.

Based on processing of experimental data on implantation 10 keV ions of hydrogen into beryllium target, a conclusion is made about formation of abnormal thin (and consequently invisible by RBS) layers with thickness less than 5 nm and very high concentration of hydrogen at a doze 5·10¹⁷ cm⁻² (structural phase transition). The origin of formation of such layers is a strong quadrupole resonance (with two lines of anomalous small width and two lines of small width) in the cross section of a capture of impurity by vacancies.

The general and obvious law is existence of unusual narrow (cold) resonances in a state of structural phase transition of substance or a nucleus.

3. Anomalous behavior of golden ions during implantation in silicon oxide/silicon (100) structure

The samples were irradiated with golden ions Au³⁺ with beam density of current near 0.2 μA/cm² at 3 MeV (\( R_p \sim 1 \) μm) up to doze 6.0·10¹⁵ cm⁻² [9].
After annealing processed at 1050 °C during 2 h second anomalous peak appear ~ 2 μm (with doze \(2.0 \cdot 10^{15} \text{ cm}^{-2}\) in area) [9]. We can see analogy with hydrogen into beryllium implantation case – ultra thin invisible layer on 2\(R_p\) formation. This 2\(R_p\) layer destroy (and visible) only after 1050 °C annealing.

### 4. Conclusion

From our results follows, that SIMOX oxide density depends on ion beam energy. The connection of this dependence (7) with the solid-state equation is obvious. Based on processing of experimental data on ions implantation into targets, a conclusion is made about formation of abnormal thin (and consequently invisible by RBS) layers on 2\(R_p\) for ions doze near structural phase transition. The origin of formation of such layers is a strong resonance in the cross section of a capture of impurity by vacancies.

The general and obvious law is existence of unusual narrow (cold) resonances in a state of structural phase transition of substance or a nucleus.

### References