AMORPHOLISM OF SILICON CRYSTAL WHEN IMPLANTED WITH LIGHT IONS

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ABSTRACT

At present, the accumulation of structural defects and the processes of transition of crystalline silicon to the amorphous state are well studied in [1, 2]. It is established by various physical methods that when ions are implanted in silicon, a large number of vacancy clusters are formed and when fully amorphous, their concentration reaches $3.2\cdot10^{20}$ см$^{-3}$. Various mechanisms have been used to explain this effect: diffusion-coagulation in [3], the result of the accumulation of defects up to the limit concentration in [4], etc. In most of the proposed mechanisms, amorphization is mainly associated with point defects. However, due to the high mobility of the interstitial atoms, the burning of vacancies is more pronounced than the formation of vacancy-type clusters with a concentration of $\sim10^{20}$ см$^{-3}$.
In [5] analyzed the results of experimental and theoretical research and proposed a new mechanism to explain the amorphization of silicon crystal in ion implantation. According to this mechanism, the curvature of the amorphous phase occurs in a disordered area, in which the inelastic energy loss of ions and the formation of point defects do not play a significant role in the amorphization process. Based on this mechanism, it was calculated that the critical dose of silicon amorphization depends on the energy and mass of the light ions being implanted.
In [6] show that the transition dose(TD) of α-β a quartz crystal is determined by the following formula:

$$\varphi_{\alpha-\beta} = \frac{k\varepsilon_0}{\sigma_{yp}\cdot E_{yp}}, \qquad (1)$$

where k=1,5÷2,5 – is the coefficient taking into account the interference of the disordered field (DF) and the return of ions from the crystal surface, the average energy of the "hot atoms" in ε_0-DF is ($\varepsilon_0\approx2$ eV), the effective cross-sectional area of elastic scattered ions with energy transfer from σ_{av} – 10^3 eV to $E_{\max} = \frac{4M_1M_2}{M_1+M_2}E$ to energy, M_1, M_2 - are the masses of ion and target atoms, E_{av} is the average energy transferred when ions collide with the target atom and used to form DF.
In ion implantation, the amorphization of α-quartz consists of two stages: α-β – transition and amorphization in [6].

In the α-β – transition, the vacancies in TD almost "disappear" due to the expansion of the crystal lattice parameters, while the emitted "hot atoms" do not have time to move away from this field and settle in adjacent crystal lattices under high voltage. As the compressed substance expands, the elastic energy obtained in the compression is transferred to the kinetic energy of the atom. Therefore, the pressure in the disordered field that occurs in the β-phase field increases strongly. In this case, the number of "hot atoms" diffusing from the expanded disordered area increases, ie the concentration of "hot atoms" in the disordered area decreases by ~10÷14 %.

The entry of large numbers of 'hot atoms' into the β-phase crystal cell and the occurrence of high pressure leads to the formation of an 'amorphous layer' around the DF. Then the atoms attached to them from DF also do not have a definite structure, i.e. they are amorphous.

If the interference of DF is taken into account, the amorphous dose of quartz is about 2-3 times higher than the α-β –transition dose. The amorphization of silicon is a much more complex process than the phase transitions in α-quartz and depends on the energy, mass, ion current density, target temperature, etc. of the ions. depends on a number of factors in [1-5].

This difference is mainly due to the mobility of the silicon interatomic atoms. When the mobility of the intergranular atoms is not very large, that is, when ions are implanted at low temperatures, the amorphization of silicon takes place approximately the same as in α-quartz. Therefore, the critical dose of silicon amorphization at low temperatures is determined by the following expression:

$$\varphi_{кр} = \frac{2\kappa\varepsilon_0}{\sigma E_{ур}}, \qquad (2)$$

It can be shown that the average energy of ions transmitted to the surface of the elastic scattering section and to the target atoms is determined by the following expressions:

$$\sigma = \frac{C_1}{E^{2/5}}\left(\frac{1}{E_н^{2/5}} - \frac{1}{E_0^{2/5}}\right) + \frac{2q}{\sqrt{E}}\left(\frac{1}{\sqrt{E_0}} - \frac{1}{\sqrt{\lambda E}}\right) + \frac{2q}{E_2}\ln\frac{\sqrt{E_0}\left(E_2+\sqrt{\lambda E}\right)}{\sqrt{\lambda E}\left(E_2+\sqrt{E\cdot E_0}\right)}; \qquad (3)$$

$$E_{ур} = \frac{\frac{B}{E}\ln\frac{E_2+\sqrt{\lambda E}}{E_2+\sqrt{EE_0}} + C_0\frac{E_0^{3/5} - E_н^{3/5}}{E^{2/5}}}{N\sigma}, \qquad (4)$$

here

$$C_1 = \frac{6{,}775\cdot\pi\gamma\cdot Z_1^{5/6}\cdot Z_2^{5/6}}{\left(Z_1^{1/2}+Z_2^{1/2}\right)^{16/15}\cdot 10^{16}}\cdot\left(\frac{M_1}{M_2}\right)^{1/5}; \quad \lambda = \frac{4M_1M_2}{(M_1+M_2)^2}; \quad \gamma = 0{,}95,$$

$$q = \frac{\pi}{8}\cdot\frac{Z_1Z_2\cdot e^2 a_T}{\left(Z_1^{1/2}+Z_2^{1/2}\right)^{2/3}}\cdot\sqrt{\frac{M_1}{M_2}}; \quad E_2 = \frac{\pi}{8}\cdot\frac{Z_1Z_2\left(Z_1^{1/2}+Z_2^{1/2}\right)^{2/3}\cdot e^2}{a_T}\cdot\sqrt{\frac{M_1}{M_2}},$$

$$E_0 \approx \frac{\sqrt{Z_1\cdot Z_2}}{1{,}5}10^3\,эВ, \quad B = 2\pi N Z_1^2 Z_2^2 e^4\cdot\frac{M_1}{M_2}, \quad C_0 = \frac{C_1}{1{,}45}\cdot N, \qquad E_н = 10^3\,эВ,$$

$a_T = 0{,}47 \cdot 10^{-8}$ *см* – In the Thomas-Fermi model, the characteristic size of the atom, Z_1, Z_2 is the sequence number of the ion and the target atom, the number of atoms in the substance N –1 sm^3, the "threshold" energy of TS formation for a silicon crystal $E_n = 10^3$ eV.

In [7] studied the structure of a silicon crystal with implants of H^+, He^+, B^+, N^+, Ar^+ ions with an energy of 100 keV in the dose range $10^{14} \div 10^{17}$ ion/sm^2. It was found that the critical dose of silicon amorphization decreases with increasing mass of bombing ions (from ~10^{17} ion/sm^2 to H^+ to $5 \cdot 10^{14}$ ion / sm^2 for Ar^+).

The authors established that when light ions are implanted, two types of local disordered areas occur simultaneously: amorphous and strongly disordered, but still retain their crystalline structure. When the concentration of "defective crystal spheres" reaches a certain critical dose as a result of subsequent irradiation, such spheres rapidly transition to the amorphous state.

Thus, the experimental results confirm that the amorphization of silicon in the implantation of light ions also consists of two stages: the accumulation and amorphization of TSs of the type "defective crystal spheres".

Table 1 shows the critical doses $\varphi_{кр}$ of silicon amorphization at low temperatures for light ions. In addition, experimental values of the silicon amorphization dose determined by the EPR study method are also given.

The critical dose φ_{kr} of silicon amorphization was assumed to be k = 2 when calculated by the formula (2). The table shows that the critical dose φ_{kr} of silicon amorphization increases with increasing ionic energy and decreases with increasing ionic mass.

As can be seen from the table, the calculation results at low temperatures are well consistent with the experimental results. As the ion energy increases, the adaptation deteriorates.

In our opinion, the increase in the critical dose of amorphization is associated with the following cases: first, one of the main conditions of the phase transition (i.e., amorphization of silicon) is a decrease in density (volume expansion) of the substance in the ion implanted layers of the crystal. As the depth of penetration of the ions increases (i.e., as the energy E increases), the dose required to expand the surface layers also increases. Second, during the implantation of light ions, "burning" of TD-type "defective crystal areas" occurs (i.e., TDs are disrupted by the formation of point defects). As the energy of the ions increases, the probability of "burning of TDs" increases.

Table 1. Critical doses (~100 K) φ_{kr} of silicon amorphization for light ions at low temperatures. ($10^{-15}\varphi_{kr}$ ion/sm^2 units)

Energy *E*, кэВ	H^+		He^+	Li^+	
	$\varphi_{кр}^{наз}$	$\varphi_{кр}^{таж}$ [7]	$\varphi_{кр}^{наз}$	$\varphi_{кр}^{наз}$	$\varphi_{кр}^{таж}$ [8]
200	35,6	-	7,36	3,25	-
180	34,1	-	7,14	3,14	~6,0
150	31,7	-	6,55	2,92	-
100	26,9	~100	5,46	2,48	4,5
80	24,6	-	5,06	2,26	4,2
60	22,0	-	4,40	1,98	2,8
40	19,5	-	3,84	1,71	-
20	14,6	-	2,98	1,35	1,60
10	-	-	2,11	1,14	-

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