

# Carbon saturation of silicon target under the action of pulsed high-intensity ion beam

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**Abstract.** The action of the pulsed high-intensity ion (carbon) beam on the silicon target is investigated by means of the theoretical model. The forming of the carbon concentration profile in depth of the silicon sample is modelled. It is argued, that there are two ways of the profile forming: short-pulsed ion (carbon) implantation and diffusion of the carbon atoms adsorbed on the silicon surface. It is shown, that the carbon atoms adsorbed on the silicon surface and diffused into the silicon target play the main role in the concentration profile forming.

## 1. Introduction

The investigation of influence of the pulsed high-intensity ion (carbon) beams (PHIIB) on the various materials is of interest to many scientific groups [1-6]. By decreasing of the PHIIB energy current (lower than  $10^7$  W/cm<sup>2</sup> [3]) it may be realized the short-pulsed implantation regime (SPIR) without surface melting. The main feature of the SPIR is characterized by rapid heating and cooling-down of the target material. The rapid process leads to high temperature gradient which promotes the diffusion process from the surface into the depth the silicon simple. The diffused particles are the carbon atoms adsorbed on the silicon surface. The sources of the adsorbed atoms can be [2]: i) the explosive plasma formed on the surface of graphite anode; ii) the impurity atoms from the residual atmosphere of the working chamber. In works [6,7] it was proposed that the beam ions penetrating into the simple by means of the ion implantation mechanism do not play a key role in the formation of the concentration profile. The assumption is based on the discrepancy between the integral implantation dose (IID) and the number of impurity ion (NIA) of a carbon: the NIA is much more than number corresponding of the IID in the experiments [6-8].

In present paper we attempt to quantitative theoretical analyze the diffusion effect at the short-pulsed ion implantation under the actions of the pulsed high-intensity ion beams. The analyze will be performed by mean of the model taking into account the rapid heating, cooling-down of the target material and the high temperature gradient producing by the PHIIB.

## 2. The Model

To analyze the diffusion process at the short-pulsed implantation the mathematical model is developed. The model allows the calculation of heating of the silicon target and the transport diffusion processes in the surface layer of the target. When there is the pulse action of PHIIB on the silicon



target, the time evolution of the temperature field  $T(x, t)$  in the depth  $x$  is determined within the framework of the Stefan task solution

$$c_p \rho_m \frac{\partial T(x, t)}{\partial t} = \lambda \frac{\partial^2 T(x, t)}{\partial x^2} + \frac{j_{beam}(t)}{e} [Q_n(x) + Q_e(x)], \quad (1)$$

where  $c_p$  is the specific heat capacity,  $\rho_m$  is the density,  $e$  is the elementary electronic charge,  $j_{beam}(t)$  is the current density function. The energy specific losses at the nuclear  $Q_n(x)$  and the electron  $Q_e(x)$  decelerations can be written as

$$Q_{n(e)}(x) = \frac{1}{\sqrt{2\pi}\Delta R_p} \int_0^{E_0} \frac{S_{n(e)}(E)}{S_{n(e)}(E) + S_{e(n)}(E)} \exp\left\{-\frac{[x - R_p(E_0) + R_p(E)]^2}{2\Delta R_p^2}\right\} dE, \quad (2)$$

where  $R_p$  and  $\Delta R_p$  are the average projected range and standard deviation respectively,  $E_0$  is the energy of beam ions,  $S_n(E)$  and  $S_e(E)$  are the sections of the nuclear and electron decelerations respectively.

The diffusion of carbon under the action PHIIB is described by the relation

$$\frac{\partial N(x, t)}{\partial t} = \frac{\partial}{\partial x} \left\{ D[T_{cd}(x, t)] \frac{\partial N(x, t)}{\partial x} \right\}, \quad (3)$$

where  $N(x, t)$  is the concentration of carbon ions on the depth. The diffusion functional is written as

$$D[T_{cd}(x, t)] = \frac{\omega(r) a_{lat}^2}{2} \exp\left[-\frac{E_{diff}}{k_B T_{cd}(x, t)}\right], \quad (4)$$

where  $a_{lat}$  is the carbon lattice constant,  $k_B$  is the Boltzmann constant. The diffusion activation energy  $E_{diff} = 2.18$  eV was defined as the difference between zero level and minimum of the potential energy  $W(\tilde{r})$  determined by the Tersoff potential [10]

$$W(\tilde{r}) = \frac{1}{2} \sum_{i, j(i \neq j)} f_C(r_{ij}) [f_R(r_{ij}) + f_A(r_{ij})], \quad (5)$$

where  $f_C$ ,  $f_R$ ,  $f_A$  are the cutoff, repulsion and attraction functions respectively,  $r_{ij}$  is the distance between particles. The absolute value of the angular frequency of the collective motion is estimated as  $\omega(\tilde{r}) = [\tilde{m}^{-1} d^2 W / d\tilde{r}^2]^{1/2}$ , where  $\tilde{m}$  is the generalized mass of the ‘‘atom-lattice’’ system. The deformation dependence of the potential energy for carbon and silicon is presented in figure 1.

The temperature dependence of the cooling-down process  $T_{cd}(x, t)$  is characterized by the relation

$$\frac{\partial T_{cd}(x,t)}{\partial t} = \frac{\lambda}{c_p \rho_m} \frac{\partial^2 T_{cd}(x,t)}{\partial x^2}, \quad (6)$$

The boundary condition can be written as

$$T_{cd}(0,t) = T_0 + (T_{ini} - T_0) \exp\left(-\frac{\lambda}{c_p \rho_m d_{Si}^2} t\right), \quad (7)$$

where  $T_{ini}$  is the temperature of the sample surface after the PHIB action,  $d_{Si} = 400 \mu\text{m}$  is the thickness of the silicon sample,  $T_0 = 300 \text{ K}$  is the ambient temperature.

The concentration implantation profile is calculated as follows

$$N_I[\tilde{X}(x,E),t] = \frac{N_{dose}}{\sqrt{2\pi}\Delta R_p(E)} \frac{k_{PRSN}}{\left[1 + \left(\frac{\tilde{X}(x,E)}{a^*}\right)^2\right]^q} \exp\left[-v^* \arctg\left(\frac{\tilde{X}(x,E)}{a^*}\right)\right], \quad (8)$$

where  $k_{PRSN} = 0.2$  is the normalization factor,

$$\tilde{X}(x,E) = [x - R_p(E)] \Delta R_p^{-1}(E), \quad (9)$$

$$a^* = \Delta R_p \sqrt{[16(\eta-1) - \beta_1(\eta-2)^2] / 16}, \quad (10)$$

$$v^* = -\frac{\eta(\eta-2)\sqrt{\beta_1}}{\sqrt{16(\eta-1) - \beta_1(\eta-2)^2}}, \quad (11)$$

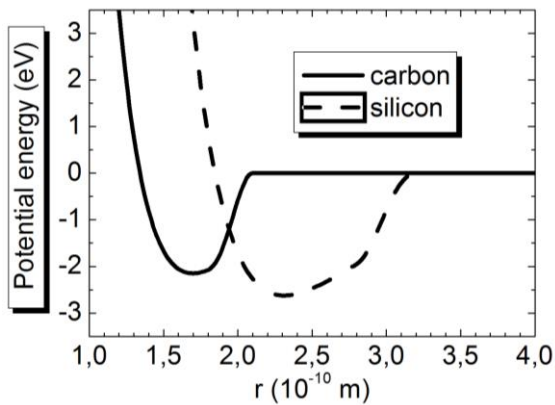
$$\eta = \frac{6(\beta_2 - \beta_1 - 1)}{2\beta_2 - 3\beta_1 - 6}, \quad (12)$$

and parameters are  $\beta_1 = 2.6896$ ,  $\beta_2 = 11.006$ .

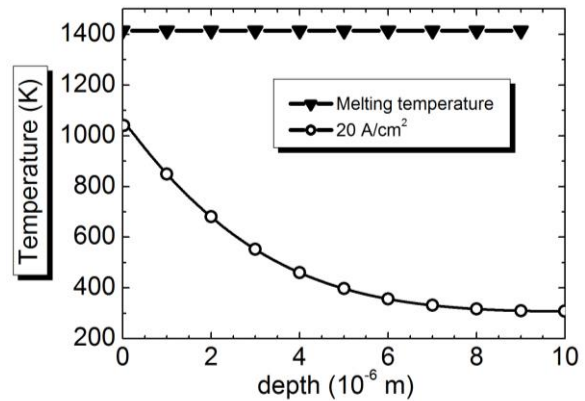
### 3. Results and discussion

The temperature profile calculated after the action (600 pulses) of one pulse is shown in figure 2. The curve at the current density  $20 \text{ A/cm}^2$  (open circles) corresponds to the experimental setup (the range of the beam current density of the TEMP-4 is  $15\text{-}20 \text{ A/cm}^2$ ). It can be seen from figure 2 that the melting processes can be neglected when mass transfer procedure is modelled.

The figure 3 shows the profile formed by the diffusion of the carbon adsorbed on the surface layer into the silicon target and implantation profile. The concentration value  $N_{norm}$  is normalized to the amorphous carbon concentration  $N_{Amorf} = 1.1 \cdot 10^{23} \text{ cm}^{-3}$  (of course,  $N_{norm} = N / N_{Amorf}$ ).

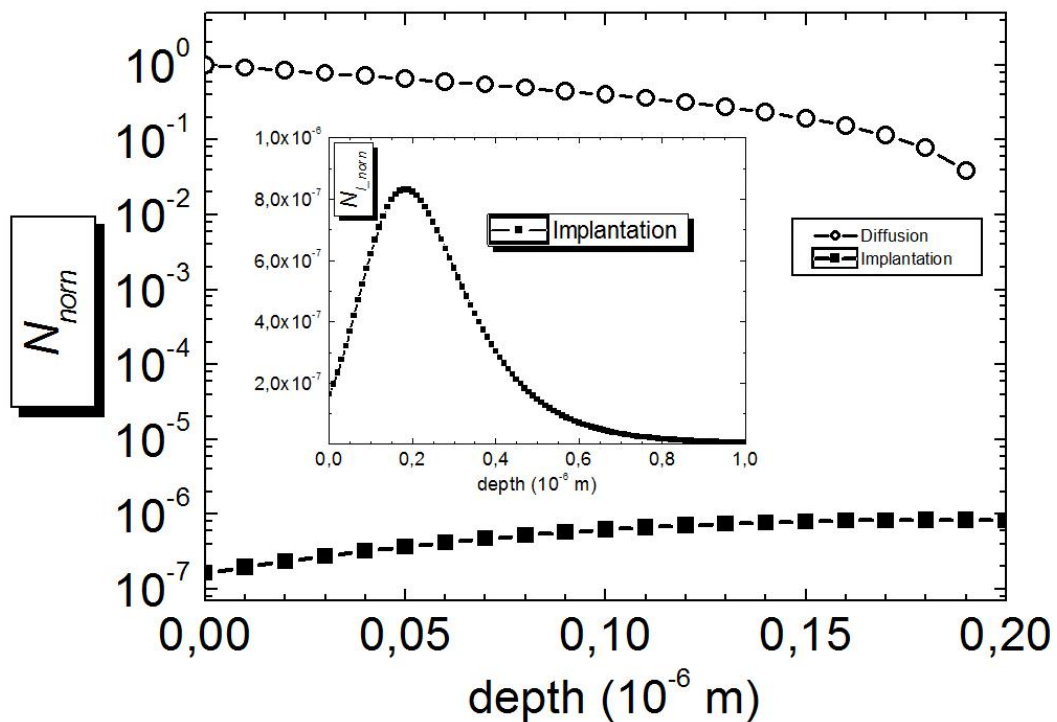


**Figure 1.** Deformation dependence of potential energy for carbon (solid) and silicon (dash)



**Figure 2.** Temperature distribution in depth of silicon target

Inside picture is the same as a dependence (square) on the main picture but it have a wide range of the depth. The discrepancy between the concentration value of the diffusion profile and implantation profile at least tree orders. Consequently, it can be concluded that the carbon saturation in the sub-surface silicon layer occurs by means of the diffusion of carbon adsorbed on the silicon surface. The contribution of the implantation ions to concentration profile is forming insignificant.



**Figure 3.** Concentration profiles: diffusion (circles), implantation (squares).

#### 4. Conclusion

The influence of the pulsed high-intensity ion beam on the silicon is studied by use the developed theoretical model. The input parameters of the model were the settings of the experimental setup of the TEMP-4. It is shown, that at the short-pulsed implantation regime of the TEMP-4 the silicon surface does not melt. However, the regime leads to the high temperature gradient which promotes the diffusion process from the surface into the depth the silicon simple. Thus, it is shown that the carbon atom diffused from the surface make the main contribution to the forming of the concentration profile. The concentration of the implanted carbon ions less more than tree orders compared with the concentration of the diffused carbon atoms.

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