Phosphorus doping of silicon by proton induced nuclear reactions

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We propose a method to dope silicon with phosphorus by means of the nuclear resonant reaction $^{30}\mathrm{Si}(p,\gamma)^{31}\mathrm{P}$, which takes place when a natural silicon target is bombarded with a few MeV proton beam. This alternative method considerably reduces the usual target damage produced by the more commonly used direct phosphorus implantation.

Direct phosphorus ion beam implantation in silicon targets[1,2] has become a well established technique to produce novel microstructures, but in spite of its many advantages the above-mentioned method has some limitations. It needs high energy phosphorus ions to implant them far from the target surface. Furthermore, ion implantation is accompanied by defect production and lattice distortion along the ion trajectory.

In this work we propose an alternative method to obtain phosphorus doped silicon by means of proton induced nuclear resonant reactions. When an energetic proton beam bombards a natural silicon target, the nuclear resonant reaction $^{30}\mathrm{Si}(p,\gamma)^{31}\mathrm{P}$ takes place; in this process, by capturing a proton, the target nucleus $^{30}\mathrm{Si}$ is transmutated into the nucleus $^{31}\mathrm{P}$. So as a final result we have a silicon matrix doped with phosphorus atoms.

The nuclear resonant reactions can only take place within small energy intervals Γ around certain energies E_r (E_r and Γ are called, respectively, the resonance energy and the resonance width of the nuclear reaction). The dependence of the cross section $\sigma(E)$ for the nuclear resonant reaction $^{30}\mathrm{Si}(p,\gamma)^{31}\mathrm{P}$ upon the proton energy can be calculated using the Breit-Wigner formula[3] for the case of a single, isolated resonance,

$$\sigma(E)=\frac{\pi\hbar^2}{4ME}\,\frac{\Gamma S(p,\gamma)}{(E-E_r)^2+\Gamma^2/4}\,, \tag{1}$$

where M and E are the proton mass and energy, respectively, and Γ and $S(p,\gamma)$ represent the total resonance width and the resonance strength, respectively. In obtaining the previous expression we have taken into account that the spins of the incident (proton) and target ($^{30}\mathrm{Si}$ nucleus) particles, are 1/2 and 0, respectively. Equation (1) was evaluated using available experimental data[4] for the nuclear reaction we are considering.

For brevity, in this letter we shall be concerned with the resonance at $E_r=942$ keV, which is the strongest one and appears clearly separated from the first nearest neighbor resonances. So in the rest of the letter we shall limit our discussion to proton beam energies around 1 MeV. A similar discussion could be done for proton energies close to the other resonance energies.

Let us consider a semi-infinite silicon target, with its surface at $x=0$, bombarded by a proton beam with an initial energy E_0 distributed according to the function $g(E_0)$. The number of phosphorus atoms, at the depth interval $(x,x+dx)$, produced per incident proton is

$$N_P(x)=c\;n_{\mathrm{Si}}\int dE\;G[g(E_0);E,x]\;\sigma(E), \tag{2}$$

where n_{Si} is the atomic density of natural silicon and $c=0.031$ is the $^{30}\mathrm{Si}$ abundance[3] in natural silicon. In the previous expression $G[g(E_0);E,x]$ is a functional of $g(E_0)$ and a function of E and x, and it represents the distribution of protons with energy E at the depth x, corresponding to a proton beam with the initial energy distribution $g(E_0)$, and is given by

$$G[g(E_0);E,x]=\int dE_0\;g(E_0)\;F(E_0-E,x), \tag{3}$$

where $F(E_0-E,x)$ stands for the distribution of protons, that having an initial energy E_0, suffer an energy loss (E_0-E) after a path length x; $F(E_0-E,x)$ is the Landau-Vavilov distribution,[5,6] which we take to be of a Gaussian form

$$F(E_0-E,x)=\frac{1}{\delta\sqrt{2\pi}}\exp\left\{-\frac{[(E_0-E)-\bar{E}\,]^2}{2\delta^2}\right\} \tag{4}$$

with $\bar{E}$ and δ representing, respectively, the mean energy loss and the energy loss fluctuation of a proton, with initial energy E_0, after travelling a path x. Then $\bar{E}=x\;S_p(E_0)$ and $\delta^2=x\;\Omega^2(E_0)$, where $S_p(E_0)$ and $\Omega^2(E_0)$ are, respectively, the stopping power and the energy loss straggling of a proton with initial energy E_0.

Only those values of E where the cross section has a relative maximum (i.e., $E=E_r$) will significantly contribute to the integration in Eq. (2). Then we obtain that the phosphorus depth distribution is given by

$$N_P(x)=c\;n_{\mathrm{Si}}\sum_{E_r}\;G[g(E_0);E_r,x]\;\sigma(E_r). \tag{5}$$

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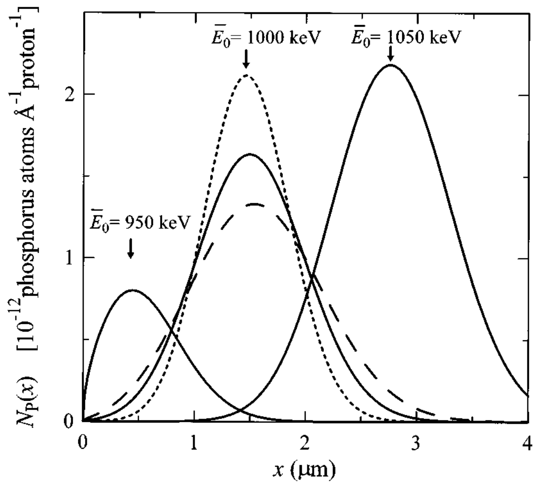

FIG. 1. Phosphorus concentration profile, $N_P(x)$, as a function of the depth x in a natural silicon target. The three solid lines correspond to $\Delta E_0 = 20$ keV, the short dashed line corresponds to $\Delta E_0 = 15$ keV and the long dashed line corresponds to $\Delta E_0 = 25$ keV. The nominal energy of the proton beam is shown on the top of each curve.

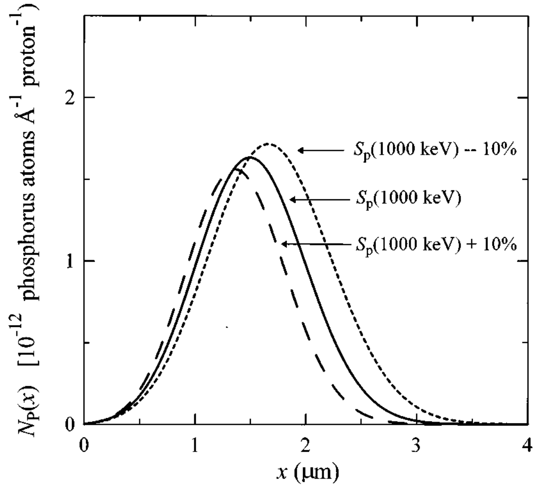

FIG. 2. Phosphorus concentration profile, $N_P(x)$, as a function of the depth x in a natural silicon target. $S_p = 4.5$ eV/Å (long dashed line), $S_p = 4.1$ eV/Å (solid line) and $S_p = 3.7$ eV/Å (short dashed line). The value $\Omega^2 = 1820$ eV^2/Å was kept constant for the three curves.

We use a Gaussian distribution for the proton beam initial energy distribution $g(E_0)$,

$$g(E_0) = \frac{1}{\Delta E_0 \sqrt{2\pi}} \exp\left\{ -\frac{(E_0 - \bar{E}_0)^2}{2(\Delta E_0)^2} \right\}, \tag{6}$$

where $\bar{E}_0$ is the nominal energy of the accelerator and ΔE_0 its energy spread. After some algebra we finally obtain the depth distribution of phosphorus atoms produced per incident proton

$$N_P(x) = c n_{\mathrm{Si}} \sum_{E_r} \sigma(E_r) \left[2\pi \left(1 + \frac{(\Delta E_0)^2}{x\Omega^2(\bar{E}_0)} \right) \right]^{-1/2} \times \exp\left\{ -\frac{1}{2} \frac{[\bar{E}_0 - E_r - x S_p(\bar{E}_0)]^2}{(\Delta E_0)^2 + x\Omega^2(\bar{E}_0)} \right\}. \tag{7}$$

Note that for the proton energies (~ 1 MeV), which is our concern in this letter and not for very thick targets (a few micrometers), only an isolated resonance (at $E_r = 942$ keV) will contribute to the summation over E_r in Eq. (7). We would need to include further resonance energies in the case of thicker targets or higher proton energies.

We shall center our discussion in the case of a proton beam with a nominal energy $\bar{E}_0$ around 1000 keV, and with an energy spread ΔE_0 around 20 keV. In Fig. 1 we show how the phosphorus depth distribution, $N_p(x)$, behaves when small variations take place in the parameters that initially characterize the proton beam: the accelerator nominal energy, $\bar{E}_0$, and the energy spread, ΔE_0. The proton stopping power we use for $\bar{E}_0 = 1000$ keV is $S_p(1000 \text{ keV}) = 4.1$ eV/Å.[7] For the energy loss straggling we use the Bohr straggling,[8] which is independent of the proton energy, and is given by $\Omega_{\mathrm{B}}^2 = 4\pi Z_1^2 e^4 n_{\mathrm{Si}} Z_2 = 1820$ eV^2/Å, where Z_1 and Z_2 are the projectile (proton) and target (silicon) atomic numbers, and e is the electronic charge. The solid curves correspond to the phosphorus concentration profile, $N_p(x)$, when the initial proton energy $\bar{E}_0 = 1000$ keV varies in $\pm 5\%$, i.e., $\bar{E}_0 =$ 950, 1000, and 1050 keV; and the proton energy spread remains constant at $\Delta E_0 = 20$ keV. For each value of these $\bar{E}_0$ we evaluated $S_p(\bar{E}_0)$ as stated in Ref. 7, and the value of the energy loss straggling was kept constant at Ω_B^2. We observe that as $\bar{E}_0$ increases the phosphorus doping profile is deeper, the concentration of phosphorus is higher and the profile broadens. So, the total number of phosphorus atoms doping the silicon matrix increases as $\bar{E}_0$ increases. The discontinuous curves illustrate the influence of the initial proton energy beam spread ΔE_0 on the phosphorus depth distribution. Now, the initial proton beam energy is kept constant at $\bar{E}_0 = 1000$ keV and ΔE_0 takes the values 15 keV (short dashed line) and 25 keV (long dashed line). We can appreciate that the uncertainties of $\pm 25\%$ in the initial energy spread produce a variation in the maximum value of $N_p(x)$, but do not affect appreciably its position, and the total number of phosphorus produced in the silicon target does not vary significantly (the areas under each one of the three curves corresponding to $\bar{E}_0 = 1000$ keV are practically the same). For a given value of $\bar{E}_0$, smaller values of the spread ΔE_0 of the proton beam energy produce sharper phosphorus profiles. Therefore the main parameter to control the depth concentration of phosphorus doping atoms is the initial energy of the proton beam, $\bar{E}_0$.

We have also evaluated the phosphorus depth concentration profile, $N_P(x)$, for typical variations of the proton energy loss magnitudes, S_p and Ω^2; the parameters that characterize the incident beam are kept constants at $\bar{E}_0 = 1000$ keV and $\Delta E_0 = 20$ keV, and the reference values for S_p and Ω_B^2 are those introduced previously: 4.1 eV/Å and 1820 eV^2/Å, respectively. In Fig. 2 we show the phosphorus depth distribution when considering typical variations ($\pm 10\%$) from that value of S_p. We can see that as S_p decreases the protons suffer the 942 keV nuclear resonant reaction farther from the target surface, and the phosphorus profile shifts toward deeper distances. The maximum value and the width of $N_P(x)$ also increase when S_p decreases, but only slightly. Although not shown in Fig. 2 we have also considered the effects on $N_P(x)$ of a variation of $\pm 25\%$ in Ω^2 around the Bohr straggling value, Ω_B^2. In this case, the position of the peak in the phosphorus distribution does not change because the stopping power is the same for the three cases depicted, but its height and its width increase for higher values of the straggling; then the total number of phosphorus atoms produced in the silicon target increases when Ω^2 increases.

In conclusion, we have shown that phosphorus atoms can be produced in a silicon sample when it is bombarded with a few MeV proton beam, due to the $^{30}Si(p,\gamma)^{31}P$ resonant nuclear reaction that takes place. This method offers an alternative procedure to the usual direct phosphorus implantation. It has the advantage of reducing the damage produced in the sample, since a light projectile is used instead of a medium-mass one. The characteristics of the dopant distribution are mainly governed by the nominal energy of the incident proton beam, $\bar{E}_0$, which determines the stopping power and energy loss straggling of the target, and also by the energy and width of the nearest resonance to $\bar{E}_0$, such that $E_r < \bar{E}_0$. In most cases the phosphorus depth distribution has an almost Gaussian shape with a broad width, compared to the narrow and asymmetric distributions obtained by direct phosphorus ion bombardment. It is worth to note that a few percent variation of the proton beam energy, $\bar{E}_0$, affects in an appreciable manner the phosphorus distribution width.

From Figs. 1 and 2 (and their respective comments) it can be seen that it is possible to choose the idoneous initial conditions of the proton beam to obtain a desired doping profile (sharper or broader, closer or farther to the target surface, etc.).

The results presented in this letter concern to individual resonances. If a thick silicon target is irradiated by protons with sufficiently high energy, there is the possibility to create simultaneously several dopant layers at fixed relative distances, depending upon the resonance energies.

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