

## **DIFFUSION IN SEMICONDUCTORS BY USING LAPLACE'S INTEGRAL TRANSFORM TECHNIQUE**

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### **Abstract**

A theoretical approach to study diffusion in semiconductors is introduced. A mass-energy model for diffusion atoms into target materials has been built up. The diffusion equation written in terms of the incident atom current density (fluence) is introduced. Laplace's Integral Transform Technique is applied to get the solution. The concentration function is obtained using Fick's first law that relates the mass transport with the concentration gradient, together with a flux balance equation. Computations for the case of time-independent incident atomic flux of different values of Phosphorus, Gallium, Indium and Arsenic diffused into

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Silicon target material are given as illustrative examples. Results show that the penetration depth of Phosphorus atoms into Silicon is much greater than that for Indium atoms, while the concentration atoms of Phosphorus atoms in Silicon is much less than that for Indium atoms. The same behavior is shown with respect to Arsenic and Gallium atoms diffused in Silicon target.

## 1. Introduction

It is well known that the selective introduction of impurities (dopants) into semiconductors and most materials by diffusion or ion implantation leads to changes in their chemical, physical, and electronic properties [1, 2]. The structure and the electrical conductivity may also be modified.

This topic has aroused the interest of many researchers due to its important applications, such as in the production of electronic devices.

Doping by diffusion is still one of the acceptable processes that have important technological applications [3, 4], such as the fabrication of the integrated circuits (IC) that forms the basis of many of the solid state device technology.

It is also useful in the preparation of alloys which possess low surface energy in the metallic surface [5]. This makes it possible to realize dropwise condensation mode on such surfaces, which has vital technological applications. Doping permits the freedom to design the desired activation energy of a dopant in a semiconductor [6]. Silicon is the main n-type dopant used in GaAs, and it is usually incorporated into GaAs by ion implantation or by diffusion employing an external source [7].

In practice, the diffusion process consists of deposition followed by diffusion (driven-in process). The development of the theoretical studies of atomic diffusion is still of great interest [8-11].

The diffusion of Boron and Phosphorus into Silicon has been investigated by the statistical moment method (SMM). A mass transfer model for doping a metal target at elevated temperatures has been built up [12] based on transport of ions in matter and radiation enhanced diffusion. The process was simulated by a dynamic Monte Carlo (MC) method to calculate the concentration-depth profiles.

In the present trial, single step diffusion is considered, where a semiconductor substrate is exposed to high concentrations of the desired impurity exceeding the level required to achieve solid solubility of the dopant at the semiconductor surface.

The aim of the present trial is to solve the parabolic diffusion equation written in terms of the current density  $J(x, t)$  of atoms rather than the concentration, together with Fick's first law and a flux balance equations. The solution is obtained analytically using Laplace integral transform technique. As illustrative examples, the obtained concentration-depth functions are computed for the diffusion of Phosphorus, Gallium, Indium and Arsenic atoms into Silicon target material. Comparison between these cases is also considered.

## 2. Mathematical Formulation of the Problem

In setting up the problem, it is assumed that a beam of impurity atoms (Phosphorus, Gallium, Indium and Arsenic) of flux density  $J_0(\text{m}^{-2} \text{sec}^{-1})$  falls normally on the front surface of the material target (Silicon) along the  $x$ -axis direction where it is partly reflected and partly driven-in into the target slab. This part is of amount  $A j_0(\text{m}^{-2} \text{sec}^{-1})$ , where,  $A = (1 - R(T))$  stands for an equivalent absorption coefficient that depends in general on the energy ( $E$ ) of the impinging atom. It may depend also on the absolute temperature  $T$  of the front surface,  $R(T)$  is the reflectivity of the front surface. It is suggested also that the impurity atoms are supplied from an undiminished infinite source for the entire duration of diffusion process [13]. This driven-in part will be redistributed within the target wafer.

The concentration function  $C(x, t)$  of such dopant extends till a penetration depth  $\delta(t)$  after which this function vanishes, i.e., the diffusion process stops at this limit.

The mathematical formulation of such a problem is given as follows:

The parabolic diffusion equation can be written in the form

$$\frac{\partial J(x, t)}{\partial t} = D \nabla_x^2 J(x, t), \quad 0 \leq x \leq d, t > 0, \quad (1)$$

where

$D(\text{m}^2/\text{sec})$  is the diffusion coefficient.

Equation (1) is subjected to the following conditions

(i) At  $t = 0$ ,  $J(x, 0) = 0$ ,

(ii) At  $x = 0$ ,  $J(0, t) = J_0(1 - R)$ ,

(iii) At  $x = \delta$ ,  $J(\delta, t) \rightarrow 0$ , and

(iv)  $C(\delta, t) \rightarrow 0$ .

$J_0(\text{m}^{-2} \text{sec}^{-1})$  is defined as the number of the incident atoms per unit area per second,  $C(x, t)(\text{m}^{-3})$  is the concentration of the doped atoms at the boundary  $x$  at time  $t$  measured from the beginning of the exposure time.

Equation (1) can be rewritten in the form

$$\nabla_x^2 J(x, t) = \frac{1}{D} \frac{\partial J(x, t)}{\partial t}. \quad (2)$$

Taking Laplace transform of equation (2) with respect to the time variable  $t$  gives

$$\frac{d^2}{dx^2} \bar{J}(x, s) = \frac{1}{D} [s\bar{J}(x, s) - J(x, 0)], \quad (3)$$

where  $\bar{J}(x, s)$  is the Laplace transform of the function  $J(x, t)$ .

The initial condition (i) makes it possible to write equation (3) in the form

$$\frac{d^2}{dx^2} \bar{J}(x, s) = \frac{s}{D} \bar{J}(x, s). \quad (4)$$

The solution is written in the form

$$\bar{J}(x, s) = Ae^{\sqrt{\frac{s}{D}}x} + Be^{-\sqrt{\frac{s}{D}}x}. \quad (5)$$

The Laplace transform of the boundary condition (ii) for  $J_0 = \text{constant}$  gives

$$\bar{J}(0, s) = \frac{J_0(1 - R(T))}{s}. \quad (6)$$

Substituting (6) into (5) at  $x = 0$ , one gets

$$A + B = \frac{J_0(1 - R(T))}{s}. \quad (7)$$

Similarly, the Laplace transform of the boundary condition (iii) gives

$$\bar{J}(\delta, s) = 0. \quad (8)$$

Substituting equation (8) into equation (5) at  $x = \delta$ , one gets

$$Ae^{\sqrt{\frac{s}{D}}\delta} + Be^{-\sqrt{\frac{s}{D}}\delta} = 0. \quad (9)$$

Solving simultaneously, equations (7) and (9), one gets

$$A = -\frac{J_0(1-R(T))}{2s \sinh\left(\sqrt{\frac{s}{D}}\delta\right)} e^{-\sqrt{\frac{s}{D}}\delta} \quad (10)$$

and

$$B = \frac{J_0(1-R(T))}{2s \sinh\left(\sqrt{\frac{s}{D}}\delta\right)} e^{+\sqrt{\frac{s}{D}}\delta}. \quad (11)$$

Substituting equations (10) and (11) into equation (5), one gets the solution in the form

$$\bar{J}(x, s) = \frac{J_0(1-R(T))}{2s \sinh\left(\sqrt{\frac{s}{D}}\delta\right)} \left[ e^{\sqrt{\frac{s}{D}}(\delta-x)} - e^{-\sqrt{\frac{s}{D}}(\delta-x)} \right], \quad (12)$$

$$\bar{J}(x, s) = \frac{J_0(1-R(T))}{s \sinh\sqrt{\frac{s}{D}}\delta} \left[ \sinh\sqrt{\frac{s}{D}}(\delta-x) \right]. \quad (13)$$

$J(x, t)$  is obtained by using the inverse Laplace transform of equation (13) (standard tables [14, 15]), in the form

$$\begin{aligned} & J(x, t) \\ &= J_0(1-R(T)) \left[ \frac{\delta-x}{\delta} + \frac{2}{\pi} \sum_{n=1}^{\infty} \left( \frac{(-1)^n}{n} \right) \left( e^{-D\left(\frac{n\pi}{\delta}\right)^2 t} \sin \frac{n\pi(\delta-x)}{\delta} \right) \right]. \end{aligned} \quad (14)$$

### 3. Determination of the Concentration Function $C(x, t)\text{m}^{-3}$

Considering Fick's first law

$$J(x, t) = -D\nabla C(x, t). \quad (15)$$

Thus

$$\int_{c(0, t)}^{c(x, t)} dC(x, t) = -\frac{1}{D} \int_0^x J(x, t) dx. \quad (16)$$

From equations (14) and (16) one gets

$$C(x, t) = C(0, t) - \frac{J_0(1 - R(T))}{D} \times \left[ \left( x - \frac{x^2}{2\delta} \right) + \sum_{n=1}^{\infty} \frac{(-1)^n 2\delta}{n^2 \pi^2} e^{-D \left( \frac{n\pi}{\delta} \right)^2 t} \left( \cos \frac{n\pi(\delta - x)}{\delta} - \cos n\pi \right) \right]. \quad (17)$$

Moreover, let us consider the balance equation for the particle flux density written in the form

$$\int_0^t J_0(1 - R(T)) dt = \int_0^{\delta} C(x, t) dx. \quad (18)$$

Substituting equation (17) into equation (18), gives the expression for  $C(0, t)$  in the form

$$C(0, t) = \frac{1}{\delta} \int_0^t J_0(1 - R(T)) dt + \frac{J_0(1 - R(T))}{D} \left[ \left( \frac{\delta}{3} \right) - \sum_{n=1}^{\infty} \frac{2\delta}{n^2 \pi^2} e^{-D \left( \frac{n\pi}{\delta} \right)^2 t} \right]. \quad (19)$$

The concentration function  $C(x, t)$  can be obtained by substituting (19) into (17) in the form

$$C(x, t) = \frac{1}{\delta} \int_0^t J_0(1 - R(T)) dt + \frac{J_0(1 - R(T))}{D} \left[ \left( \frac{\delta}{3} - x + \frac{x^2}{2\delta} \right) - \sum_{n=1}^{\infty} \frac{(-1)^n 2\delta}{n^2 \pi^2} e^{-D \left( \frac{n\pi}{\delta} \right)^2 t} \cos \frac{n\pi(\delta - x)}{\delta} \right]. \quad (20)$$

#### 4. Determination of the Diffusion Penetration Depth $\delta(m)$

Using the boundary condition (iv) at  $x = \delta$  in equation (20) one gets

$$0 = \frac{1}{\delta} \int_0^t J_0(1 - R(T))dt + \frac{J_0(1 - R(T))}{D} \left[ \left( -\frac{\delta}{6} \right) - \sum_{n=1}^{\infty} \frac{(-1)^n 2\delta}{n^2 \pi^2} e^{-D \left( \frac{n\pi}{\delta} \right)^2 t} \right]. \quad (21)$$

Considering the order of the terms in equation (21), one can neglect the term

$\sum_{n=1}^{\infty} \frac{(-1)^n 2\delta}{n^2 \pi^2} e^{-D \left( \frac{n\pi}{\delta} \right)^2 t}$  with respect to  $\left| \frac{\delta}{6} \right|$ . Thus one finally gets the diffusion penetration depth function as

$$\delta \equiv \sqrt{6Dt}. \quad (22)$$

#### 5. Computations

Computations are carried out according to values in Table 1, considering constant incident particle flux  $J_0 = 5 \times 10^{15} \text{ m}^{-2} \text{ sec}^{-1}$ ,  $D = D_0 \text{Exp}(E_v / kT)$   $\text{m}^2 \text{ sec}^{-1}$  and  $R(T)$  for silicon  $= 0.322 + 3.12 \times 10^{-5} T$ ) [16] in the range (300 K - 1685 K).

**Table 1.** The values of  $D_0$ ,  $E_v$  for the diffused elements of Phosphorus, Gallium, Indium and Arsenic diffused into Silicon target material [17]

Parameters Element	$D_0$ , $\text{m}^2/\text{sec}$	$E_v$ , eV
Arsenic	3.2 E-5	3.56
Phosphorus	3.0 E-4	3.68
Indium	16 E-4	3.9
Gallium	3.6 E-4	3.51

It is suggested that the relative size of the dopant atom relative to the host medium atoms plays also an important role in the diffusion process. Table 2 gives the size of the impurity Gallium and Indium atoms relative to Silicon [18].

**Table 2.** Size of some impurity atoms relative to Silicon [18]

Element	Size relative to Silicon
Gallium	1.07
Indium	1.22

The electron configuration of neutral atoms in their ground states is related also to the size of the diffused atoms.

**Table 3.** The outer configuration for some neutral atoms in their ground states

Element	Electron configuration
Si <sup>14</sup>	3s <sup>2</sup> 3p <sup>2</sup>
P <sup>15</sup>	3s <sup>2</sup> 3p <sup>3</sup>
Ga <sup>31</sup>	4s <sup>2</sup> 4p <sup>1</sup>
As <sup>33</sup>	4s <sup>2</sup> 4p <sup>3</sup>
In <sup>49</sup>	5s <sup>2</sup> 5p <sup>1</sup>

The following special cases are considered:

(i)  $t = 1$  sec

The concentration function  $C(x, t)$  against the depth  $x$  is computed for the diffusion of Indium, Phosphorous, into Silicon (Figure 1, for  $R = 3.313 \text{ E-1}$  for  $T = 300 \text{ K}$ , and Figure 3, for  $R = 3.5 \text{ E-1}$  and  $T = 900 \text{ K}$ ). The same dependence for the diffusion of Arsenic and Gallium, into Silicon (Figure 2, for  $R = 3.313 \text{ E-1}$  and  $T = 300 \text{ K}$ , Figure 4, for  $R = 3.5 \text{ E-1}$  and  $T = 900 \text{ K}$ ).

(ii) At  $x = (\delta/10) \text{ m}$

The concentration function  $C(x, t)$  against the diffusion time  $t$  is computed for the diffusion of Indium, Phosphorous, into Silicon (Figure 5, for  $R = 3.313 \text{ E-1}$ ,  $T = 300 \text{ K}$  and Figure 7, for  $R = 3.5 \text{ E-1}$ ,  $T = 900 \text{ K}$ ). The same dependence for the diffusion of Arsenic and Gallium, into Silicon (Figure 6, for  $R = 3.313 \text{ E-1}$  and



$T = 300$  K, Figure 8, for  $R = 3.5 \text{ E-1}$  and  $T = 900$  K).

## 6. Discussions

1. The obtained expression for the concentration function  $C(x, t) \text{ m}^{-3}$  (equation (20)) reveals that it depends principally on the flux density  $J_0, \text{ m}^{-2}\text{s}^{-1}$ . The dependence is linear for constant flux density.

2. The same function depends fundamentally on the diffusion coefficient  $D, \text{ m}^2\text{s}^{-1}$ .

3. The diffusion penetration depth depends basically on the diffusion coefficient  $D, \text{ m}^2\text{s}^{-1}$  which in turn depends on the absolute temperature  $T$ . So the penetration depth becomes greater and the concentration becomes smaller at  $T = 900$  K than that at  $T = 300$  K. Such depth depends also on the size of the dopant atom relative to the host atom, this is evident in Figures 1, 2, 3 and 4.

4. Dopants of higher relative sizes are more accumulated than dopants of smaller relative sizes at a certain layer and at a certain diffusion time (Figures 5, 6, 7 and 8).

## 7. Conclusions

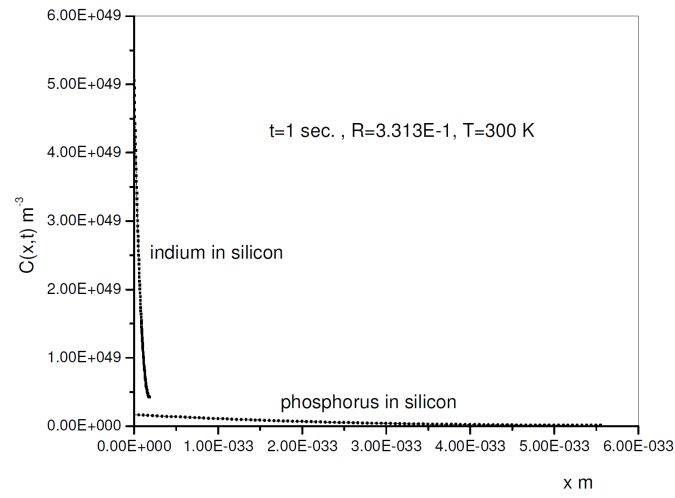
1. The concentration of the Indium and Arsenic dopants into Silicon at a certain layer with time is greater than that for Phosphorous and Gallium dopants into Silicon for the same operating conditions.

2. The penetration depth of the Indium and Arsenic are less than that for Phosphorous and Gallium into Silicon for the same operating conditions.

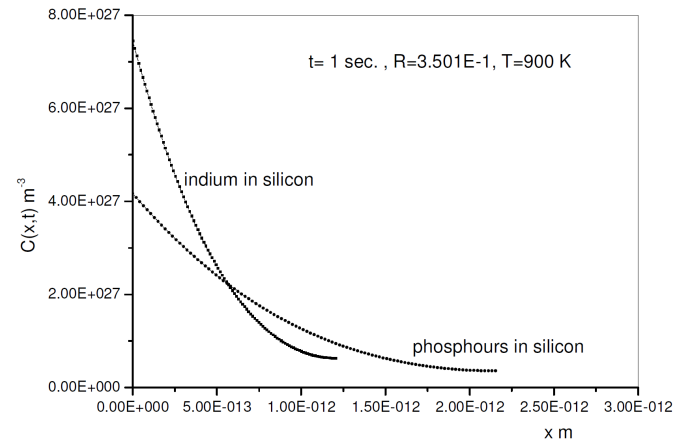
## References

- [1] G. Carter and W. A. Grant, Ion Implantation Semiconductors, Edward Arnold, London, 1976.
- [2] S. W. Jones, Diffusion in Silicon, IC Knowledge LIC, 2000, pp. 1-12.
- [3] S. M. Gary and M. S. Simon, Fundamental of Semiconductor Fabrication, 1st ed., John-Wiley & Sons, 2004.
- [4] V. Hung, P. Hong and B. Khue, Boron and Phosphorus diffusion in Silicon;

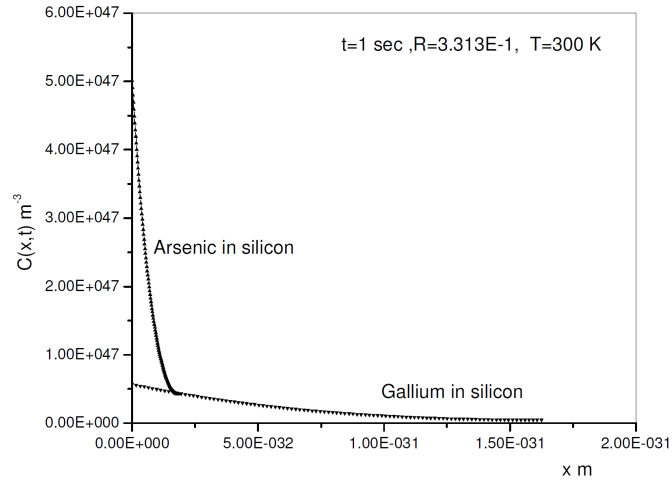
- interstitial, vacancy, and combination mechanisms, *Prac. Nalt. Conf. Theor. Phys.* 35 (2010), 73.
- [5] Q. Zhao, D. C. Zhang and J. F. Lin, Surface materials draperies condensation mode by ion-implantation technology, *Int. J. Heat Mass Transfer* 34(11) (1991), 2833.
  - [6] W. T. Tsang, E. F. Schubert and J. E. Cunningham, *Appl. Phys. Lett.* 60(1) (1992), 115.
  - [7] T. Ahlgren, J. Likonen, J. Slotte, J. Raisanen, M. Rajatora and J. Keinonen, Concentration dependent and independent Si diffusion in ion implanted GaAs, *Phys. Rev. B* 56(8) (1997).
  - [8] H. W. Chang and M. K. Lei, Mass transfer of metal ion implantation into metal target at elevated temperature, *Computational Material Science* 33 (2005), 459.
  - [9] A. Chreneos, H. Bracht, R. W. Grimes and B. P. Uberuaga, *Appl. Phys. Lett.* (2008), 172103.
  - [10] D. V. Morgan and K. Board, *An Introduction to Semiconductor Micro Technology*, 2nd ed., John-Wiley & Sons, 1990.
  - [11] J. F. Ready, Effects due to absorption of laser radiation, *J. Appl. Phys.* 36 (1965), 462.
  - [12] M. Narayanan and H. Al-Nashash, Introducing undergraduate students to simulation of semiconductor doping technique, *Computer and Electrical Engineering* 10 (2008), 1016.
  - [13] P. Ranade, H. Takeuchi, V. Subramanian and T. King, Observation of Boron and Arsenic mediated inter diffusion across Germanium/Silicon interfaces, *Electrochemical and Solid State Letters* 5(2) (2002), G5-G7.
  - [14] M. R. Spiegel, *Laplace Transforms*, Schaum's Outline Series, McGraw-Hill Book Company, New York, USA, 1965.
  - [15] G. E. Robers and H. Kaufman, *Table of Laplace Transforms*, Saunders Company, London, 1966.
  - [16] A. Battacharyya and B. G. Streetman, Dynamics of pulsed CO laser annealing of silicon, *J. Appl. Phys.* 14 (1981), L67-L72.
  - [17] R. B. Fair, Concentration profiles of diffuse dopants in Silicon, *Impurity Dopant Processes in Silicon*, F. Y. Y. Yang, ed., North Holland, 1981.
  - [18] Sorab K. Ghandhi, *The Theory and Practice of Micro Electronics*, John Wiley, 1968.



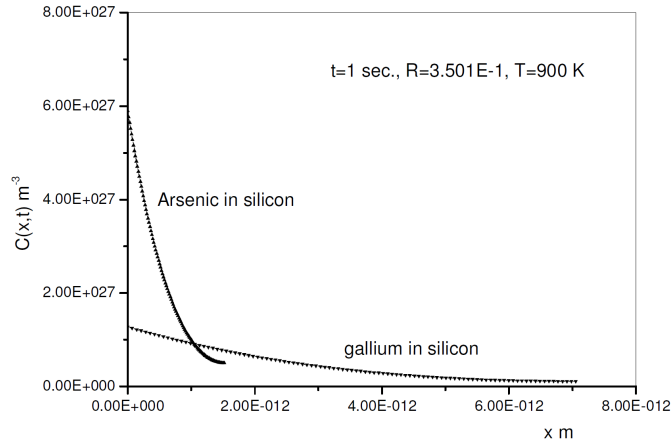
**Figure 1.** Shows the concentration of Indium and Phosphorus in Silicon as a function of the depth in the Silicon target. At  $t = 1$  sec,  $R = 3.313 \text{ E-}1$  and  $T = 300 \text{ K}$ .



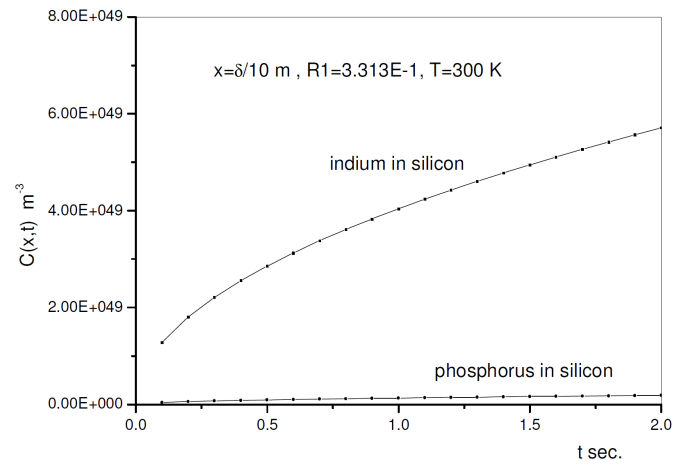
**Figure 2.** Shows the concentration of Indium and Phosphorus in Silicon as a function of the depth in the Silicon target. At  $t = 1$  sec,  $R = 3.501 \text{ E-}1$  and  $T = 900 \text{ K}$ .



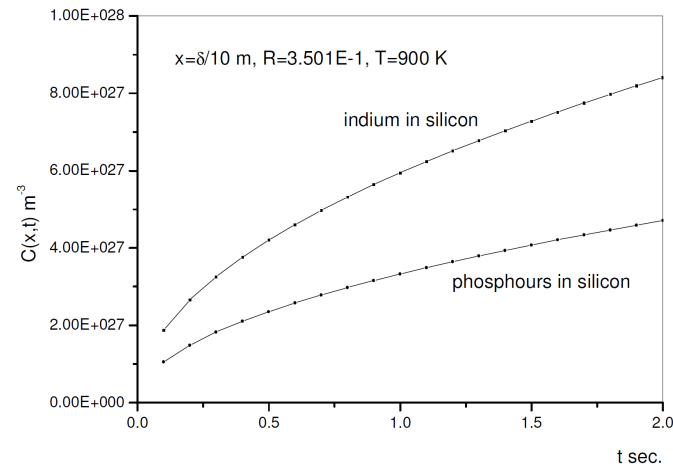
**Figure 3.** Shows the concentration of Arsenic and Gallium in Silicon as a function of the depth in the Silicon target. At  $t = 1$  sec,  $R = 3.313 \text{ E-}1$  and  $T = 300 \text{ K}$ .



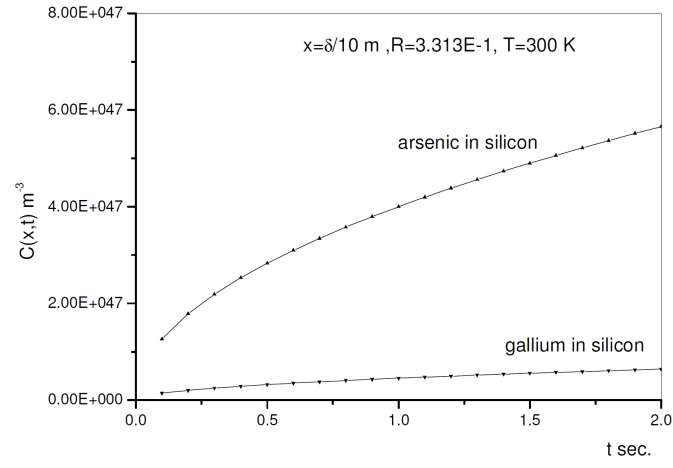
**Figure 4.** Shows the concentration of Arsenic and Gallium in Silicon as a function of the depth in the Silicon target. At  $t = 1$  sec,  $R = 3.3501 \text{ E-}1$  and  $T = 900 \text{ K}$ .



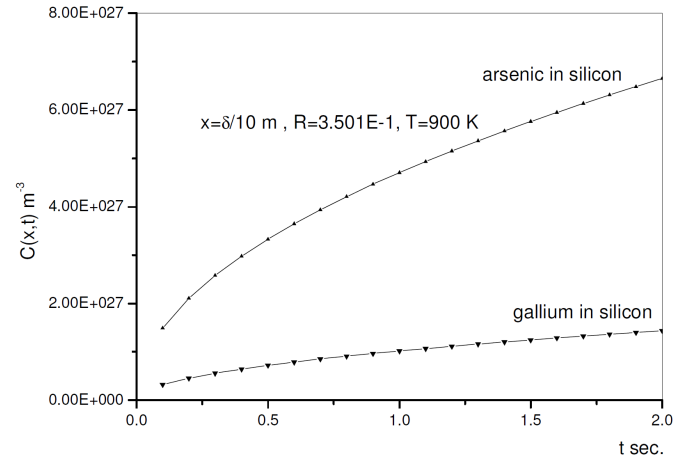
**Figure 5.** Shows the time dependence of the concentration of Indium and Phosphorus in Silicon target. At  $x = \delta/10 \text{ m}$ ,  $R = 3.313 \times 10^{-1}$  and  $T = 300 \text{ K}$ .



**Figure 6.** Shows the time dependence of the concentration of Indium and Phosphorus in Silicon target. At  $x = \delta/10 \text{ m}$ ,  $R = 3.3501 \times 10^{-1}$  and  $T = 900 \text{ K}$ .



**Figure 7.** Shows the time dependence of the concentration of Arsenic and Gallium in Silicon target. At  $x = \delta/10$  m,  $R = 3.313\text{E}-1$  and  $T = 300$  K.



**Figure 8.** Shows the time dependence of the concentration of Arsenic and Gallium in Silicon.  $x = \delta/10$  m,  $R = 3.3501\text{E}-1$  and  $T = 900$  K.