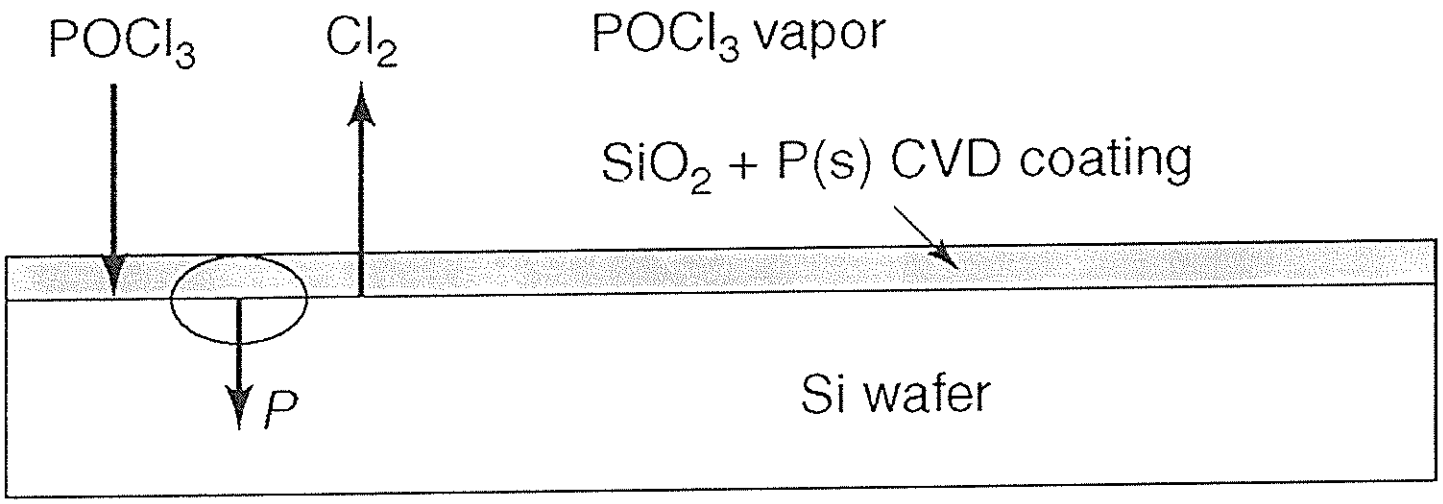
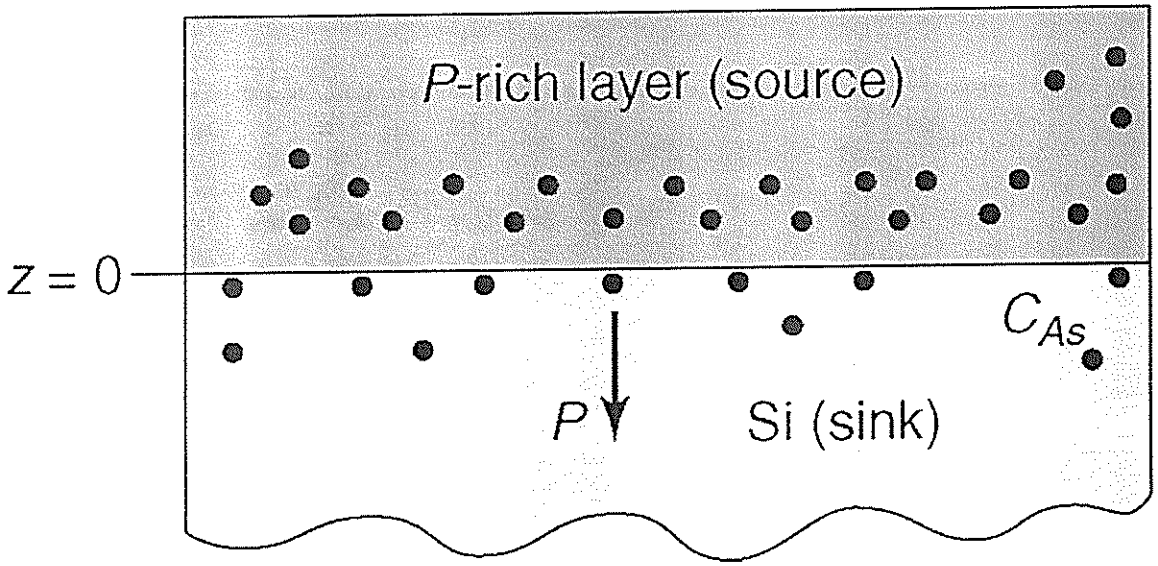
Θέμα 3ο



$$Si(s) + 2POCl_3(g) \longrightarrow SiO_2(s) + 3Cl_2 + 2P(s)$$



solid serves as a semi-infinite sink for the diffusion process. It is desirable to predict the properties of the Si-P thin film as a function of doping conditions. The concentration profile of the doped phosphorous atoms is particularly important for controlling the electrical conductivity of the semiconducting thin film.

Consider the phosphorous doping of crystalline silicon at 1100°C, a temperature high enough to promote phosphorous diffusion. The surface concentration of phosphorous (c_{As}) in the silicon is 2.5×10^{20} atoms P/cm^3 solid Si, which is relatively dilute, since pure solid silicon is 5×10^{22} atoms Si/cm^3 solid. Furthermore, the phosphorous-rich coating is considered as an infinite source relative to the amount of P atoms transferred, so that c_{As} is constant. Predict the depth of the Si-P thin film after 1 hour, if the target concentration is 1% of the surface value (2.5×10^{18} atoms P/cm^3 solid Si), and the concentration profile of P atoms after one hour.

Based on the assumptions given in the problem statement, the partial differential equation describing the one-dimensional, unsteady-state concentration profile $c_A(z, t)$ of phosphorous (species A) in solid silicon (species ~~B~~) is

$$\frac{\partial c_A}{\partial t} = D_{AB} \frac{\partial^2 c_A}{\partial z^2} \tag{27-1}$$

For a semi-infinite medium, the initial and boundary conditions are

$$t = 0,\ c_A(z, 0) = c_{Ao} = 0 \quad \text{for all } z$$
$$z = 0,\ c_A(0, t) = c_{As} = 2.5 \times 10^{20} \text{ atoms P/cm}^3 \text{ solid Si, for } t > 0$$
$$z = \infty,\ c_A(\infty, t) = c_{Ao} = 0 \quad \text{for all } t$$

If the diffusion coefficient D_{AB} is a constant, then the analytical solution is

$$\frac{c_{As} - c_A}{c_{As} - c_{Ao}} = \text{erf}\left(\frac{z}{2\sqrt{D_{AB}t}}\right) = \text{erf}(\phi)$$

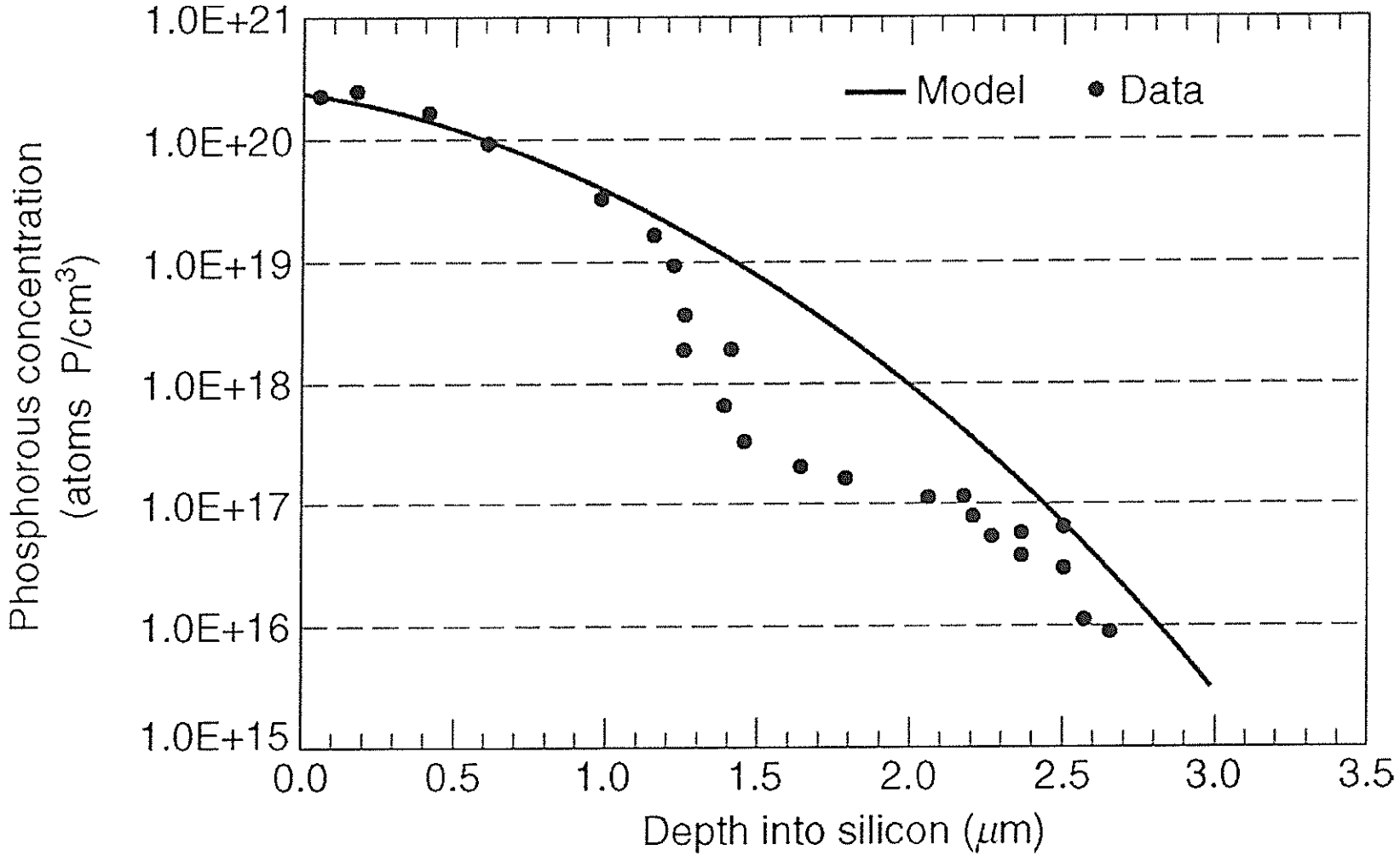
Note that the depth z is imbedded in ϕ, the argument of the error function. The value for $\text{erf}(\phi)$ is calculated from the dimensionless concentration change

$$\frac{c_{As} - c_A}{c_{As} - c_{Ao}} = \frac{2.5 \times 10^{20} \text{ atoms P/cm}^3 - 2.5 \times 10^{18} \text{ atoms P/cm}^3}{2.5 \times 10^{20} \text{ atoms P/cm}^3 - 0} = 0.990 = \text{erf}(\phi)$$

From Appendix Table L, the argument of the error function at erf(ϕ) = 0.990 is $\phi = 1.82$. From Figure 24.8 the solid-diffusion coefficient of P atoms (species A) in crystalline silicon (species B) is 6.5×10^{-13} cm^2/s at 1100°C (1373 K). The depth z can be backed out from ϕ by

$$z = \phi \cdot 2\sqrt{D_{AB}t} = 1.82 \cdot 2 \cdot \sqrt{\left(6.5 \times 10^{-13}\,\frac{\text{cm}^2}{\text{s}} \cdot \frac{10^8\,\mu\text{m}^2}{1\,\text{cm}^2}\right)\left(1\,\text{h} \cdot \frac{3600\,\text{s}}{1\,\text{h}}\right)} = 1.76\,\mu\text{m}$$

Prediction of the concentration profile after 1 hour requires the calculation of ϕ at different values of z, followed by the calculation of erf(ϕ) and finally, $c_A(z, t)$. Repetitive calculation of erf(ϕ) is best carried out with the help of a mathematics software package such as Mathcad (MathSoft Inc., Cambridge, Mass.). The predicted phosphorous concentration profile is compared with the data of Errana and Kakati* obtained under similar process conditions, as shown in Figure 27.3. It is known that the molecular-diffusion coefficient of phosphorous in crystalline silicon is function of phosphorous concentration. The concentration-dependent diffusion coefficient creates a "dip" in the observed phosphorous concentration profile. A detailed model of this phenomenon is provided by Middleman and Hochberg.†


Model
Data
1.0E+21
1.0E+20
1.0E+19
1.0E+18
1.0E+17
1.0E+16
1.0E+15
Phosphorous concentration (atoms P/cm3)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Depth into silicon (μm)