# Answers to Question Sheet 1, Atomic Diffusion

1. A steady–state flux allows the application of Fick's first law $J = -D(\partial C/\partial x)$. Given that the hydrogen concentration in the steel in contact with air can be assumed to be zero,

$$\begin{aligned} J &= 0.1 \times 10^{-6} \exp\left\{\frac{-13400}{8.3143 \times 298}\right\}\frac{4.2-0}{4 \times 10^{-3}} \\ &= 4.7 \times 10^{-7}\,\mathrm{moles\,m^{-2}\,s^{-1}} \end{aligned}$$

Therefore, to dissipate 20 moles over an area of 2 $\mathrm{m}^2$ will take $20/(4.7 \times 10^{-7} \times 3600 \times 2) = 5910$ h. These calculations are for atomic hydrogen whereas hydrogen is stored in its molecular $H_2$ form which has negligible solubility in iron. Dissolved hydrogen severely embrittles iron; by reducing the energy required to create new surfaces (making fracture easy; by the accumulation of high pressure gaseous hydrogen at defects).

2. The error function solution is appropriate:

$$C\{x,t\} = A + B\,\mathrm{erf}\left\{\frac{x}{2\sqrt{Dt}}\right\} \qquad \text{with} \qquad C\{0,t\} = C_s \quad \text{and} \quad C\{x,0\} = C_0$$

$$\text{so that} \qquad C\{x,t\} = C_s - (C_s - C_0)\,\mathrm{erf}\left\{\frac{x}{2\sqrt{Dt}}\right\}$$

We require $C$ to be the eutectoid concentration $\simeq 0.8$ wt%, so that

$$\mathrm{erf}\left\{\frac{x}{2\sqrt{Dt}}\right\} = \frac{C_s - C}{C_s - C_0} = \frac{1.5-0.8}{1.5-0.05} = 0.48$$

On substituting $D = 3.59 \times 10^{-4}\,\mathrm{mm^2\,s^{-1}}$ and $x = 0.3\,\mathrm{mm}$, we get $t = 298\,\mathrm{s}$ or about 5 min.

3. A plot of $\log\{D\}$ vs $T^{-1}$ has a slope $-Q/R\ln\{10\}$ when linear. From the illustration below, both samples are dominated by lattice diffusion at high temperatures. The gradient for the high temperature regime gives an activation energy of about 140 kJ mole$^{-1}$.

At low temperatures lattice diffusion does not contribute much to the flux. Much of the flux is via defect assisted diffusion. The defect density is larger in the cold–worked sample and hence the larger apparent diffusivity relative to the annealed sample. We hope that the measurements are not affected by changes in the defect density during the experiments.

4. Sample $M0$ shows a decarburised surface. Carbon was removed from the surface region during heat treatment in air. The carbon at the steel surface combines with oxygen in the air; fresh supplies continuously arrive at the surface by diffusion from the interior of the steel, leading to decarburisation. We therefore obtain a gradient of microstructure with pearlite in the centre and increasing quantities of ferrite as the surface is approached. You can see micrographs and a description of specimen $M0$ on

   http://www.msm.cam.ac.uk/Department/Teaching/online.html

   Decarburisation can be minimised by heat treatment in a vacuum, in an inert environment or by painting a protective ceramic powder coating on the steel. Small samples can be wrapped in stainless steel foil as a measure of protection.

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