



The rates at which atoms diffuse around in solids determine the lifetimes of solid-state devices, are critical to the processing and aging of industrial materials, and govern the behavior of hydrogen storage for automotive fuel cells. To go from one site to another the diffusing atom must cross a barrier, i.e. go through a high-energy intermediate state. (In the picture that would be the halfway state where the diffusing atom has to squeeze through the others.) The chance of making it to the top of that high-energy barrier, with “activation energy”  $\Delta E$  up from the stable states, is reduced by a Boltzmann factor:  $e^{-\Delta E/kT}$ .

The net rate for making hops of distance  $L$  is then  $f_A e^{-\Delta E/kT}$ , where  $f_A$  (the ‘attempt rate’) is roughly the frequency the atom is rattling around in the crystal. Then the diffusion constant is,

$$D = \frac{1}{6} L^2 f_A e^{-\Delta E/kT}.$$

1. Hydrogen diffuses in niobium with  $D = 10^{-5} \text{ cm}^2/\text{s}$  at  $T=300 \text{ K}$ . The activation energy for its hops is  $\Delta E = 107 \text{ meV}$ . What is its diffusion constant at  $T=330\text{K}$ ?

Only the Boltzmann factor (the probability of getting over the hill) has changed.

$$e^{-\Delta E/kT_2} / e^{-\Delta E/kT_1} = 1.46, \text{ so } D \text{ becomes } 1.46 \times 10^{-5}.$$

2. In a complicated silicon-based device, the hydrogen diffusion rate is found to show an activation energy  $\Delta E = 0.32 \text{ eV}$ . If the device operates at  $330 \text{ K}$  rather than  $300 \text{ K}$ , by what factor does the hydrogen diffusion speed up?

This is almost the same problem as in part 1, but rather than redoing the exponentials, we can simply use scaling.  $\Delta E$  is larger by a factor of  $0.32/0.107$ :  $1.46^{0.32/0.107} = 3.10$ .

This is the reason why electronics lasts longer at low temperatures.