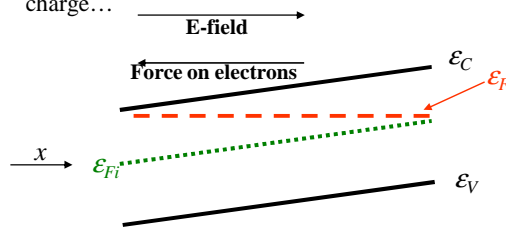


Graded Impurity Distribution

- Consider a non-uniformly doped n-type semiconductor (i.e. it has a graded impurity distribution.). Assume that the doping concentration **decreases** as x increases.
- If semiconductor in equilibrium, then Fermi energy level is constant throughout.
- There will be a diffusion of majority carrier electrons from the region of high to low concentration (+ x direction), leaving behind positively charged donor ions.
- This separation of charge induces an electric field opposes the diffusion process.
- When equilibrium is reached, the mobile carrier concentration is not exactly equal to the fixed impurity concentration, and the induced electric field prevents any further separation of charge...



Graded Impurity Distribution

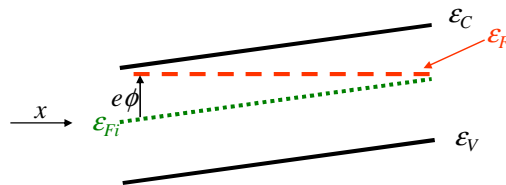
- However, usually the space-charge induced by the diffusion process is a small fraction of the impurity concentration, thus the mobile carrier concentration is not too different from the impurity dopant density.
- Electric potential is related to the electron potential energy by the electron charge:

$$\phi = -\frac{1}{e}(\mathcal{E}_{Fi} - \mathcal{E}_F)$$

- Hence in 1D

$$E_x = -\frac{d\phi}{dx} = \frac{1}{e} \frac{d\mathcal{E}_{Fi}}{dx} \quad (1)$$

i.e. if intrinsic Fermi level changes as a function of distance throughout a semiconductor in thermal equilibrium, then an electric field exists.



Graded Impurity Distribution

- Assume a quasi-neutrality condition in which the electron concentration is almost equal to the donor impurity concentration, then we can still write

$$n_0 = n_i \exp\left[\frac{\mathcal{E}_F - \mathcal{E}_{Fi}}{k_B T}\right] \approx N_d(x)$$

$$\mathcal{E}_F - \mathcal{E}_{Fi} = k_B T \ln\left(\frac{N_d(x)}{n_i}\right)$$

- The Fermi level is constant for thermal equilibrium, so we obtain

$$-\frac{d\mathcal{E}_{Fi}}{dx} = \frac{k_B T}{N_d(x)} \frac{dN_d(x)}{dx}$$

- Combining equation (1) on previous slide with the equation above:

$$E_x = -\frac{d\phi}{dx} = \frac{1}{e} \frac{d\mathcal{E}_{Fi}}{dx} \quad E_x = -\frac{k_B T}{e} \frac{1}{N_d(x)} \frac{dN_d(x)}{dx} \quad (2)$$

The Einstein relation

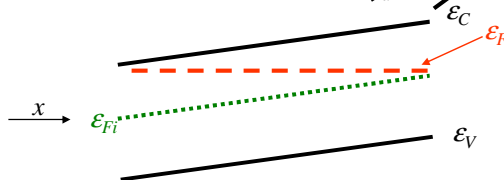
- Consider the non-uniformly doped semiconductor again, and assume that there are no electrical connections so the semiconductor is in thermal equilibrium.
- Hence the individual electron and hole currents must be zero.
- For electrons:

$$J_e = 0 = en\mu_e E_x + eD_e \frac{dn}{dx}$$

$$E_x = -\frac{k_B T}{e} \frac{1}{N_d(x)} \frac{dN_d(x)}{dx}$$

- Assuming quasi-neutrality, so that $n(x) \approx N_d(x)$, and substitute in equation (2) from previous slide to obtain

$$0 = -eN_d(x)\mu_e \left(\frac{k_B T}{e}\right) \frac{1}{N_d(x)} \frac{dN_d(x)}{dx} + eD_e \frac{dN_d(x)}{dx}$$



The Einstein relation

- This equation is valid for the condition

$$\frac{D_e}{\mu_e} = \frac{k_B T}{e}$$

- Similarly, the hole current must also be zero, hence

$$\frac{D_h}{\mu_h} = \frac{k_B T}{e}$$

- Combining these two equations:

$$\frac{D_e}{\mu_e} = \frac{D_h}{\mu_h} = \frac{k_B T}{e}$$

	μ_e	D_e	μ_h	D_h
Si	1350	35	480	12.4
GaAs	8500	220	400	10.4
Ge	3900	101	1900	49.2

Typical mobility and diffusion current values at 300K and low doping concentrations $\mu(\text{cm}^2 \text{V}^{-1} \text{s}^{-1})$; $D(\text{cm}^2 \text{s}^{-1})$

- i.e.* the diffusion coefficient and mobility are not independent parameters. This relation is known as the **Einstein relation**

Note: Mobilities are a strong function of temperature (slides 15.6), as are the diffusion coefficients. Hence the specific temperature dependence given in the Einstein relation is only a small fraction of the real temperature characteristic.



Thermal Properties of Solids

- We need to understand **phonons** (a quantisation of the elastic energy of sound waves) to discuss the thermal properties of solids:
 - Insulators and semiconductors: Debye theory \rightarrow heat capacity, thermal conduction
 - Metals (again) but including lattice effects as well as electrons: heat capacity \rightarrow thermal conduction, electrical resistance and Weidemann-Franz law.

- The thermal equilibrium number of phonons with frequency ω

$$n_{ph}(\hbar\omega) = \frac{1}{\exp[(\hbar\omega)/k_B T] - 1} \quad (\text{Planck distribution})$$

... a special case of **Bose-Einstein statistics** determines the statistical distribution of identical indistinguishable bosons over the energy states in thermal equilibrium.

- Bosons, unlike fermions, are not subject to the Pauli exclusion principle: an unlimited number of particles may occupy the same state at the same time (Bose-Einstein condensate).

- $\hbar\omega \gg k_B T \rightarrow n_{ph} \approx \exp(-\hbar\omega/k_B T)$

i.e. small probability of a phonon being excited so for $T = 0$: no vibrations (phonons)

- $k_B T \gg \hbar\omega \rightarrow n_{ph} \approx \frac{1}{1 + \hbar\omega/k_B T - 1} = \frac{k_B T}{\hbar\omega}$

i.e. number of phonons is very high



Phonons: Debye approximation

treats the vibrations of the atomic lattice (heat) as phonons in a box.

- Assumes identical oscillators, and neglects dispersion of acoustic waves. This is continuum approximation is valid because the interatomic spacing \ll wavelength).
- i.e. assume a linear dependence $\omega = v_s k$ (dotted line) (v_s , speed of sound).

- Number of allowed states in range $k \rightarrow k + dk$ — volume of spherical shell in k -space

3 acoustic modes

$$G(k)dk = 3 \cdot \frac{4\pi k^2 dk}{(2\pi/L)^3} = \frac{12\pi\omega^2 d\omega}{(2\pi/L)^3 v_s^3}$$

volume occupied by a single quantum state in k -space ($V = L^3$)

$$G(\omega) = \frac{G(k)dk}{d\omega} = \frac{3V}{2\pi^2} \frac{\omega^2}{v_s^3}$$

- We define ω_D such that above this cutoff there are no modes. We consider the total number of states

There are $3N$ vibrational modes of a 3D solid of N atoms

$$3N = \int_0^{\omega_D} G(\omega) d\omega = \frac{V}{2\pi^2} \frac{\omega_D^3}{v_s^3} \quad (1)$$

Debye frequency



Phonons: Debye temperature

- We can define the Debye temperature, θ_D

$$\hbar\omega_D = k_B\theta_D$$

- By rearranging (1) on previous slide for ω_D and substituting it into above equation:

$$\theta_D = \frac{\hbar v_s}{k_B} \left(\frac{6\pi^2 N}{V} \right)^{1/3} \quad (1)$$

Density = n

- i.e. $\theta_D \sim v_s n^{1/3} \sim (Y/\rho)^{1/2} n^{1/3} \sim (Y/M)^{1/2}$, where Y = elastic constant (Young's modulus, and $M = nM$)

- Therefore the stiffer the crystal, and the smaller the M , the higher the θ_D
- Examples of Debye temperatures: Si: 650K, Cu: 340K, C: 1860K, Pb: 102K

- It is the is the temperature of a crystal's highest normal mode of vibration, i.e., the highest temperature that can be achieved due to a single normal vibration.

