

Semiconductors

1. Evaluate the free electron concentration in the conduction band of a non degenerate semiconductor
2. Evaluate the free hole concentration in the valence band of a non degenerate semiconductor
3. Derive the intrinsic concentration (n_i) expression in an intrinsic semiconductor
4. Derive the mass action law for a doped non degenerate semiconductor in thermal equilibrium
5. Derive the temperature dependence of the intrinsic concentration in a non degenerate semiconductor
6. Derive Shockley equations for a non degenerate semiconductor
7. Evaluate the position of the Fermi level in a semiconductor sample in the following three cases:
 - (a) intrinsic;
 - (b) n doped and non degenerate;
 - (c) p doped and non degenerate;
8. Assuming that all doping atoms are ionized, derive the expression for the majority carrier concentration in a non degenerate semiconductor in the following three cases:
 - (a) n doped with doping concentration N_D ;
 - (b) p doped with doping concentration N_A ;
 - (c) concentration N_D of donor atoms and N_A of acceptor atoms (assume $N_A > N_D$)
9. Derive microscopic Ohm's law for a semiconductor and evaluate the electrical conductivity for an intrinsic, n doped and p doped semiconductor

Semiconductor mathematical model

1. Derive the free electron continuity equation in a semiconductor
2. Derive the free hole continuity equation in a semiconductor
3. Derive, in stationary (i.e., static) conditions, the behaviour of the minority carrier excess concentration (e.g., electrons in a p sample) under the quasi-neutrality condition with zero electric field, and assuming that the injected excess concentration in $x = 0$ is known, while it becomes zero at the sample limit $x = L$

SEMICONDUCTORS

- 1 In order to evaluate the free carriers concentrations the energy distribution function is exploited. For free electrons in the conduction band the function is defined as $f_m(E)$ such that $dn = f_m(E) dE$, where dn is the number of free electrons per unit volume having energy between E and $E + dE$. By integration on the conduction band the total number of free electrons n is computed as $n = \int_{E_c}^{+\infty} f_m(E) dE$ [1] [as $f_m(E \rightarrow +\infty) \rightarrow 0$ it's possible to integrate from E_c to $+\infty$]

$f_m(E)$ is defined as $f_m(E) = N_m(E) f_m(E)$ where
 N_m : number of available states per unit volume, energy
 $N_m(E) = \gamma_m \sqrt{E - E_c}$, $\gamma_m = 4\pi h^{-3} (2m_m^*)^{3/2}$

$f_m(E)$: probability that a state is occupied. For electrons in thermal equilibrium, f_m is given by the Fermi Dirac distribution

$$f_m(E) = \left[1 + \exp\left(\frac{E - E_F}{k_B T}\right) \right]^{-1} \quad \text{where } E_F \text{ (Fermi level) is such that: } f_m(E_F) = \frac{1}{2}, \forall T$$

considering (*) it can be written

$$n = \gamma_m \int_{E_c}^{+\infty} \frac{\sqrt{E - E_c}}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} dE \quad [2] \text{ (no closed form is available)}$$

for non degenerate semiconductors (semicond. such that the Fermi level is within the bandgap: $E_v < E_F < E_c$) as the integration takes place in the conduction band (from E_c to $+\infty$)
 $E - E_F \gg 0 \Rightarrow \exp\left(\frac{E - E_F}{k_B T}\right) \gg 1$ so the probability density

function can be approx as $f(E) \approx \exp\left(-\frac{E - E_F}{k_B T}\right)$ which is the exp. occupation probab. for classical non interacting particle gas described by Boltzmann statistics by applying Boltzmann approx to [2]

$$n \approx \gamma_m \exp\left(\frac{E_F}{k_B T}\right) \int_{E_c}^{+\infty} \sqrt{E - E_c} \exp\left(-\frac{E}{k_B T}\right) dE = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

where $N_c = \frac{\gamma_m}{2} \sqrt{\pi} (k_B T)^{3/2}$ is the effective density of states in the CB

2 In order to evaluate the free carriers concentrations the energy distribution function is exploited. For free holes in the valence band the function is defined as $p_p(E)$ such that $dp = p_p(E) dE$, where dn is the number of free holes per unit volume having energy between E and $E + dE$. By integration on the valence band the total number of free holes p is computed as $p = \int^{E_v} p_p(E) dE$ [1] [as $p(E \rightarrow -\infty) \rightarrow 0$ it's possible to integrate from $-\infty$ to E_v]

$p_p(E)$ is defined as $p_p(E) = N_p(E) f_p(E)$ where
 N_p : number of available states per unit volume, energy
 $N_p(E) = \gamma_p \sqrt{E_v - E}$, $\gamma_p = 4\pi h^{-3} (2m_p^*)^{3/2}$

$f_p(E)$: probability that a state is occupied. For electrons in thermal equilibrium, f_m is given by the Fermi Dirac distribution:

$$f_m(E) = \left[1 + \exp\left(\frac{E - E_F}{k_B T}\right) \right]^{-1} \text{ where } E_F \text{ (Fermi level) is such that: } f_m(E_F) = \frac{1}{2}, \forall T$$

$$f_p(E) = 1 - f_m(E) = \left[1 + \exp\left(-\frac{E - E_F}{k_B T}\right) \right]$$

considering (*) it can be written

$$p = \gamma_p \int_{-\infty}^{E_v} \frac{\sqrt{E_v - E}}{1 + \exp\left(-\frac{E - E_F}{k_B T}\right)} dE \quad [2] \text{ (no dosed form is available)}$$

for non degenerate semiconductors (semicond. such that the Fermi level is within the bandgap: $E_v < E_F < E_c$) as the integration takes place in the valence band (from $-\infty$ to E_v) $E - E_F < 0 \Rightarrow \exp\left(-\frac{E - E_F}{k_B T}\right) \gg 1$ so the probability density

function can be approx as $f_p(E) \approx \exp\left(\frac{E - E_F}{k_B T}\right)$ (Boltzmann statistics)

$$p \approx \gamma_p \exp\left(\frac{-E_F}{k_B T}\right) \int_{-\infty}^{E_v} \sqrt{E_v - E} \exp\left(\frac{E}{k_B T}\right) dE = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

where $N_v = \frac{\gamma_p}{2} \sqrt{\pi} (k_B T)^{3/2}$ is the effective density of states in the CB

3 For an **intrinsic** semiconductor (non degenerate) the number of **free charges** is the **result** of the **equilibrium** between **two phenomena**:

- **generation** of e-h couple (e in VB absorb energy \leftrightarrow h in CB
thermal generation

optical generation: due to the absorption of photons having energy $E > E_g$

impact generation: perfect periodicity of the crystal is only ideal. Where periodicity is broken "free" carriers interact with the crystal by mechanical collision, losing kinetic energy. If the energy lost is greater than $E_g \Rightarrow$ generation e⁻/h couple

- **recombination** of e-h couple (random formation of covalent bond)

as the **phenomena** takes place in **couples of carriers**

$n = p = n_i = p_i$ where n_i is the intrinsic concentration for a non degenerate semiconductor, as Boltzmann approx

$$np = N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right) N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right) = N_c N_v \exp\left(-\frac{E_g}{k_B T}\right)$$

as for an undoped (intrinsic) semicon $n = p = n_i$

$$n_i^2 = N_c N_v \exp\left(-\frac{E_g}{k_B T}\right)$$

4 For a **non degenerate** semiconductor, **Boltzmann approx.** hold

$$n \approx N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right) ; p \approx N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right)$$

deriving the product np we get

$$np = N_c N_v \exp\left(-\frac{E_c - E_F}{k_B T} - \frac{E_F - E_v}{k_B T}\right) = N_c N_v \exp\left(-\frac{E_g}{k_B T}\right)$$

where E_g is the bandgap of the particular semiconductor utilized and it's defined as $E_g = E_v - E_c$

the product np is **independent of the doping level** as it is **independent of E_F** but **depends** only on the **material** (E_g) and the **temperature** (T)

as for an **intrinsic** material $\Leftrightarrow n = p = n_i$

it can be written $n_i^2 = N_c N_v \exp(-E_g/k_B T)$ **MASS ACTION LAW**

the **law** holds if two **requirements** are met:

- **thermal equilibrium** condition
- **non degenerate** semiconductor

5 Exploiting the **mass action law**

$$np = n_i^2 = N_c N_v \exp\left(-\frac{E_g}{k_B T}\right)$$

where N_c, N_v are the effective density of states in the CB, VB defined as

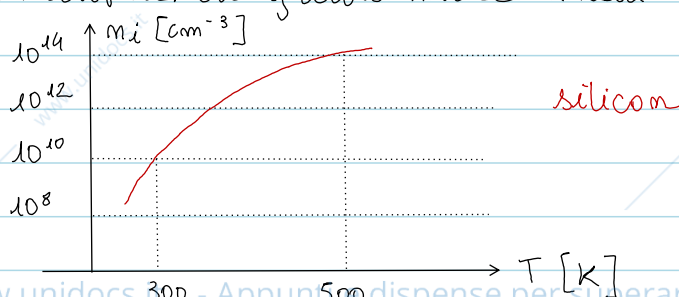
$$N_c = \frac{\gamma_m \sqrt{\pi}}{2} (k_B T)^{3/2} ; N_v = \frac{\gamma_p \sqrt{\pi}}{2} (k_B T)^{3/2}$$

substituting in the mass action law

$$np = \frac{\gamma_m \gamma_p \pi}{4} (k_B T)^3 \exp\left(-\frac{E_g}{k_B T}\right)$$

from which is clear that $n_i^2 \propto T^3 \exp\left(-\frac{E_g}{k_B T}\right)$

the result is that the intrinsic concentration grows more than exponentially with temperature



6 As Boltzmann approx holds for non degenerate semiconductor defining E_{Fi} as the Fermi level in the intrinsic case

$$n_i = N_c \exp\left(-\frac{E_c - E_{Fi}}{k_B T}\right); \quad p_i = N_v \exp\left(-\frac{E_{Fi} - E_v}{k_B T}\right)$$

isolating N_c, N_v from the previous relations

$$N_c = n_i \exp\left(\frac{E_c - E_{Fi}}{k_B T}\right); \quad N_v = p_i \exp\left(\frac{E_{Fi} - E_v}{k_B T}\right)$$

substituting N_c, N_v in the general relations for the free carriers concentration of a non degenerate semiconductor

$$n = n_i \exp\left(\frac{E_c - E_{Fi}}{k_B T}\right) \exp\left(-\frac{E_c - E_F}{k_B T}\right) = n_i \exp\left(\frac{E_F - E_{Fi}}{k_B T}\right)$$

$$p = p_i \exp\left(\frac{E_{Fi} - E_v}{k_B T}\right) \exp\left(-\frac{E_F - E_v}{k_B T}\right) = p_i \exp\left(\frac{E_{Fi} - E_F}{k_B T}\right)$$

SCHOKLEY
EQUATIONS

these equations are equivalent to the Boltzmann relations. Schokley equations holds the same conditions of non degenerate semiconductor and th. equilibrium

the formulation of Boltzmann relations provided by Schokley highlights the physical meaning of the Fermi level as the center of gravity for the free carriers distributions

intrinsic material $E_F = E_{Fi}$

n-doping ($n > p$) $\Rightarrow E_F > E_{Fi}$

p-doping ($p > n$) $\Rightarrow E_F < E_{Fi}$

as at th. eq. the mass action law $np = n_i^2$ must hold, increasing the concentration of a free carrier causes the other free carrier's concentration to decrease for example:

$$\begin{array}{l} \text{increasing } n \Rightarrow E_F > E_{Fi} \\ \swarrow \\ n = n_i \exp\left(\frac{E_F - E_{Fi}}{k_B T}\right) \uparrow \\ \searrow \\ p = p_i \exp\left(\frac{E_{Fi} - E_F}{k_B T}\right) \downarrow \end{array}$$

In conclusion, at th. equil. the free carriers concentrations cannot be changed independently

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a) Exploiting **Schokley equations** (non degenerate sc) and as for an **intrinsic** sc must be **$n = p$**

$$N_c \exp\left(-\frac{E_c - E_{Fi}}{k_B T}\right) = N_v \exp\left(-\frac{E_{Fi} - E_v}{k_B T}\right)$$

$$\frac{N_c}{N_v} = \exp\left(\frac{E_v - E_{Fi} + E_c - E_{Fi}}{k_B T}\right) = \exp\left(\frac{E_v + E_c - 2E_{Fi}}{k_B T}\right)$$

$$\frac{E_v + E_c - 2E_{Fi}}{k_B T} = \ln\left(\frac{N_c}{N_v}\right) \Leftrightarrow -2E_{Fi} = k_B T \ln\left(\frac{N_c}{N_v}\right) - E_v - E_c$$

$$E_{Fi} = -\frac{k_B T}{2} \ln\left(\frac{N_c}{N_v}\right) + \frac{E_c + E_v}{2} \quad \text{as} \quad \begin{aligned} N_c &= \gamma_m \sqrt{E - E_c} \\ N_v &= \gamma_p \sqrt{E_v - E} \end{aligned}$$

$$\text{where } \gamma_m = 4\pi h^{-3} (2m_m^*)^{3/2}, \quad \gamma_p = 4\pi h^{-3} (2m_p^*)^{3/2}$$

as N_c, N_v differs only for the different values of the effective masses m_m^*, m_p^* . If this difference is **negligible** then $\frac{N_c}{N_v} \approx 1$

$E_{Fi} \approx \frac{E_c + E_v}{2}$ from which it can be noted that the intrinsic Fermi level falls almost in the middle of the material energy bandgap

b) for a non degenerate n-doped semicond. assuming a **donor concentration** N_D , at **thermal equilibrium** condition and assuming **complete ionization** **$n \approx N_D$**

from Boltzmann relations

$$n = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right) = N_D \Leftrightarrow \frac{E_F - E_c}{k_B T} = \ln \frac{N_D}{N_c} \Leftrightarrow E_F = E_c - k_B T \ln \frac{N_c}{N_D}$$

- c) for a **non degenerate** p-doped semiconductor, assuming an **acceptor concentration** N_A , at **thermal equilibrium** condition and assuming complete ionization

$$p \approx N_A$$

from **Boltzmann relations**

$$p = N_V \exp\left(-\frac{E_F - E_V}{k_B T}\right) = N_A \Leftrightarrow \frac{E_F - E_V}{k_B T} = -\ln \frac{N_A}{N_V} \Leftrightarrow E_F = E_V + k_B T \ln \frac{N_V}{N_A}$$

- 8 evaluation of majority carriers concentration (n. deg. sc.) assuming complete ionization

- a) for n-doped, doping conc. N_D
defining $N^+ = N_D^+ - N_A^- = N_D - N_A$

$$\begin{cases} n - p = N^+ & \text{local neutrality condition} \\ n \cdot p = n_i^2 & \text{mass action law} \end{cases}$$

substituting $p = \frac{n_i^2}{n}$ in the neutrality condition

$$n - \frac{n_i^2}{n} = N^+ \Leftrightarrow n^2 - N^+ n - n_i^2 = 0 \Leftrightarrow n = \frac{N^+ + \sqrt{(N^+)^2 + 4n_i^2}}{2} \Leftrightarrow$$

$$n = \frac{N^+}{2} \left[1 + \sqrt{1 + \left(\frac{2n_i}{N^+}\right)^2} \right] \text{ for } N^+ \gg n_i \text{ (doping cond.)} \Rightarrow n \approx N^+$$

complete ionization, n-doping $N^+ \approx N_D \Rightarrow n \approx N_D$

- b) for p-doped non degenerate semiconductor.

$$\begin{cases} n - p = -|N^+| & \text{neutrality cond.} \\ n \cdot p = n_i^2 & \text{mass action law} \end{cases} \Rightarrow n = \frac{n_i^2}{p}$$

$$\frac{n_i^2}{p} - p = -|N^+| \Leftrightarrow p^2 - |N^+| p - n_i^2 = 0 \Leftrightarrow p = \frac{|N^+| + \sqrt{|N^+|^2 + 4n_i^2}}{2}$$

$$p = \frac{|N^+|}{2} \left[1 + \sqrt{1 + \left(\frac{2n_i}{|N^+|}\right)^2} \right] \text{ for } |N^+| \gg n_i \text{ (doping condition)} \Rightarrow p \approx |N^+|$$

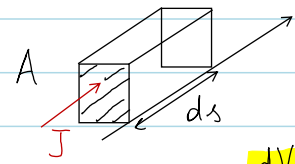
complete ionization, p-doping $N^+ \approx N_A \Rightarrow p \approx N_A$

- c) the majority carriers for a semiconductor where $N_A > N_D$ are the free holes referring to point b)

$$p = \frac{|N^+|}{2} \left[1 + \sqrt{1 + \left(\frac{2mi}{|N^+|} \right)^2} \right]$$

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- a) considering **n-doped** sample, $p \approx 0$ applying a uniform **electric field** \mathcal{E}



$$dV = A \cdot ds$$

$$I = \frac{dQ}{dt} = \frac{dQ}{ds} \frac{ds}{dt} = \frac{dQ}{dV} A v_m = -q n A v_m = q n A \mu_n \mathcal{E} \quad [1]$$

where v_m is the **average drift velocity** for electrons defined $v_m = -\mu_n \mathcal{E}$ where μ_n is the corresponding **mobility**
 $[\mu_n] = \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$

considering the **current density** $J = \frac{I}{A} = \sigma \mathcal{E}$ where σ is the **electric conductivity**

from [1] $\sigma = q n \mu_n$

- b) considering **p-doped** sample, $n \approx 0$ applying **uniform** \mathcal{E}

$$I = \frac{dQ}{dt} = \frac{dQ}{ds} \frac{ds}{dt} = \frac{dQ}{dV} A v_p = q p A v_p = q p A \mu_p \mathcal{E} \quad v_p = \mu_p \mathcal{E}$$

$$J = \frac{I}{A} = \sigma \mathcal{E} \quad q p \mu_p \mathcal{E} = \sigma \mathcal{E} \Leftrightarrow \sigma = q p \mu_p \mathcal{E}$$

- c) considering an **intrinsic** semiconductor when applying a **uniform** \mathcal{E} the **total current** will be the **sum of electrons and holes contribution** from previous results

$$I = q n A \mu_n \mathcal{E} + q p A \mu_p \mathcal{E} \quad J = \frac{I}{A} = \sigma \mathcal{E} \Leftrightarrow$$

$$(q n \mu_n + q p \mu_p) \mathcal{E} = \sigma \mathcal{E} \Leftrightarrow \sigma = q (n \mu_n + p \mu_p)$$

SEMICOND. MATH. MODEL

1) considering electrons crossing a volume $dV = A dx$

$$\frac{\partial m}{\partial t} dV = \frac{\partial m}{\partial t} A dx$$

variation of electrons are due to four contributions

1) e entering the volume per u. time $\Phi_e(x) = [J(x)/-q] \cdot A$

2) e exiting the volume per u. time $\Phi_e(x+dx) = [J(x+dx)/-q] \cdot A$

3) generation per u. time $G_m A dx$

4) recombination per u. time $R_m A dx$

where R_m, G_m are the e recomb. and generation rate per u. time and u. volume

substituting

$$\frac{\partial m}{\partial t} A dx = \frac{J_m(x)}{-q} A - \frac{J_m(x+dx)}{-q} A + G_m A dx - R_m A dx$$

considering the flow contributions

$$\frac{J_m(x)}{-q} - \frac{J_m(x+dx)}{-q} = \frac{1}{q} [J_m(x+dx) - J_m(x)]$$

as $dx \rightarrow 0 \Rightarrow$ first order approx $J_m(x+dx) \approx J_m(x) + \frac{\partial J_m}{\partial x} dx$

$$\text{substituting } \frac{1}{q} [J_m(x+dx) - J_m(x)] \approx \frac{1}{q} \left[\frac{\partial J_m}{\partial x} dx \right]$$

considering generation/recomb. contrib.

as the net recombination rate for e is defined as

$$U_m = R_m - G_m \quad G_m dx - R_m dx = -U_m dx$$

substituting the expressions in [1] and considering $dx \rightarrow 0$

$$\frac{\partial m}{\partial t} = \frac{1}{q} \frac{\partial J_m}{\partial x} - U_m \quad e^- \text{ CONTIN. EQ.}$$

2

considering holes crossing a volume $dV = A dx$

$$\frac{\partial p}{\partial t} dV = \frac{\partial p}{\partial t} A dx$$

flux contributions $\Phi_p(x) = \frac{J_p(x)}{q} A$, $\Phi_p(x+dx) = \frac{J_p(x+dx)}{q} A$

gen/recomb. contrib. $R_p A dx$, $G_p A dx$

$$\frac{\partial p}{\partial t} A dx = \frac{J_p(x)}{q} A - \frac{J_p(x+dx)}{q} A + G_p A dx - R_p A dx$$

considering flux contributions

$$\frac{J_p(x)}{q} - \frac{J_p(x+dx)}{q} = \frac{1}{q} [J_p(x) - J_p(x+dx)]$$

as $dx \rightarrow 0$ $J_p(x+dx) \approx J_p(x) + \frac{\partial J_p}{\partial x} dx$ substituting

$$\frac{1}{q} [J_p(x) - J_p(x+dx)] \approx -\frac{1}{q} \left[\frac{\partial J_p}{\partial x} dx \right]$$

considering gen/recomb. contrib.

$$G_p dx - R_p dx = -U_p dx$$

substituting and considering $dx \rightarrow 0$

$$\frac{\partial p}{\partial t} = -\frac{\partial J_p}{\partial x} - U_p \quad \text{h CONTINUITY EQ.}$$

3

$$m'(x) = m(x) - m_0$$

considering the **free e continuity eq.**

$$\frac{dm}{dt} = \frac{1}{q} \frac{d}{dx} J_m - U_m$$

stationary condition $\Rightarrow \frac{dm}{dt} = 0 = \frac{1}{q} \frac{d}{dx} J_m - U_m$

quasi-neutral condition, $\epsilon = 0$ $\Rightarrow J_m = J_{m,diff} = q D_m \frac{dm}{dx}$
 $[Vx, m'(x) = p'(x)]$

e^- diffusivity $D_m = \mu_m V_T$

lifetime approx for net recomb. rate $U_m \approx \frac{m'}{\tau_m} \rightarrow e^-$ lifetime
 substituting

$$\frac{1}{q} \frac{d}{dx} \left[q D_m \frac{dm}{dx} \right] - \frac{m'}{\tau_m} = 0 \quad \text{as } m_0 \text{ is const} \Rightarrow \frac{dm}{dx} = \frac{dm'}{dx}$$

$$D_m \frac{d^2 m'}{dx^2} - \frac{m'}{\tau_m} = 0 \quad \text{diffusion length } L_m = \sqrt{D_m \tau_m}$$

$$\frac{d^2 m'}{dx^2} - \frac{m'}{L_m^2} = 0 \quad \text{in order to solve 2 boundary conditions are needed}$$

first b. cond. $m'(x=0)$ (Hp: Known quantity)

second b. cond. $m'(x=L) = 0$ (Hp: for $x=L$ back to equilib.)

$$m'(x) = A e^{-x/L_m} + B e^{x/L_m} \quad \text{general solution}$$

$$\begin{cases} A = m'(0) - B & \text{first bound. cond.} \end{cases}$$

$$\begin{cases} A e^{-L/L_m} + B e^{L/L_m} = 0 & \text{second bound. cond} \end{cases}$$

$$[m'(0) - B] e^{-L/L_m} + B e^{L/L_m} = 0 \Leftrightarrow m'(0) e^{-L/L_m} - B \left(e^{-L/L_m} - e^{L/L_m} \right) = 0$$

$$B = \frac{m'(0) e^{-L/L_m}}{[e^{-L/L_m} - e^{L/L_m}]} \quad \text{substituting in } A = m'(0) - B$$

$$A = m'(0) - \frac{m'(0) e^{-L/L_m}}{(e^{-L/L_m} - e^{L/L_m})} = \frac{m'(0) e^{L/L_m} - m'(0) e^{L/L_m} - m'(0) e^{-L/L_m}}{(e^{-L/L_m} - e^{L/L_m})}$$

substituting in the general solution

$$m'(x) = m'(0) \frac{e^{\frac{-L-x}{L_m}} - e^{\frac{L-x}{L_m}}}{e^{\frac{-L}{L_m}} - e^{\frac{L}{L_m}}} \cdot \frac{2}{2} = m'(0) \frac{\sinh\left(\frac{L-x}{L_m}\right)}{\sinh\left(\frac{L}{L_m}\right)}$$