

# Finding $E_F$ : charge neutrality and the $\log(N)$ graph

*Semiconductor physics, Academic year 2020-2021*

# Recap: n, p

Charge carriers in the band structure obey Fermi-Dirac statistics  $f_{E_F}(E)$ .

The probability of an energy level containing a carrier is proportional to the statistical probability of that energy level times the density of available states at that energy. The total number of carrier is then an integral:

$$n = \int_{E_c}^{+\infty} dE \text{ DOS}_{C,e^-}(E) \cdot f_{E_F}(E)$$

*and*

$$p = \int_{-\infty}^{E_V} dE \text{ DOS}_{V,p^+}(E) \cdot [1 - f_{E_F}(E)]$$

# Recap: n, p

Working out these integrals one obtains:

$$n = N_C F_{1/2} \left( \frac{E_F - E_C}{k_B T} \right) \quad \text{and} \quad p = N_V F_{1/2} \left( \frac{E_V - E_F}{k_B T} \right)$$

Which simplify to  $F_{1/2}(\varepsilon) \rightarrow \exp(\varepsilon)$  for  $\varepsilon \rightarrow -\infty$  :

**non-degenerate semiconductors**

$$n \approx N_C \exp \left( \frac{E_F - E_C}{k_B T} \right) \quad \text{and} \quad p \approx N_V \exp \left( \frac{E_V - E_F}{k_B T} \right)$$

## Recap: n, p

Plotting these on a logarithmic graph as functions of  $E_F$  will yield **two regions** with the transition limit usually  $4k_B T$  away from band edge:

Degenerate semiconductor: Maxwell-Boltzmann cannot be used

Non-degenerate semiconductor: Maxwell-Boltzmann can be used.

The plot will be a straight line on a logarithmic graph, with slope:

$$\log_{10} \left( \exp \left( \frac{\pm E_F}{k_B T} + \dots \right) \right) = \pm \frac{\log_{10}(e)}{k_B T} E_F + \dots$$

And starting points:

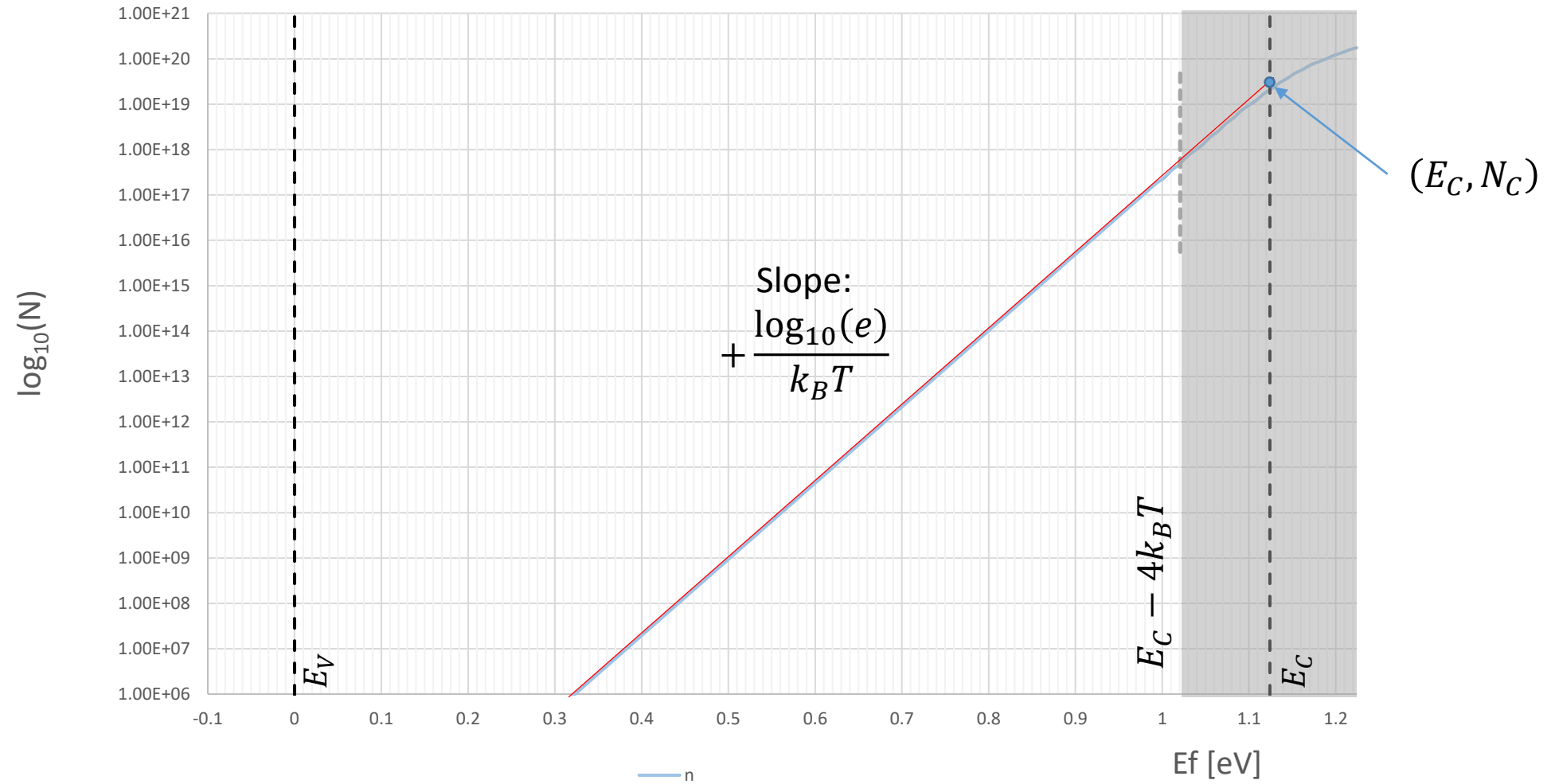
$$n: (E_F, N) = (E_C, N_C) \quad \text{and} \quad p: (E_F, N) = (E_V, N_V)$$

# Log(n)

Non-degenerate  
semiconductor =  
**MB**

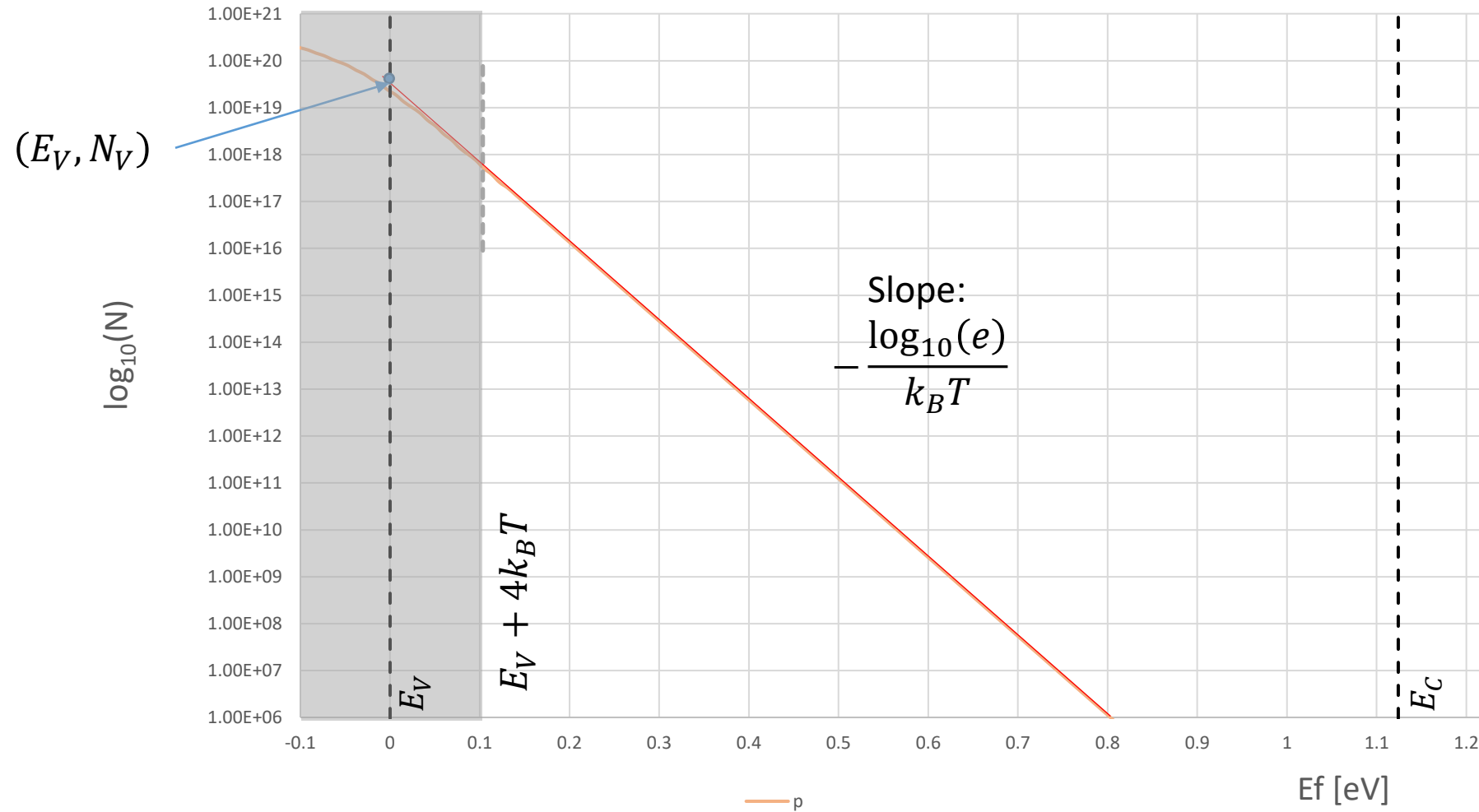
Degenerate  
semiconductor =  
**FD**

Log(N) vs. Ef



# Log(p)

Degenerate semiconductor = **FD**  
 Non-degenerate semiconductor = **MB**  
 Log(N) vs. Ef



Recap:  $N_A^-$ ,  $N_D^+$

Dopant levels obey modified Fermi-Dirac statistics:

The probability of a dopant state being ionized is a function of the statistical probability of that energy level being occupied, and the degeneracy of the different ways in which it can be ionized.

$$N_A^- = \frac{N_A}{1 + 4 \exp\left(\frac{E_A - E_F}{k_B T}\right)} \quad \text{and} \quad N_D^+ = \frac{N_D}{1 + 2 \exp\left(\frac{E_F - E_D}{k_B T}\right)}$$

Recap:  $N_A^-$ ,  $N_D^+$

**Three regions** can be distinguished.

Full ionization: where all ions are full ionized:

$$N_A \approx N_A^- \quad \text{for} \quad E_F > E_A + 4k_B T + k_B T \ln(4)$$

$$N_D \approx N_D^+ \quad \text{for} \quad E_F < E_D - 4k_B T - k_B T \ln(2)$$

Exponential region: where Maxwell-Boltzmann can be used

$$N_A^- \approx N_A \cdot \frac{1}{4} \exp\left(\frac{E_F - E_A}{k_B T}\right) \quad \text{for} \quad E_F < E_A - 4k_B T + k_B T \ln(4)$$

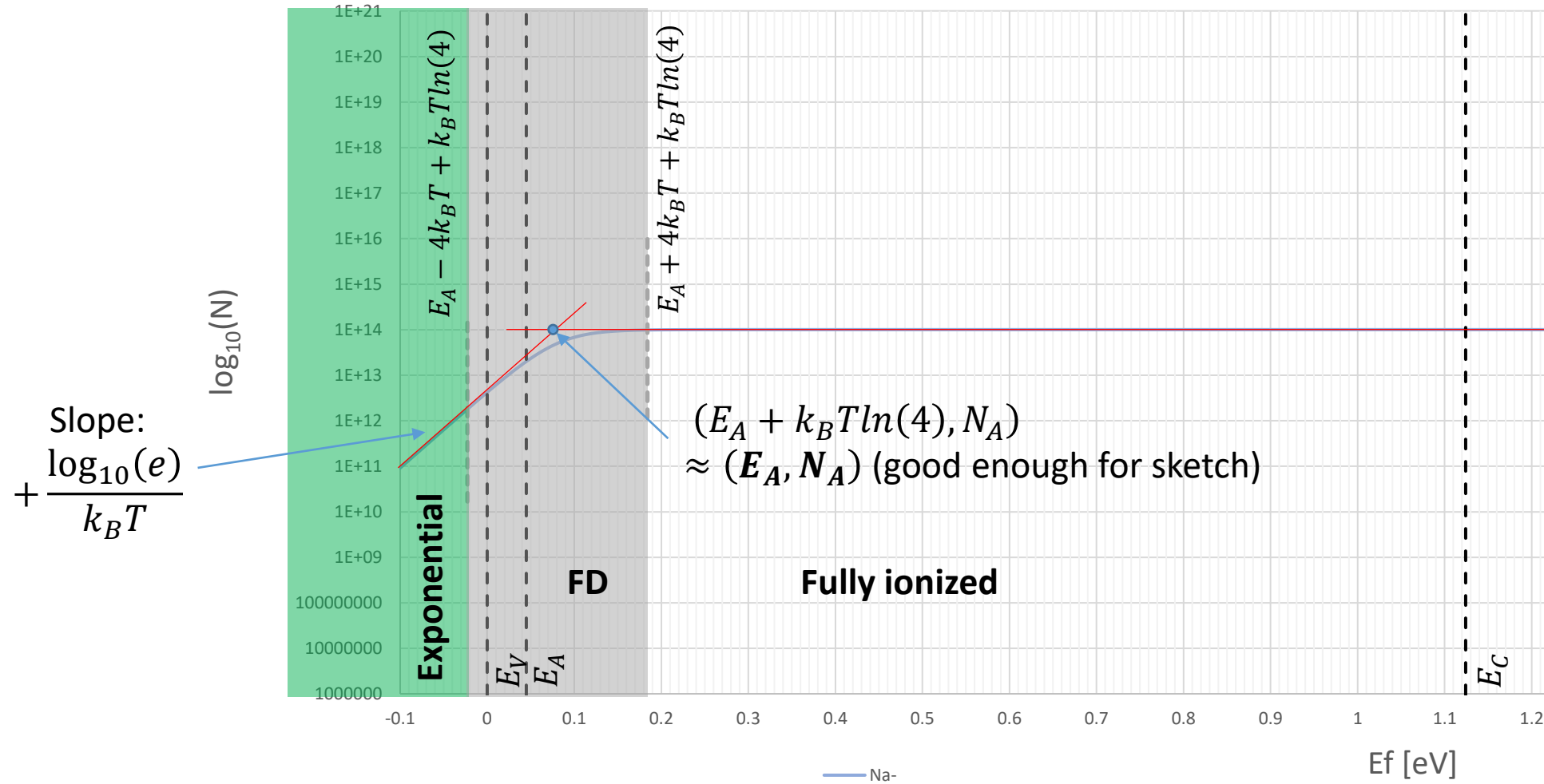
$$N_D^+ \approx N_D \cdot \frac{1}{2} \exp\left(\frac{E_D - E_F}{k_B T}\right) \quad \text{for} \quad E_F > E_D + 4k_B T - k_B T \ln(2)$$

Intermediate: where no simplifications can be made.



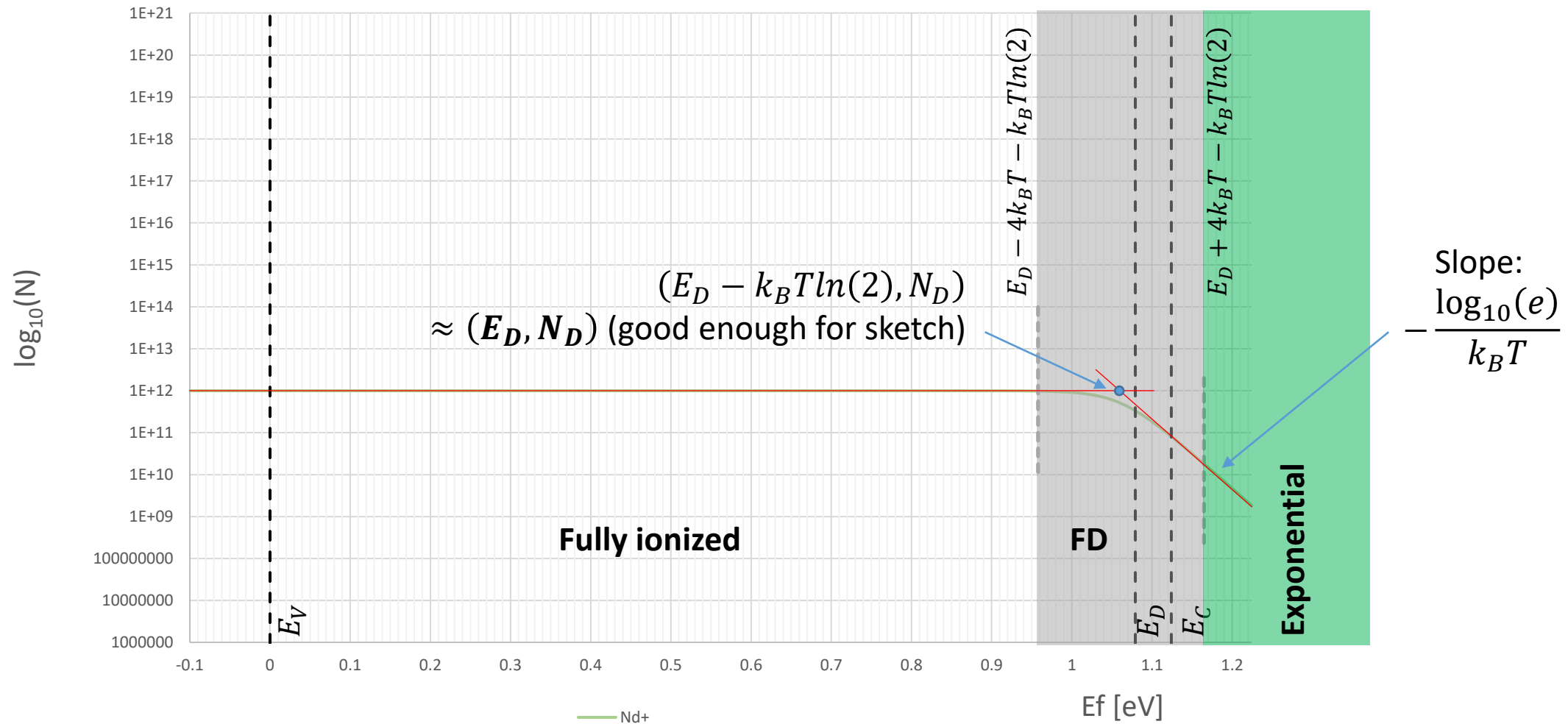
# Log( $N_{A^-}$ )

Log(N) vs. Ef



# Log( $N_D^+$ )

Log(N) vs. Ef



# Charge neutrality

The overall sample must have no static electric charge, so:

$$Q_{total+} = Q_{total-} \quad \text{thus} \quad n + N_A^- = p + N_D^+$$

We've seen so far that these are all functions of  $E_F$ . The Fermi-level  $E_F$  takes on the value which satisfies charge neutrality.

Finding this point on the log(N)-graph amounts to plotting both the left- and right-hand sums, and finding their intersection point.

Let's first look at the sums separately

# Sums in CN equation

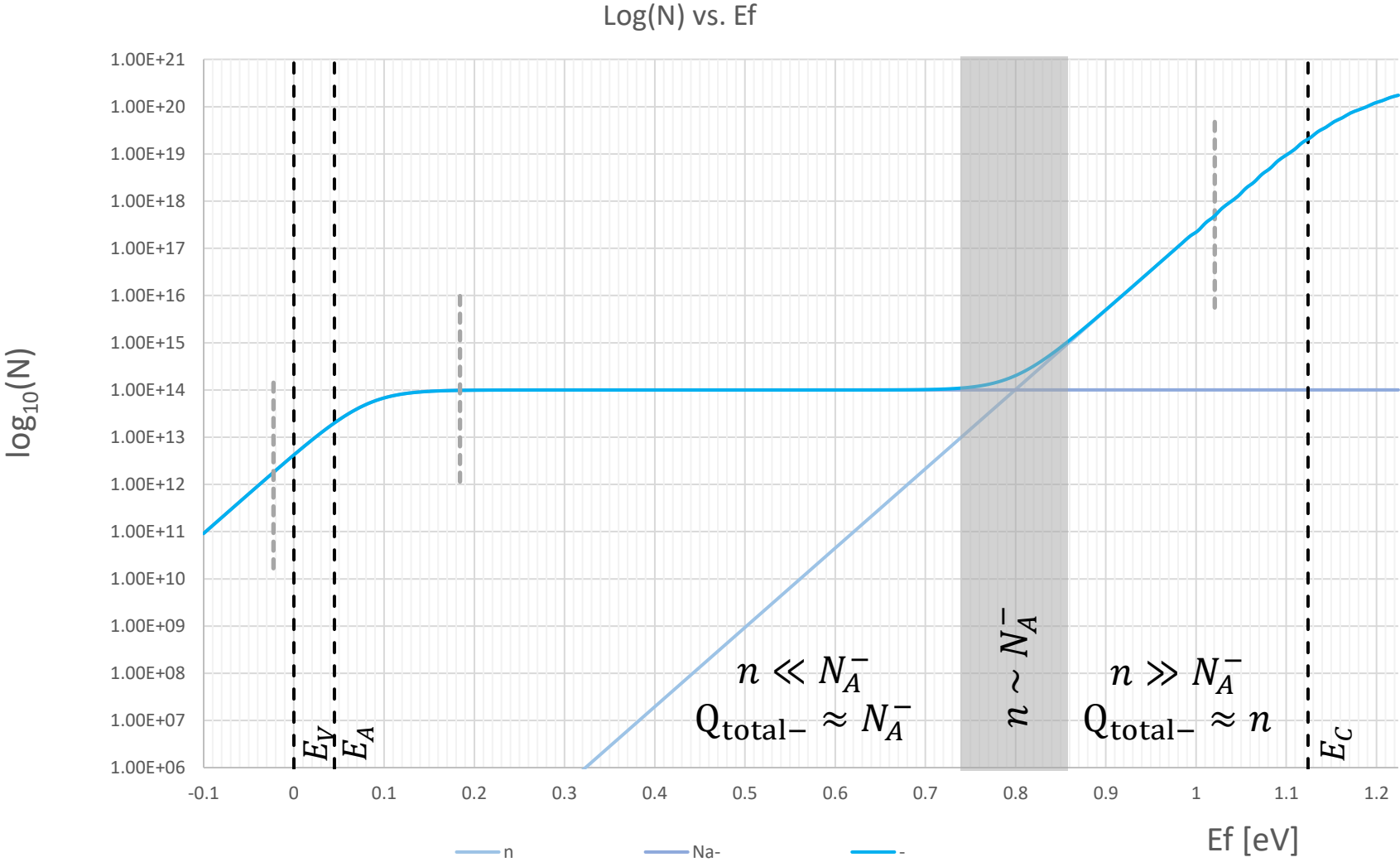
**Three regions** can be distinguished for each sum (three for  $n + N_A^-$  and three for  $p + N_D^+$ ), which are in parallel with the regions seen before.

Intrinsic: Most of the positive(/negative) charges come from the band structure  $p(/n)$ , hence  $N_D^+ (/ N_A^-)$  can be neglected

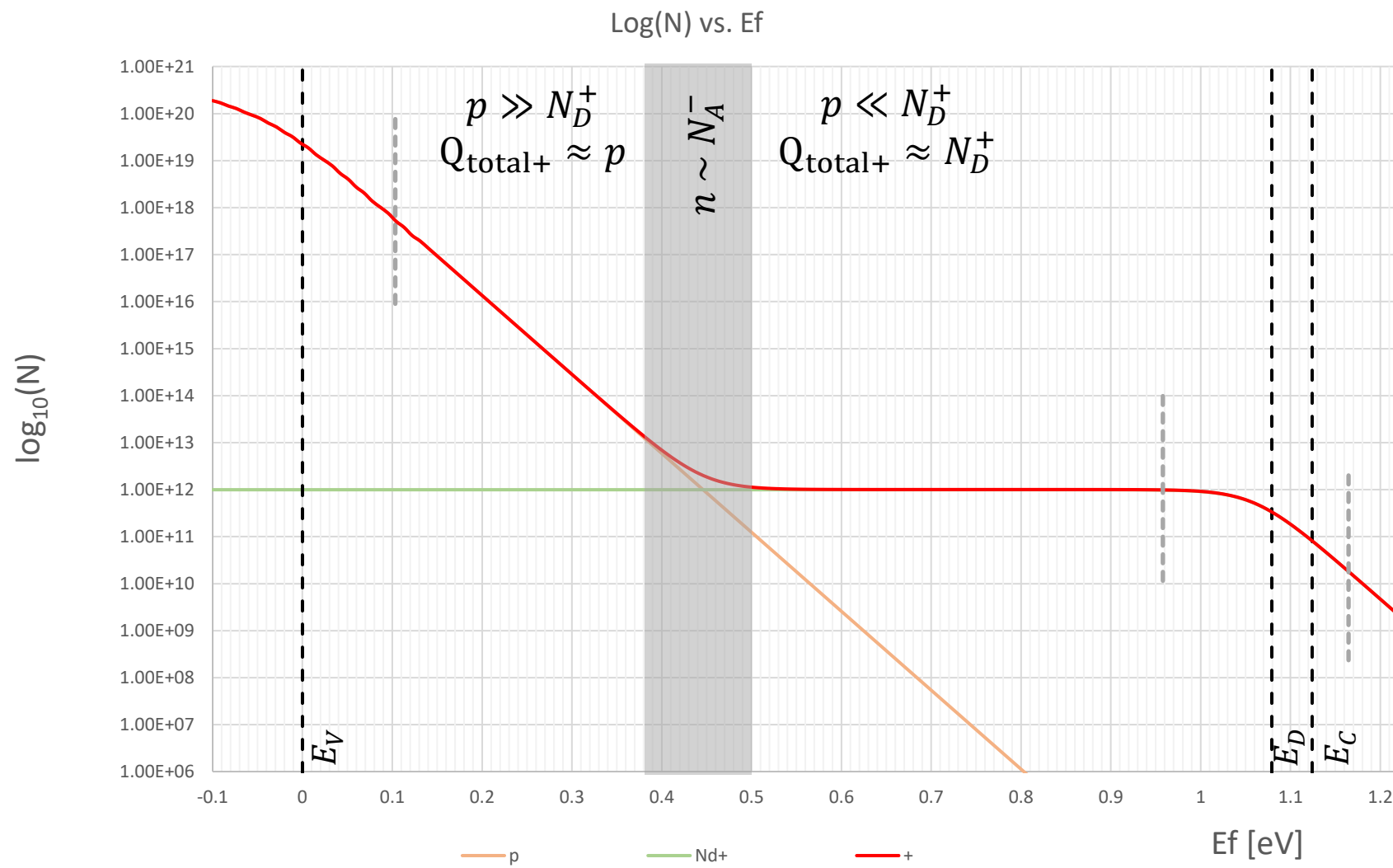
Extrinsic: Most of the positive(/negative) charges come from the ionized dopants  $N_D^+ (/N_A^-)$ , hence  $p(/n)$  can be neglected.

Intermediate: Neither  $p(/n)$  nor  $N_D^+ (/N_A^-)$  can be neglected, since their values are in of the same order of magnitude.

$$n + N_A^-$$



$p + N_D^+$



# Charge neutrality: intrinsic

Without the presence of dopants, charge neutrality amounts to

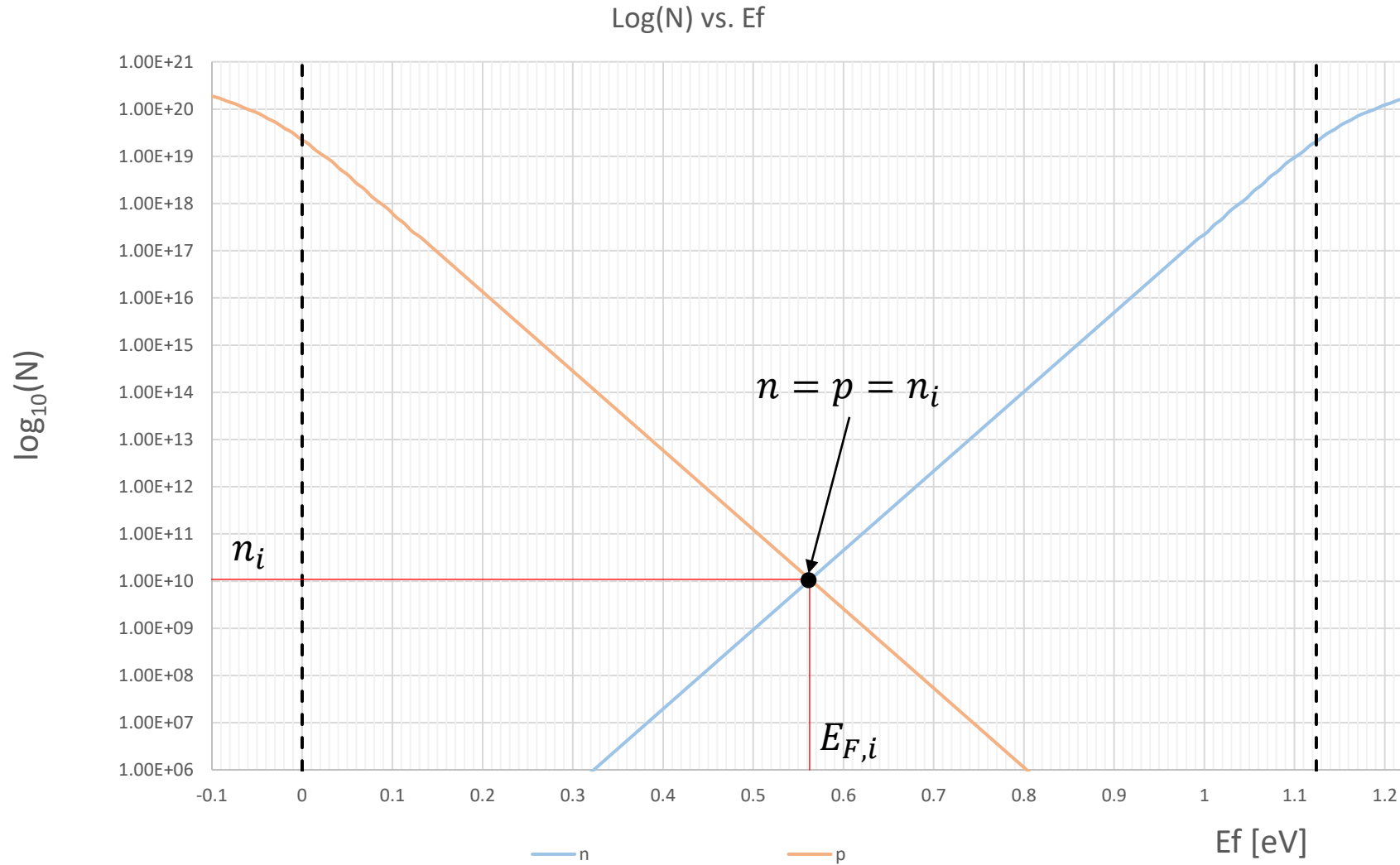
$$p = n = n_i,$$

with  $n_i$  called the intrinsic carrier concentration. There are equal amounts of electron and hole charge carriers, so the sample is neither p- nor n-type. We say it is intrinsic.

This does not mean that  $E_F$  lies in the middle of the bandgap, though for some semiconductors this is a good approximation. The associated  $E_F$  is labeled  $E_{F,i}$ , and depends on the difference in density of states between the valence and conduction bands.

# Charge neutrality: intrinsic

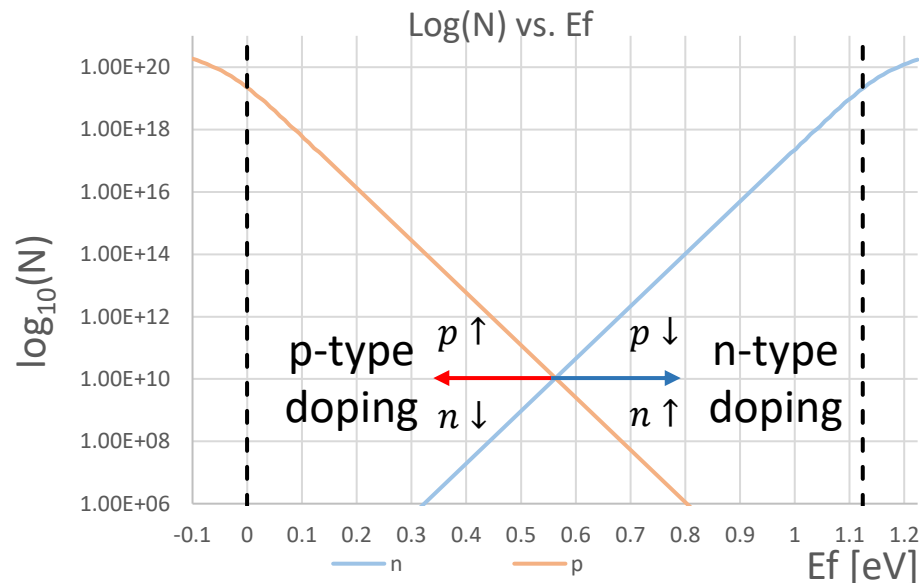
$$N_C \cdot \exp\left(\frac{E_{F,i} - E_C}{k_B T}\right) = N_V \cdot \exp\left(\frac{E_{V,i} - E_F}{k_B T}\right) = n_i$$





# Mass action law

The slope (in the log()) plot) of both  $n$  and  $p$  are equal in magnitude and opposite in sign. This means that any shift in  $E_F$  will lead to an increase in one and an equal and opposite reduction of the other.



Thus, their product will remain constant, as long as we remain in the Maxwell-Boltzmann regime (non-degenerate):

$$n \cdot p = n_i^2$$

# Charge neutrality: with dopants

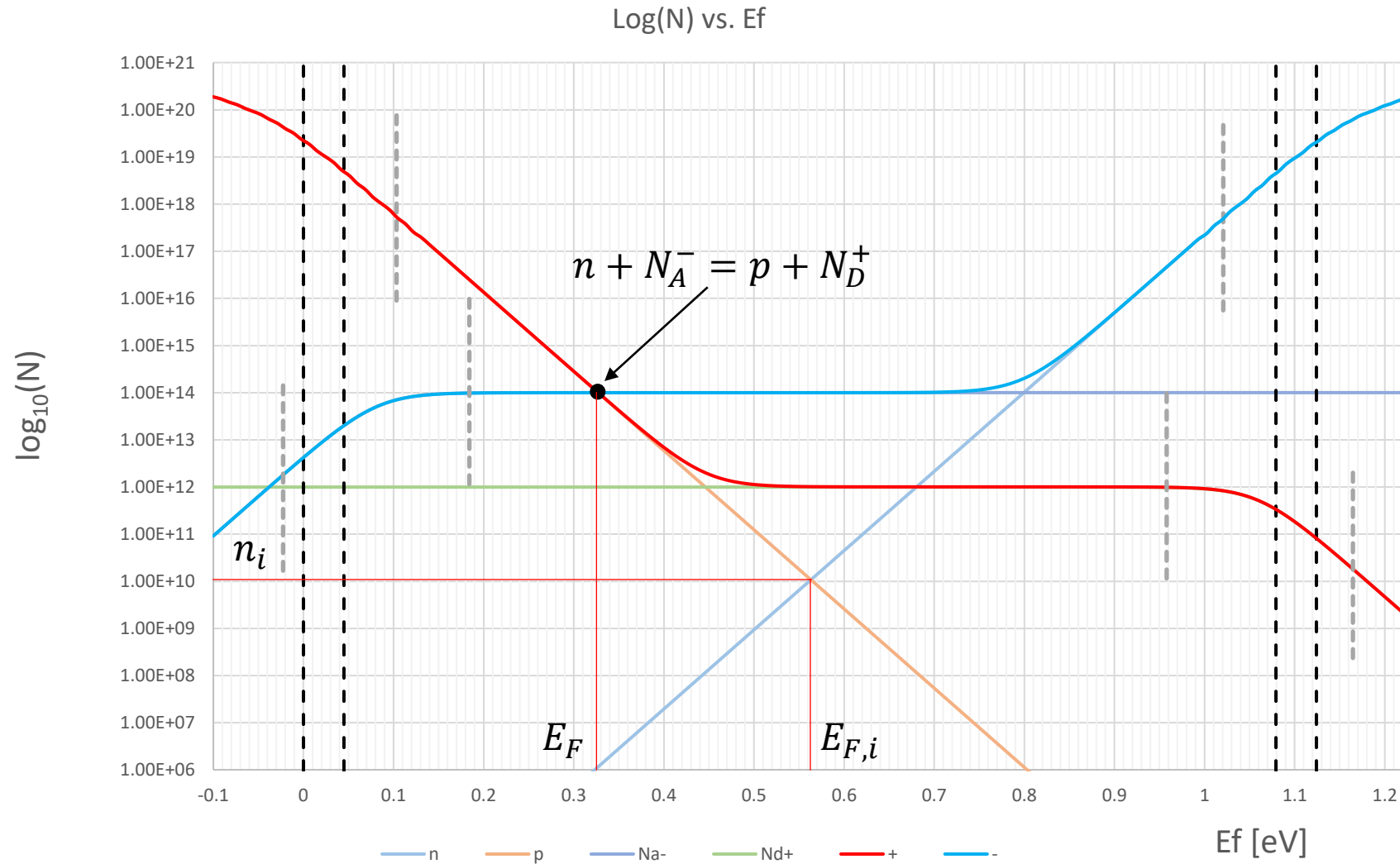
If the sample is doped with levels of dopants above  $n_i$ , then the p/n line will intersect with  $N_A^-/N_D^+$  instead of n/p respectively.

This creates an imbalance between n and p: we have created majority and minority charge carriers. If  $E_F < E_{F,i}$  then the sample has become p-type, and if  $E_F > E_{F,i}$  the sample has become n-type.

Full charge neutrality (CN), without assumptions, takes on the form:

$$N_C \cdot F_{\frac{1}{2}} \left( \frac{E_F - E_C}{k_B T} \right) + \frac{N_A}{1 + 4 \exp \left( \frac{E_A - E_F}{k_B T} \right)} = N_V \cdot F_{\frac{1}{2}} \left( \frac{E_V - E_F}{k_B T} \right) + \frac{N_D}{1 + 2 \exp \left( \frac{E_F - E_D}{k_B T} \right)}$$

# Charge neutrality: p-type example



# Regimes: saturation

p-type example

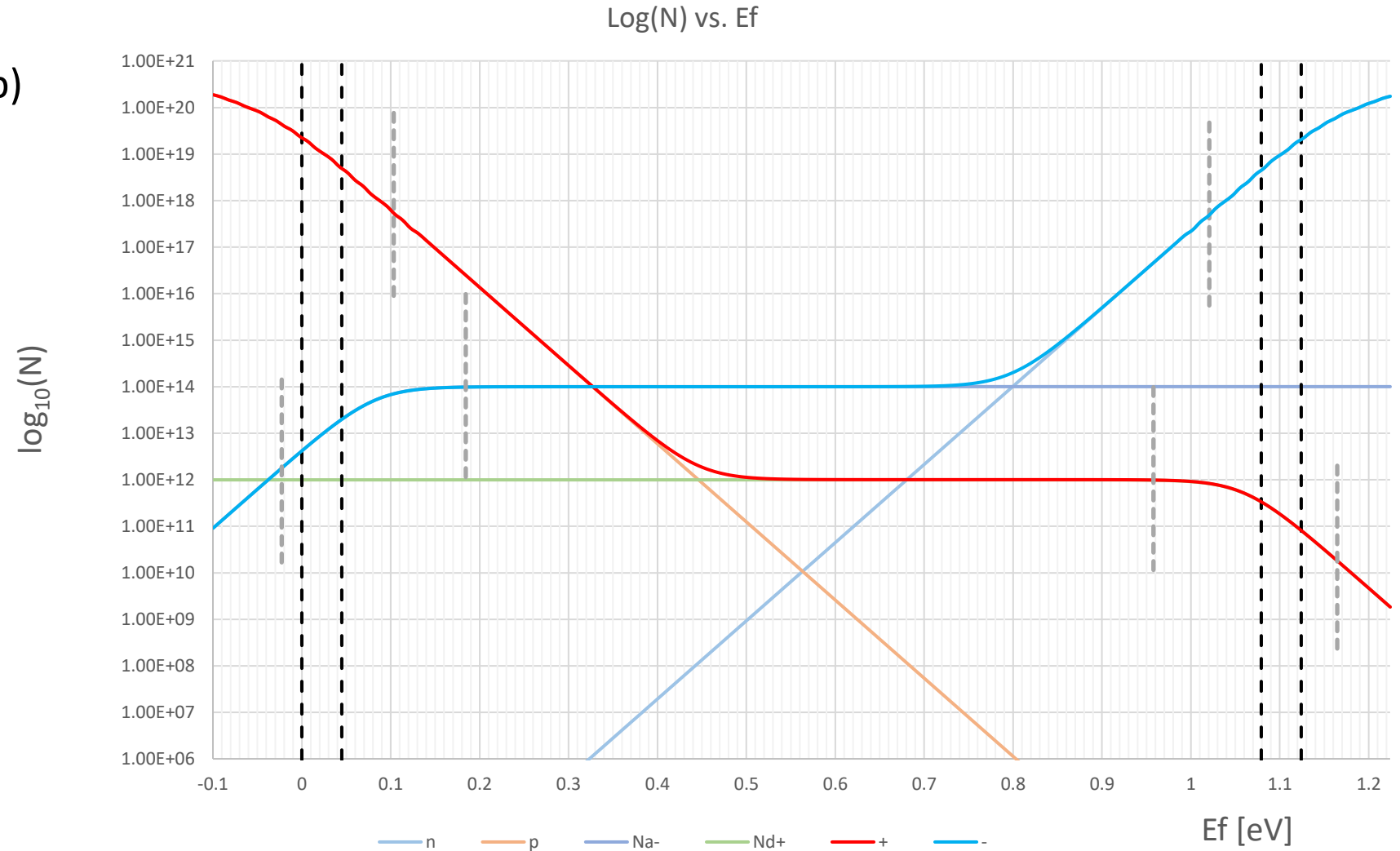
One of the carrier lines (n/p) crosses one of the fully ionized dopant lines ( $N_A^-$  /  $N_D^+$ ).

CN (p-type):

$$N_A - N_D = N_V \cdot \exp\left(\frac{E_V - E_F}{k_B T}\right)$$

CN (n-type):

$$N_D - N_A = N_C \cdot \exp\left(-\frac{E_C - E_F}{k_B T}\right)$$



# Regimes: low-temperature/freeze-out

The majority dopant is no longer fully ionized, and crosses with either:

- **Uncompensated:** The carrier line of opposite charge
- **partially compensated:** The minority dopant line which will be fully ionized

# Regimes: uncompensated freeze-out

n-type:

$$\frac{N_A}{1+4 \exp\left(\frac{E_A-E_F}{k_B T}\right)} = N_V \cdot \exp\left(\frac{E_V-E_F}{k_B T}\right)$$

p-type:

$$\frac{N_D}{1+2 \exp\left(\frac{E_F-E_D}{k_B T}\right)} = N_C \cdot \exp\left(\frac{E_F-E_C}{k_B T}\right)$$

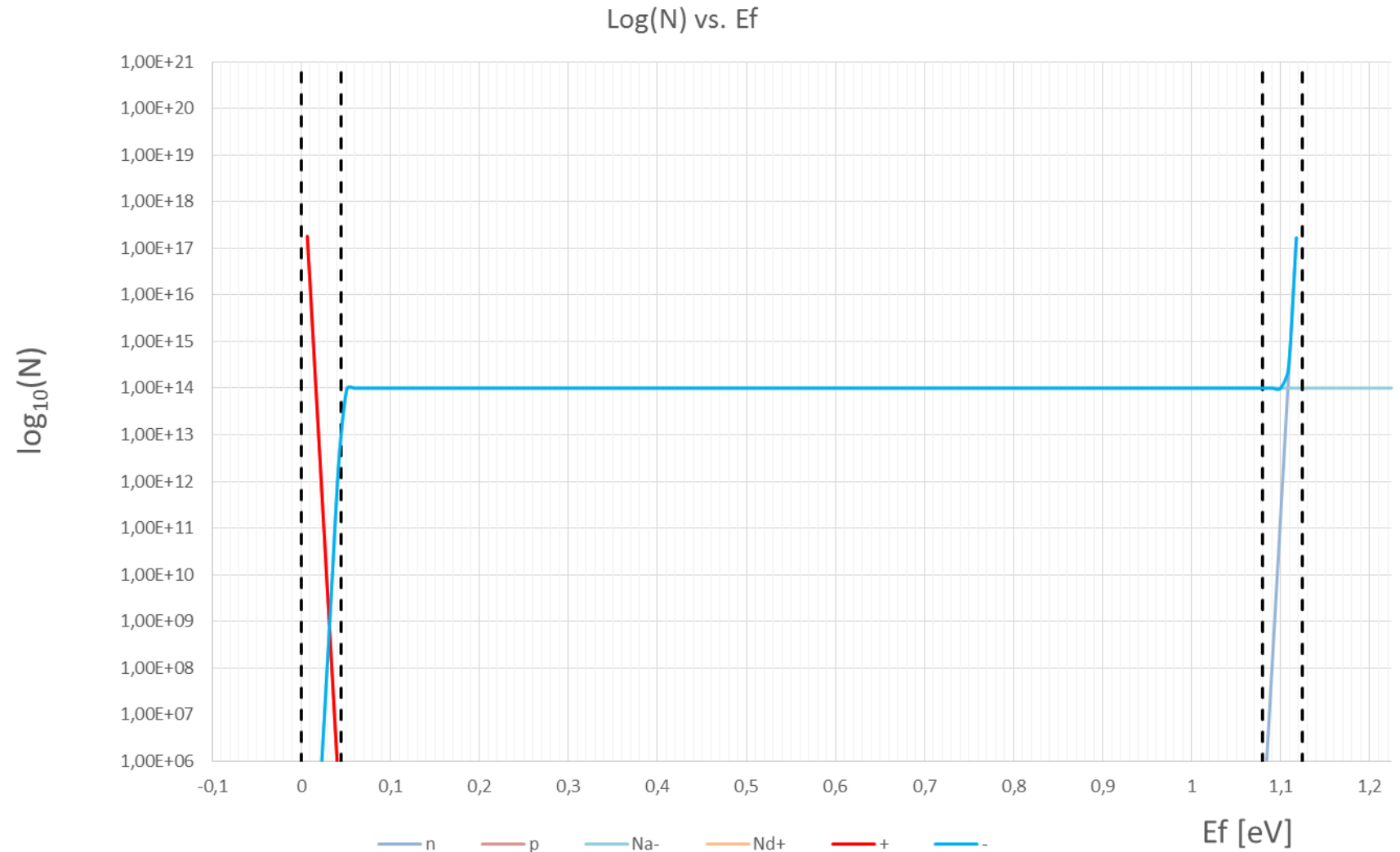
Possibly make use of MB:

n-type:

$$\frac{N_A}{4} \exp\left(-\frac{E_A-E_F}{k_B T}\right) = N_V \cdot \exp\left(\frac{E_V-E_F}{k_B T}\right)$$

p-type:

$$\frac{N_D}{2} \exp\left(-\frac{E_F-E_D}{k_B T}\right) = N_C \cdot \exp\left(\frac{E_F-E_C}{k_B T}\right)$$



# Regimes: Partially compensated freeze-out

n-type:

$$\frac{N_A}{1 + 4 \exp\left(\frac{E_A - E_F}{k_B T}\right)} = N_D$$

p-type:

$$\frac{N_D}{1 + 2 \exp\left(\frac{E_F - E_D}{k_B T}\right)} = N_A$$

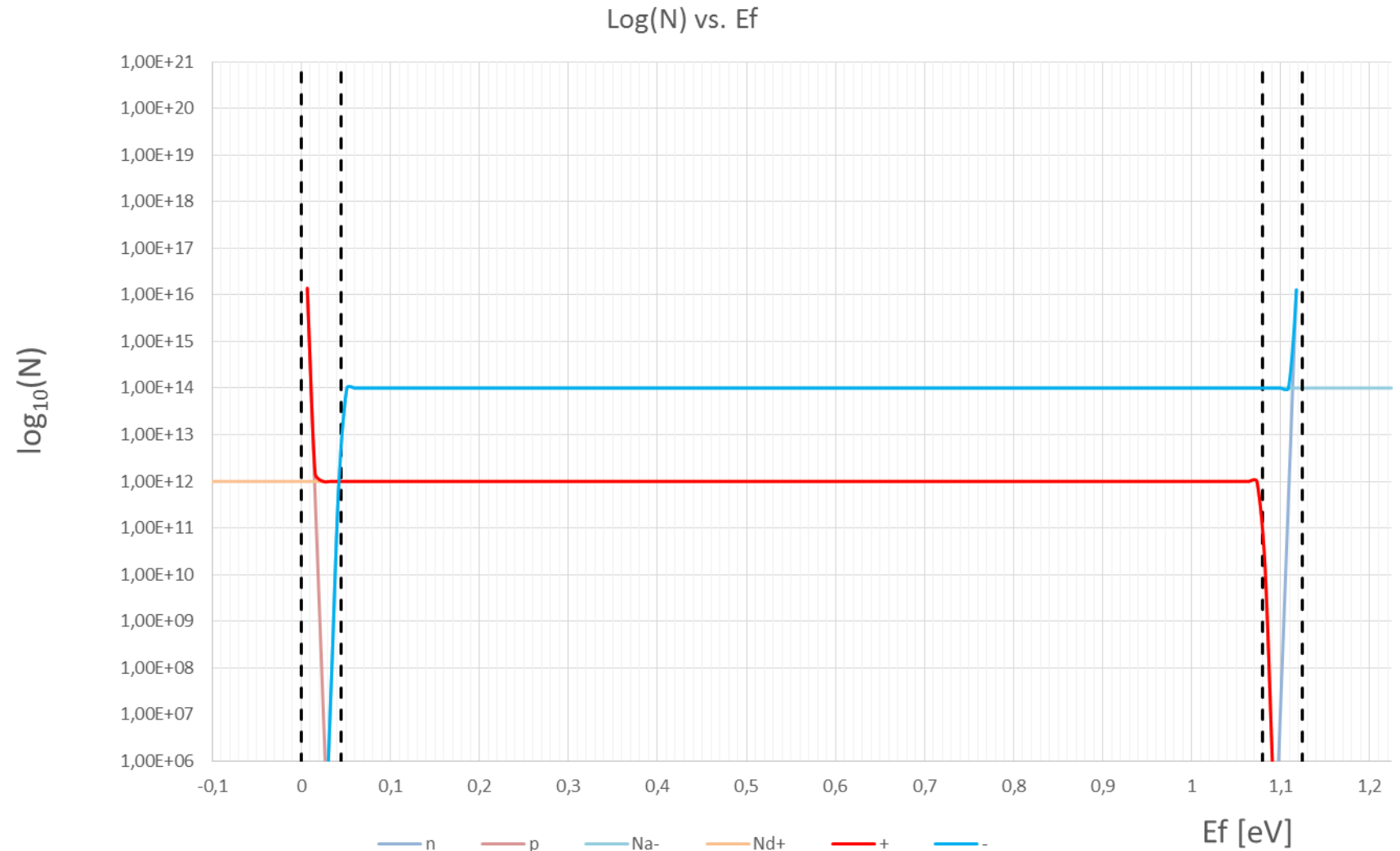
Possibly make use of MB:

n-type:

$$\frac{N_A}{4} \exp\left(-\frac{E_A - E_F}{k_B T}\right) = N_D$$

p-type:

$$\frac{N_D}{2} \exp\left(-\frac{E_F - E_D}{k_B T}\right) = N_A$$



# Regimes: High temperature

As the temperature is increased from the saturation regime, no more carriers are added from the dopants (already fully ionized), but a larger fraction of the carriers will be provided from the bands.

There comes a point, where the minority carriers are no longer negligible ( $n \approx p$ ): we have entered the high temperature regime.

If the temperature is increased further, the contribution from the dopants becomes negligible ( $n \approx p \gg N_A^- \text{ or } N_D^+$ ). The sample has returned to fully intrinsic. (see previously)



# Regimes: High temperature

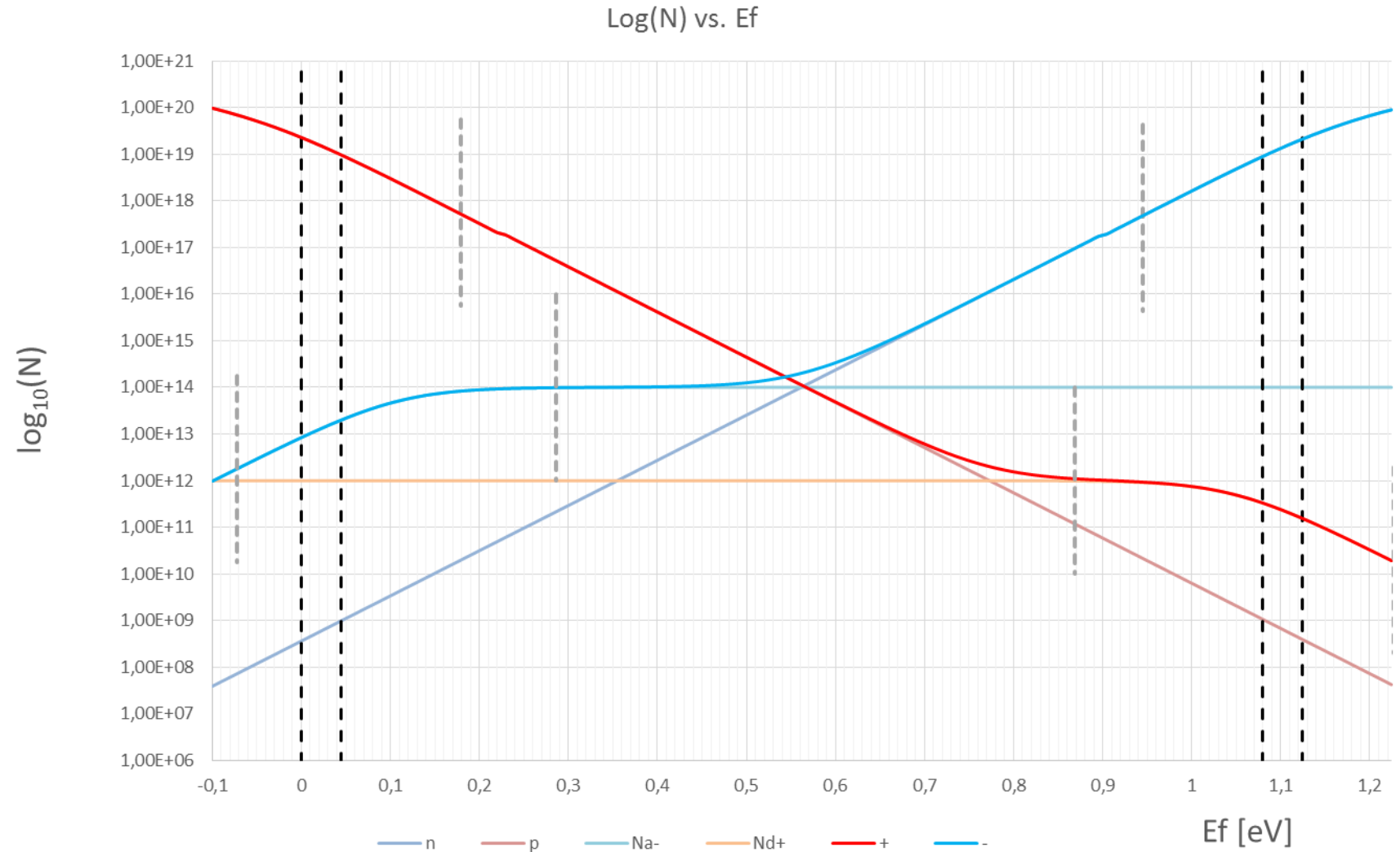
CN:

$$n + N_A = p + N_D$$

$$N_C \cdot \exp\left(\frac{E_F - E_C}{k_B T}\right) + N_A = N_V \cdot \exp\left(\frac{E_V - E_F}{k_B T}\right) + N_D$$

Which will need the mass action law to solve:

$$n \cdot p = n_i^2$$



# General method

- Start by sketching out the  $\log(N)$  graph for the given situation.
- No matter what the required value is, start with charge neutrality (CN) because that is the constraining equation. Using the sketched graph determine which simplifications you could apply to CN if necessary.
- If all goes well, you should be able to analytically solve for the desired unknown. Possibly in function of other unknowns. (e.g. session 4.1.d). In some cases, using the mass action law may be required.
- Look back at what assumptions you made, and check whether or not their condition is met. If not, a related regime (set of assumptions) must be used instead. Usually this will be because you oversimplified and find out some values are non-negligible.