5. Fundamentals of Optoelectronics

5.1 Materials and Radiative Recombination

5.1.1 Basic Questions and Material Issues

Basic Questions

- With "**optoelectronics**" in the context of this lecture we mean *only* electronic devices based on semiconductors where *recombination processes emit light*. We call this radiation process **spontaneous emission** of light, because it just happens statistically without any other ingredients but electrons and holes.
  - We thus do not (yet) look at the opposite process - the *absorption* of light, important in photo-diodes (or solar cells as already discussed before).
  - *Transmission* of light in waveguides (which might be integrated on a chip) is also not considered here.
- We have seen that silicon is an indirect semiconductor and recombination proceeds via deep levels. The energy released does not produce photons in an appreciable amount and **Si** is therefore not useful for optoelectronic applications.
  - This is, however, not a general truth. While recombination via *deep levels* as the required third partner does not produce light, indeed, recombination proceeding via some other third partner may. We will see that there are indirect semiconductors that emit enough light to be useful for practical applications.
  - But generally, we are looking for *direct* semiconductors where it can be expected that recombination does result in light production.
- This leads us to some general questions which can be translated to requests for material properties. Let us consider the more fundamental ones:
- The *first* question is: *What is the wavelength of the light produced?*
  - If the light is produced by direct band-to-band recombination, we have of course

$$h \cdot \nu = E_C - E_V$$

  - If the radiative recombination proceeds from some other energy states we simply replace $E_C - E_V$ by ΔE, the relevant energy difference.
  - With $c_{mat} = \nu \cdot \lambda$, and c_{mat} = velocity of light in the material = c_0 / n (with c_0 = velocity of light in vacuum, and n = refractive index of the material), we obtain

$$\lambda = \frac{h \cdot c_0}{\Delta E \cdot n}$$

- This leaves us with further material-related questions:
  - *First*, we are asking about the value of ΔE, or in most cases $E_C - E_V$, for optoelectronic materials. The answer comes from the band diagram and from finer details, still to be considered.
  - *Second*, we now must know the (possibly complex) **refractive index** of the material. This is not only important for the value of the wave length *in* the material, but especially for the transmission of light *out* of the material – where the difference in the refractive indices between two materials is a prime property of interest. The **refractive index** of a semiconductor is a new property that we did not address before.
- The *second* question coming to mind is: *How much light is produced by recombination*, or more precisely, what is the **quantum efficiency** η_{qu}, defined as the fraction of recombination events producing light?
  - For this we have to look at the various pathways open for recombination. In the preceding chapters we have discussed recombination in general and for *one* particular mechanism in detail.
  - However, there might be several mechanisms for recombination open to minority carriers, and only one might produce light. We thus must consider recombination in optoelectronic materials in more detail.
- *Third*, we may wonder about the *absolute intensity* or even more specific, *the intensity density* we can produce.
  - In other words, how many light producing recombination events per second are attainable in a *given volume* of material? What is the limit and which factors determine it?
  - Or, reformulated in technical terms: How do we produce a large non-equilibrium density of minorities (and majorities, too)? How do we inject electronically (by currents driven by external voltages) high densities of carriers in small volumes with no way out but recombination?
  - This question leads to the overwhelmingly complex issue of heterojunctions, quantum-wells, and the like.
- Now that we produced light, we must ask our *fourth* question: *How do we get it out of the semiconductor* ? Which percentage of the light produced will actually escape – some light, for sure, will be absorbed *in* the material.
  - Will it come out in all directions, with a preferred direction, or even as a ***LASER*** beam?
  - What do we have to do to optimize whatever we want?
  - How do we meet the two basic requirements for LASER activity – *inversion* and *feed-back* (whatever that means; we will come back to it)?
- We now ask the *fifth* question: *What can we do to modify the wavelength of the emitted light?*

- Can we "tune" a given semiconductor, or mix different ones? What are the criteria for success?

And *finally*, for question number *six*, we must consider the technology: *How do we make the needed materials and devices?*

- What technologies exist, what are the pros and cons?
- What can we use from **Si** technology? What kind of technologies do we need that are specific to optoelectronics ?

All these questions are interrelated; very often we can not deal with just one at a time. In other words, if you optimize one property, you will change most of the others, too.

- Selecting materials and processes for an optimized device is a complex process and still a topic of front-end research.
- While much progress has been made during the last **20** years or so, there is still no cheap and reliable *blue* semiconductor *Laser* although first prototypes based on the fairly new *technical* semiconductor **GaN** (gallium nitride) have been introduced around **1998**.
- It is a safe bet that we will see a lot more progress for the next **20** years, and that it will come from rather involved physics and materials research employing quite a bit of quantum theory, new concepts like "**photonic crystals**" and "**spintronics**" – buzz words that you, the student, may not have heard yet, but that may well become part of your professional career.

Material Issues

Pondering the questions from above, it becomes clear very quickly that we need several suitable semiconductors to cover all aspects of optoelectronics.

- It also becomes clear that we have to look at more properties than we did for **Si** – the *dielectric constant*, e.g., is a prime parameter now.
- The value of the band gap, too, is now of prime importance. (We wouldn't have cared much if it would have been somewhat different in **Si**!)
- The precise mechanisms for recombination are a prime matter of interest. In **Si**, all that counted was that you had some, but not too many deep level around midgap, giving a large recombination life time. With optoelectronics we may have to make sure that recombination proceeds exactly as needed.
- Let's start with looking at major semiconductors and their properties in detail. (If you are interested in more data, or in other semiconductors, have a look at the relevant data collection of the Ioffe Institute or at that of Derek Palmer.)

Properties	Si	Ge	GaAs	InP	InSb	$In_{0.53}Ga_{0.47}As$	GaP	GaN	SiC	Diamond	Remarks
Crystal											
Unit weight [mol]	29.09		144.63	145.79		168.545					
Density [g/cm^3]	2.33	5.32	5.32	5.49	5.77	5.49	4.14	6.1	3.166 (cubic) 3.211 (hex)	3.51	
Crystal structure	Diamond	Diamond	Zincblende (Sphalerite)	Zincblende	Zincblende	Zincblende	Zincblende	Wurtzite	Many variants: cubic, hex, rhombohedral	Diamond	
Lattice constant [nm]	0.5431	0.565	0.565	0.587	0.648	0.5867	0.545	a = 0.319 c = 0.519	a = 0.30 c many values	0.357	
Transport properties											
Band gap [eV]	1.12	0.66	1.42	1.35	0.17	0.75	2.26	3.4	2.39 - 3.26	5.47	
Type	indirect	indirect	direct	direct		direct	indirect	direct	indirect	indirect	
Effective e$^-$ mass [m^*/m_0]	0.98						0.35	0.2	0.24 - 0.7		
Effective h$^+$ mass [m^*/m_0] light heavy	0.16 0.49		0.082 0.45	0.12 0.56	7.3	0.051 0.50	0.14 0.79	0.3 1.4	0.9		
N_{eff} of CB [10^{18} cm^{-3}]	28 (32)	10.4	0.47	0.54	0.042	0.21	18				
N_{eff} of VB [10^{18} cm^{-3}]	10 (18)	6	7	2.9		7.4	19				
n_i [10^6 cm^{-3}]	6,600 (13,000)		2.2	5.7		63,000					
Mobility (undoped) [cm^2/Vs] μ_n μ_h	1,500 450	1,900 3,900	8,500 450	5,000 200	80,000 1,250	14,000 400	300 150	1,000 200	500 - 1,000 20 - 50	200 - 2,200 1,800 - 2,100	

Lifetime (general) [µs]	2,500		0.01	0.005		0.02					
Mechanism of lumines-cence	none		band-band	band-band		band-band	**exciton, if doped**	band-band			
Dielectric properties											
Dielectric constant at high frequency (static)	11.7	16	10.9 (12.9)	9.6 (12.4)	15.7 (16.8)	13.7	9.1 (11.1)	ϵ_{xx}, ϵ_{zz}: 5.35, 5.8 (9.5, 10.4)	ϵ_{xx}, ϵ_{zz}: 6.5, 6.7 (9.7, 10)	5.5	
Breakdown field strength [kV/cm]	300		350	400		100		5,000			
Specific intrinsic resistance [MΩcm]	0.2		310	11		0.000,8					
Electron affinity [eV]	4.0	4.05	4.07	4.4	4.59	4.63	4.3	4.1			
Thermal Properties											
Expansion coefficient [10^{-6} /K]	2.6	5.9	6.86	4.75	5.37	5.66	5.3	5.59 (a) 3.17 (c)		1	
Therm. conductivity [W/cmK]	1.5	0.58	0.45	0.68	0.18	0.05	1.1	1.3	5.0	22	Cu: 4.01
Specific heat [J/gK]	0.7	0.31	0.35	0.31	0.2	0.29	0.43	0.49	0.671	0.428	Cu: 0.38
Melting point [°C]	1,412	937	1,238	1,062	527	970	1,457	2,500			

- Silicon is included as a reference (if there are several numbers, they are from different sources). We find expected properties, but also, perhaps, some unexpected ones.
  - *Dielectric constants are relatively large* even at the very high optical frequencies. This is not necessarily self-evident since at least for **Si** the only polarization mechanism operational is atomic polarization, i.e. the shift of electrons relative to the atom core.
  - There is at least one recombination mechanism not mentioned before: *Exciton* recombination.
- Let's continue by looking at recombination mechanisms in more detail.