



UiO : **Department of Physics**
University of Oslo

Low energy loss; electronic structure and dielectric properties

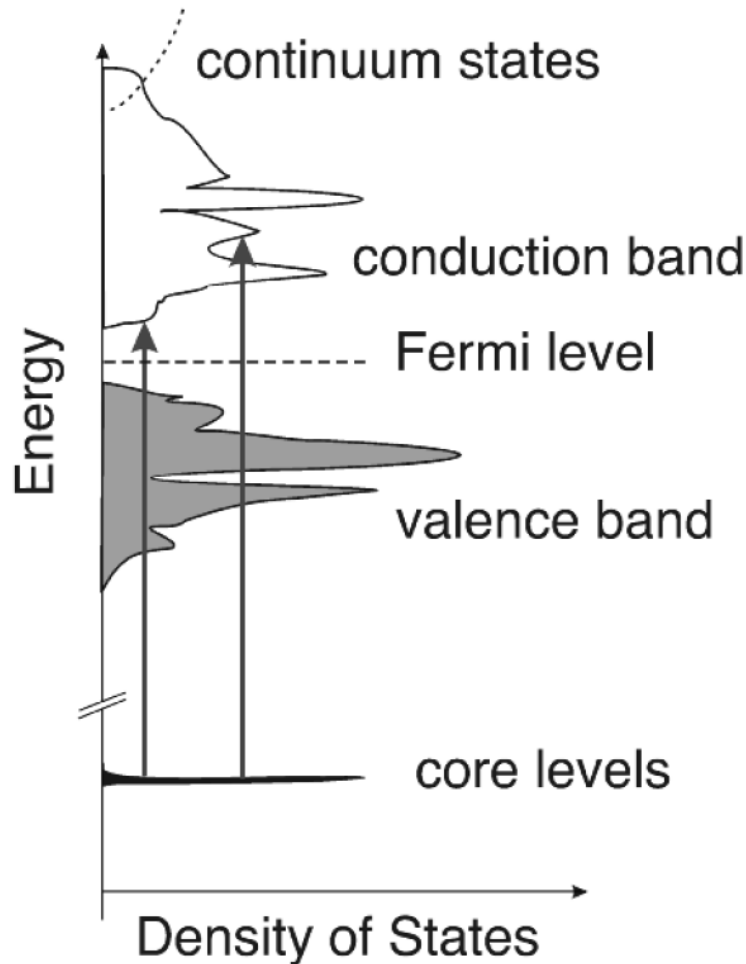
FYS5310/FYS9320

Lecture 7

02.03.2017



FYS5310 teaching schedule						
Preliminary schedule only! You should keep the class-times on Wednesdays and Thursdays open unless notified by email (or in this schedule) that there is no class						
References to the textbook to Fultz & Howe unless stated otherwise.						
Date		Time	Lecture/lab	Topic	Chapters	Homework
Wednesday	18.01.2017	14:15-16:00	Lecture	Introduction to the course. Derivation of the structure factor (01)	4.1, 4.3.1, 6.1	Exercise set 1 (handout)
Thursday	19.01.2017	12:15-14:00	Lecture	No class (SMN seminar)		
Wednesday	25.01.2017	13:15-16:00	Lab/Colloquium	Going through exercise set 1 + Lecture: The atomic form factor (02)	4.3	Excercise set 2 (handout)
Thursday	26.01.2017	12:15-14:00	Lecture	No class		
Wednesday	01.02.2017	14:15-16:00	Lab/colloquium	Going though exercise set 2		
Thursday	02.02.2017	12:15-14:00	Lecture	Uses of EELS and EELS instrumentation (03)	5.1, 5.2; W&C 37	Exercise set 3 (handout)
Wednesday	08.02.2017	14:15-16:00	Lab/colloquium	Going though exercise set 3		
Thursday	09.02.2017	12:15-14:00	Lecture	Inelastic form factors (04)	5.4.1-5.4.3 + primer on Dirac notation	
Wednesday	15.02.2017	12:15-16:00	Lab/colloquium	No class		
Thursday	16.02.2017	12:15-14:00	Lecture	Inelastic form factors, scattering cross sections, dipole selection rules (05)	5.4.4-5.4.7, W&C 39, plus Brehm and Mullin on parity and dipole selection rules	
Wednesday	22.02.2017	12:15-16:00	Lab/colloquium	No class		
Thursday	23.02.2017	12:15-14:00	Lecture	Core losses: Quantification and electronic structure (06)	5.4, W&C 39+40	Exercise set 4 (handout)
Wednesday	01.03.2017	12:15-16:00	Lab/colloquium	Going through exercrise set 4		
Thursday	02.03.2017	12:15-14:00	Lecture	Low energy loss; electronic structure and dielectric properties pt 1 (07)	5.3, W&C 38	Exercise set 5 (handout)
Wednesday	08.03.2017	12:15-16:00	Lab/colloquium	Computer lab + going through exercise set 5		
Thursday	09.03.2017	12:15-14:00	Lecture	Low energy loss; electronic structure and dielectric properties pt 2 (08)	5.3, W&C 38	
Wednesday	15.03.2017	12:15-16:00	Lab/colloquium	No class		
Thursday	16.03.2017	12:15-14:00	Lecture	No class		
Wednesday	22.03.2017	12:15-16:00	Lab/colloquium	Computer lab		



- If the initial states are sharply peaked in energy, then all transitions originate at this energy
- One particular E_i and one particular E takes you to a single point in the conduction band E_f
- In effect we are convoluting the conduction band DOS with a delta function

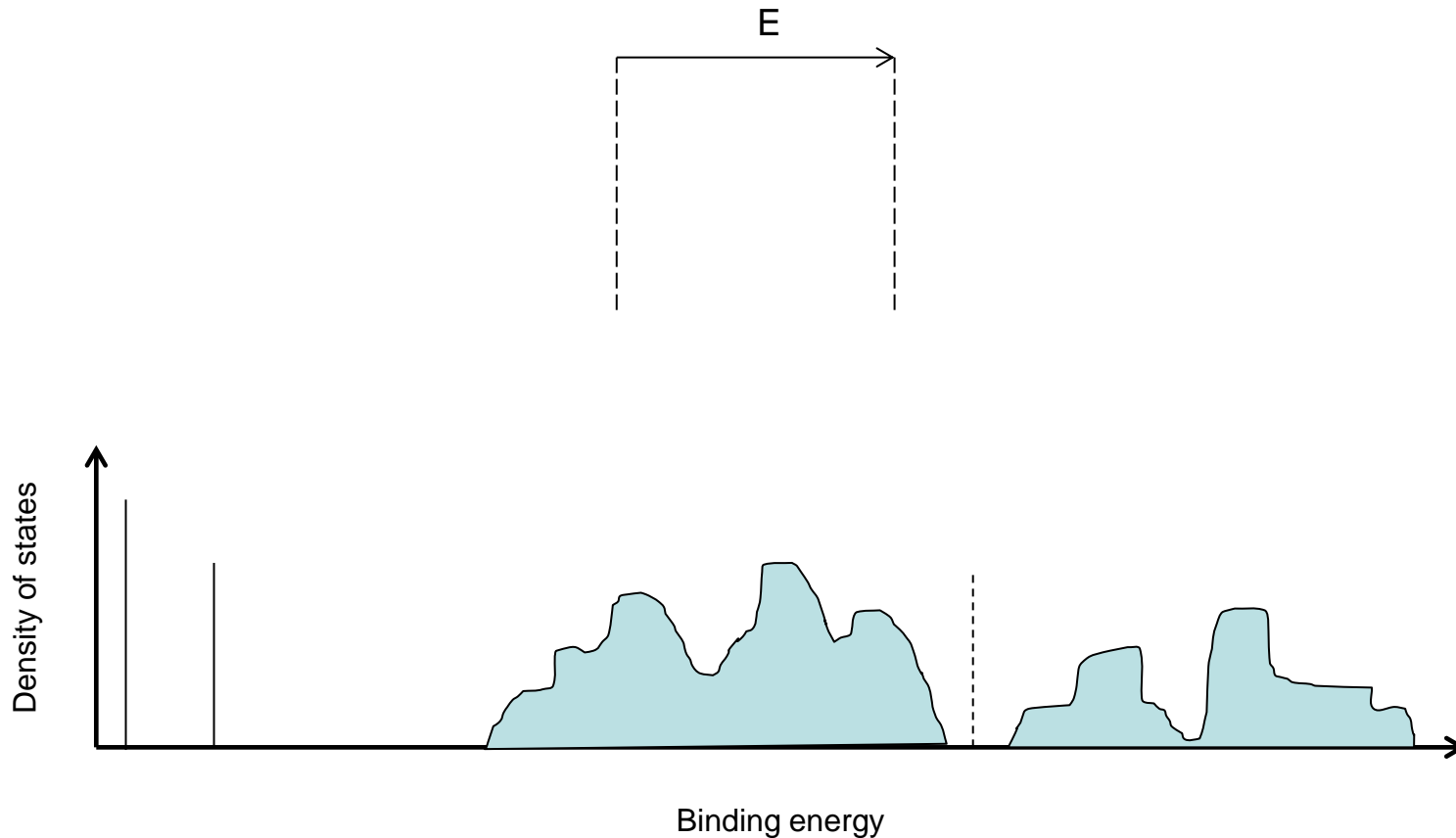
$$\text{Delta function} \otimes cDOS = cDOS$$

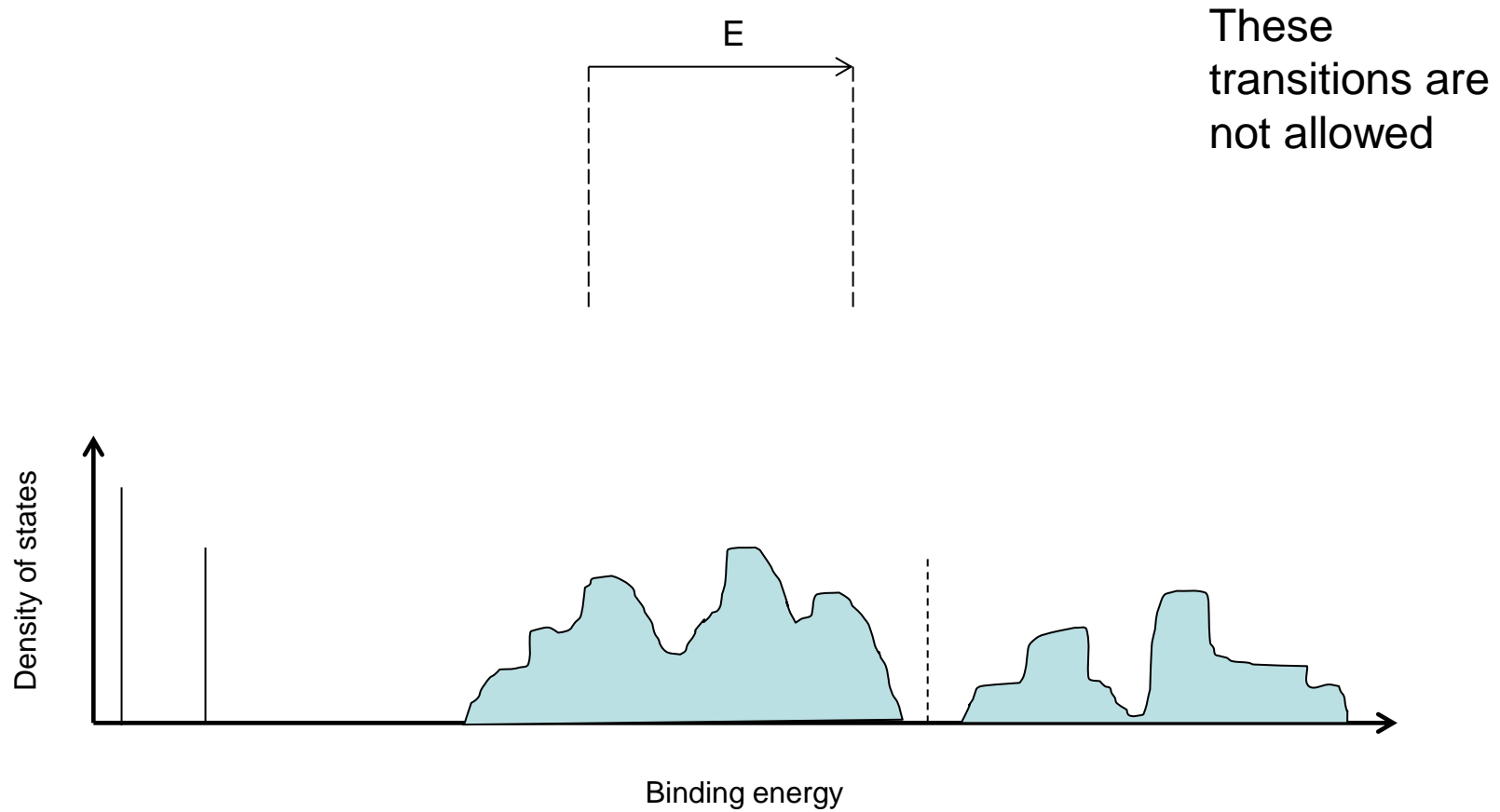
- The spectrum reflects a scaled conduction band DOS

$$vDOS \otimes cDOS = ?$$

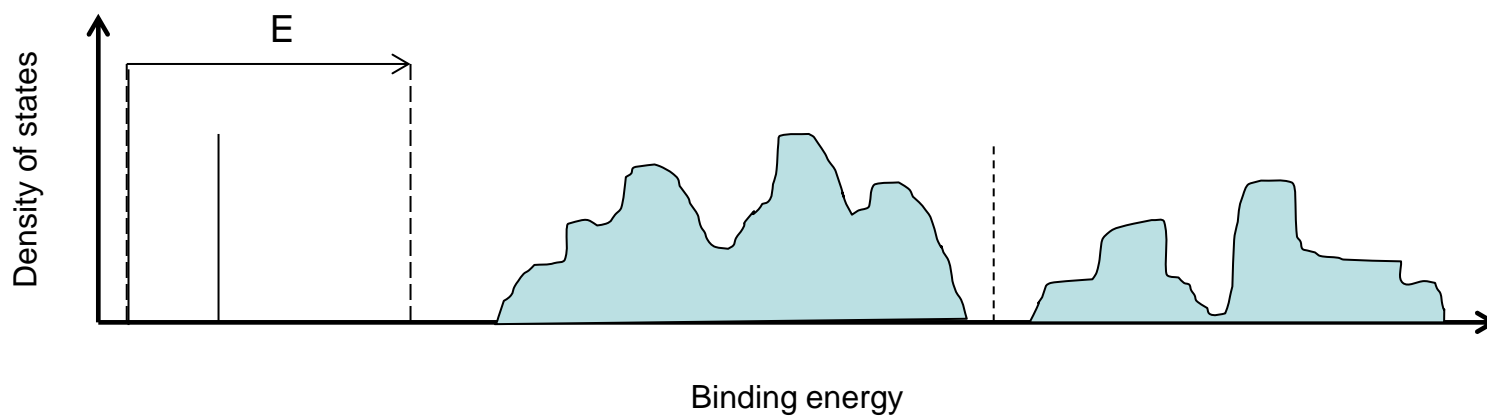
- But what if the initial states are in the valence band?

Possible transitions contributing to one point in the energy loss spectrum

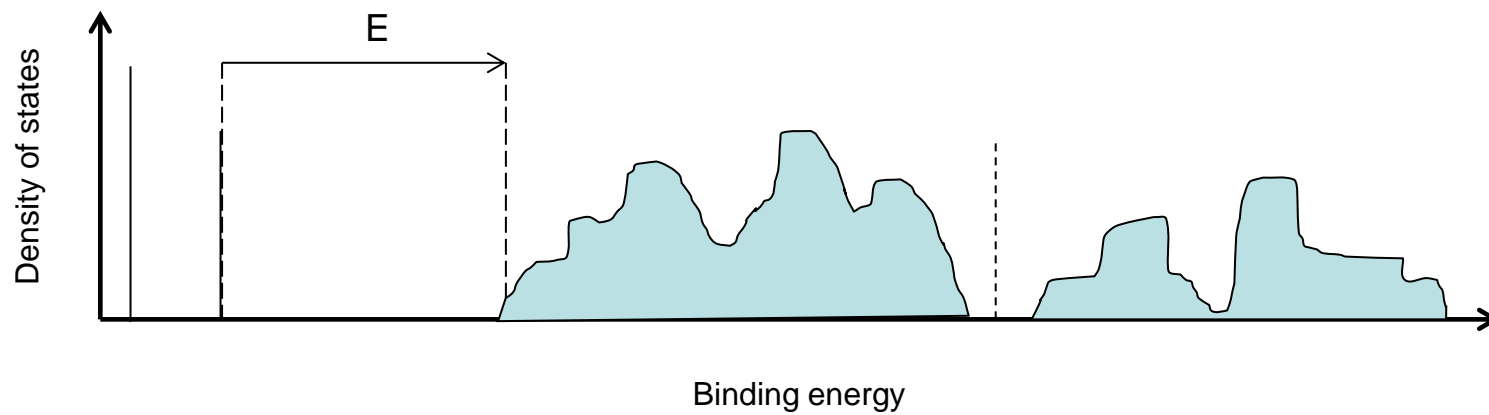




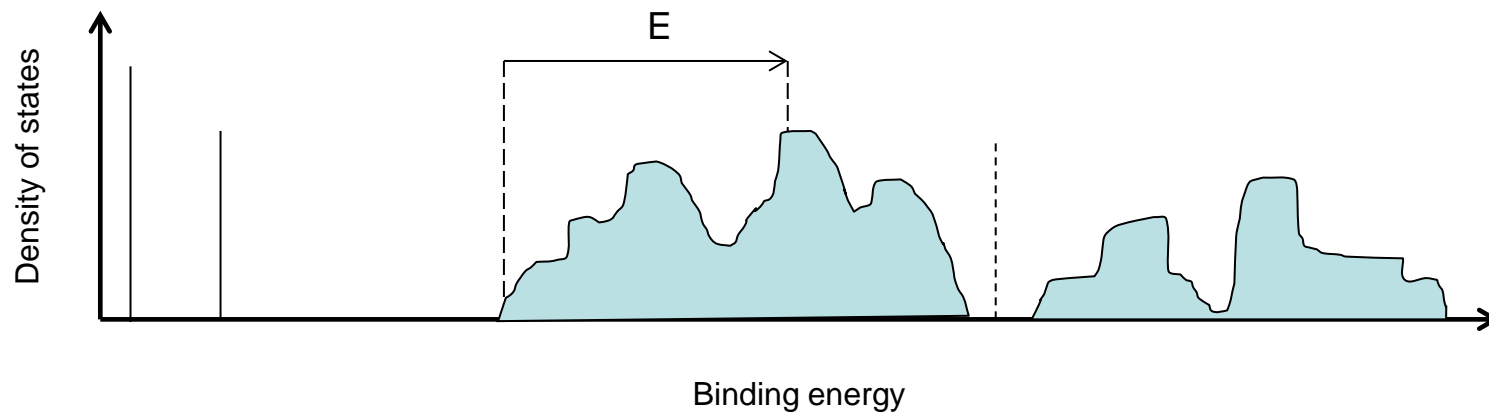
...still no
contribution to
the EELS
spectrum



What about
now?

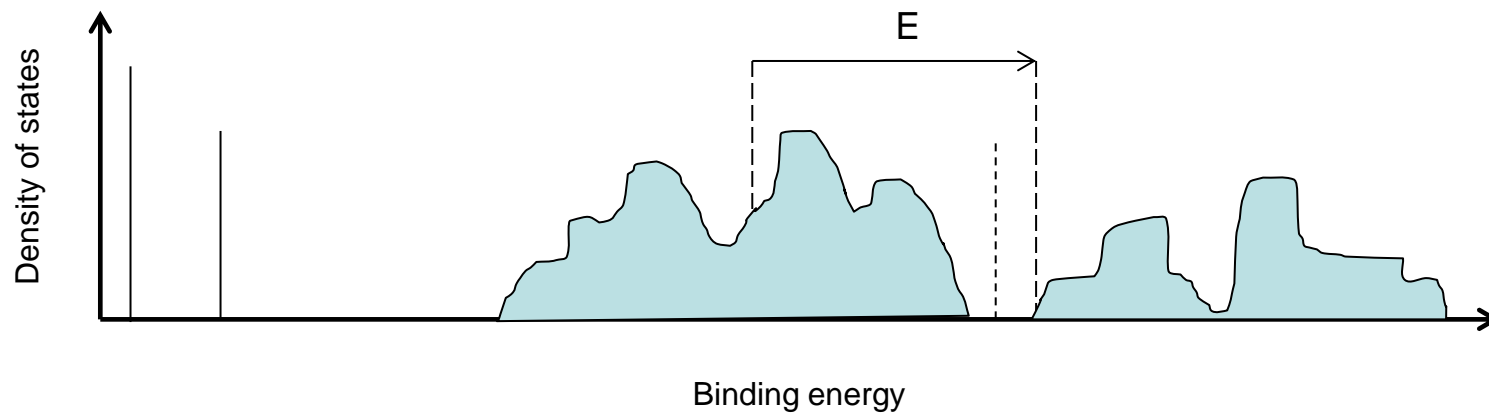


Here we see the first transition that contributes to the EELS spectrum



And this is the
final transition
that contributes

Repeat for the
next energy loss E



The EELS spectrum as a Joint Density of States

This is good for core losses:

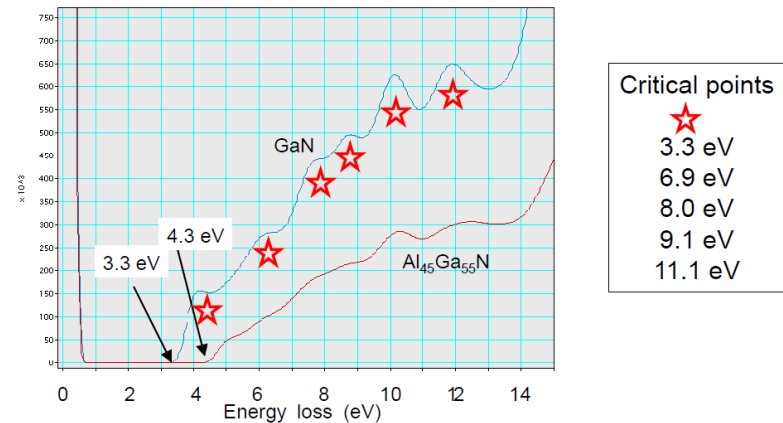
$$\frac{d^2\sigma(\Delta\mathbf{k}, E)}{d\Omega dE} = \frac{4}{a_0^2 \Delta k^4} \rho(E) |\langle\beta|e^{-i\Delta\mathbf{k}\cdot\mathbf{r}}|\alpha\rangle|^2$$

But for single electron transitions in the low loss region we need to consider the convolution of valence DOS with conduction DOS (also called Joint Density of States, JDOS):

$$I(E) \propto \int_{\varepsilon_F - E}^{\varepsilon_F} |\langle\Psi_f|e^{iq\cdot r}|\Psi_i\rangle|^2 \rho_{vb}(E_i) \rho_{cb}(E_i + E) dE_i$$

No dipole approximation?

- The low loss spectrum can be used to detect band gaps and so-called critical points in the JDOS.
- These features are very important for optical properties



Detection of band gap and critical points

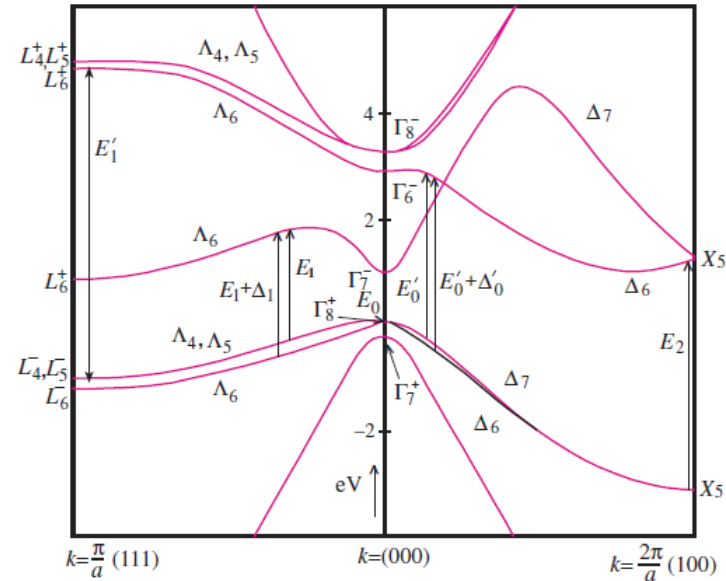


Fig. 6.13. The band structure of Ge showing the various direct transitions responsible for the structures in the imaginary part of the dielectric function shown in Fig. 6.12. The transitions giving rise to the various structures in the dielectric function are identified

Table 6.3. The measured energies [eV] of the prominent structures in the optical spectra of some diamond and zinc-blende-type semiconductors. All energies are low temperature values except that of the E_0 transition in Si, which was measured at room temperature. Compiled from data listed in [6.27], [6.28] and [6.29].

Transition	Si	Ge	GaAs	InP	GaP	GaN
E_0	4.185	0.898	1.5192	1.4236	2.869	3.302 ^a
$E_0 + \Delta_0$	4.229	1.184	1.859	1.532	2.949	3.319 ^a
E_1	3.45	2.222	3.017	3.287	3.780	7.03
$E_1 + \Delta_1$	—	2.41	3.245	3.423	3.835	
E'_0	3.378	3.206	4.488	4.70	4.72	
$E'_0 + \Delta'_0$	—	3.39	4.659	5.17	4.88	
E_2	4.330	4.49	5.110	5.05	5.22	7.63
E'_1	5.50	5.65	6.63		6.8	

^a Grown on MgO.

The dielectric function

- Describes the response of the material to an external field
- Not a constant

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

- The real term describes the polarizability
- The imaginary term describes absorption
- The «single scattering distribution» is given by

$$I(E) = \frac{2I_0 t}{\pi a_0 m_0 v^2} \operatorname{Im} \left(-\frac{1}{\varepsilon(E)} \right) \ln \left(1 + \left[\left(\frac{\beta}{\Theta_E} \right)^2 \right] \right)$$

$$\operatorname{Im} \left(-\frac{1}{\varepsilon(E)} \right) = \frac{\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}$$

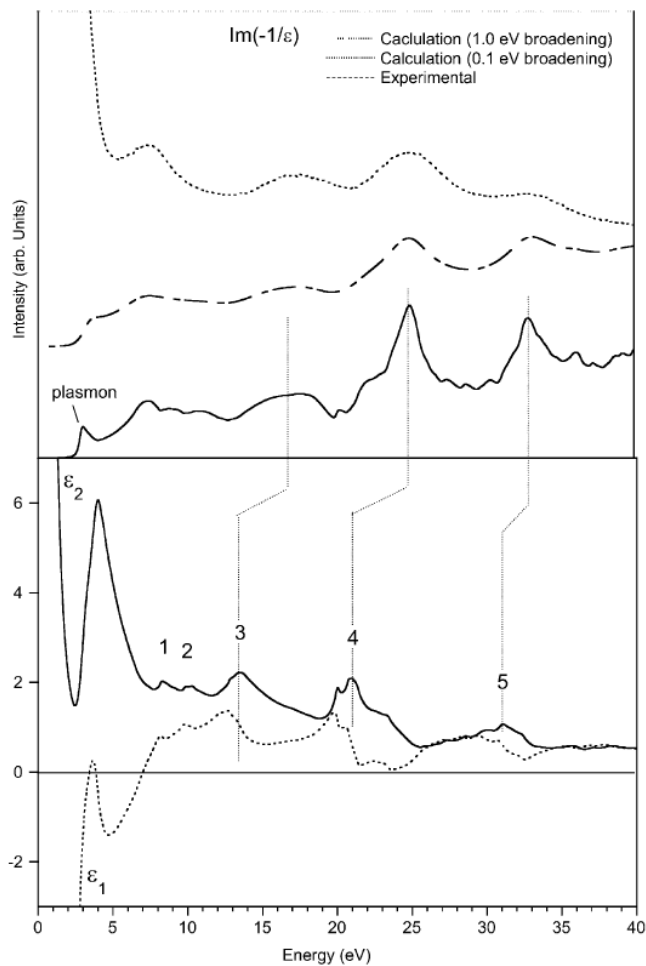


Fig. 7. ϵ_1 , ϵ_2 and the loss-function for Ag compared to the experimental loss-function. The ZLP has not been removed from the experimental spectrum. Some of the interband transitions in ϵ_2 are labeled 1–5 and these correspond to peaks in the loss-function at a higher energy, as indicated.

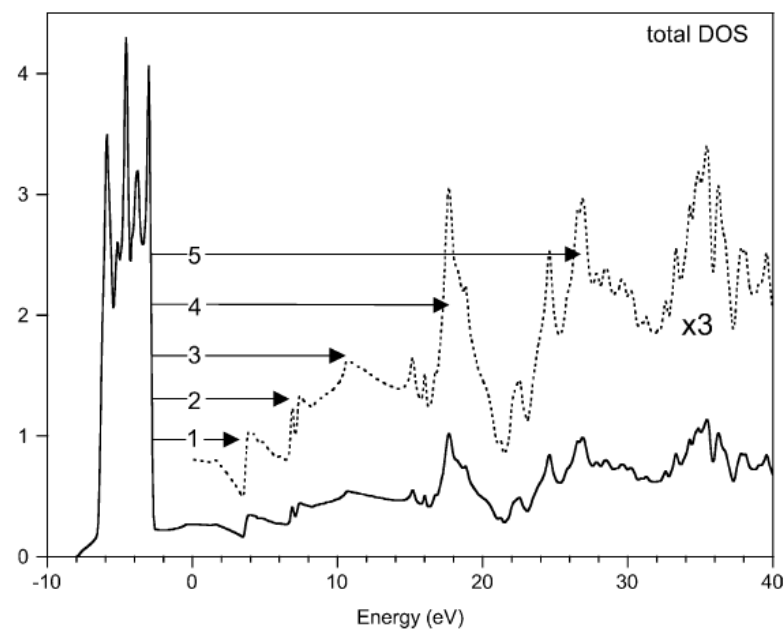


Fig. 8. Total DOS for Ag. The interband transitions for the peaks in ϵ_2 in Fig. 7 are indicated.

The dielectric polarization of the material

The polarization of a material subjected to a time varying electric field is:

$$\mathbf{P}(\omega) = \varepsilon_0 [\varepsilon(\omega) - 1] \mathbf{E}(\omega)$$

The displacement (total field) in the material is then:

$$\begin{aligned} \mathbf{D}(\omega) &= \varepsilon_0 \mathbf{E}(\omega) + \mathbf{P}(\omega) \\ &= \varepsilon_0 \mathbf{E}(\omega) + \varepsilon_0 [\varepsilon(\omega) - 1] \mathbf{E}(\omega) \\ &= \varepsilon(\omega) \varepsilon_0 \mathbf{E}(\omega) \end{aligned}$$

So what happens if $\varepsilon(\omega)=0$?

The dielectric function in the Drude model

- For free electrons in a uniform background potential, the dielectric function is

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega + i\omega/\tau}$$

- Where ω_p is a harmonic oscillator resonance frequency given by

$$\omega_p = \sqrt{\frac{ne^2}{m_0\varepsilon_0}}$$

- τ is the scattering time/damping factor

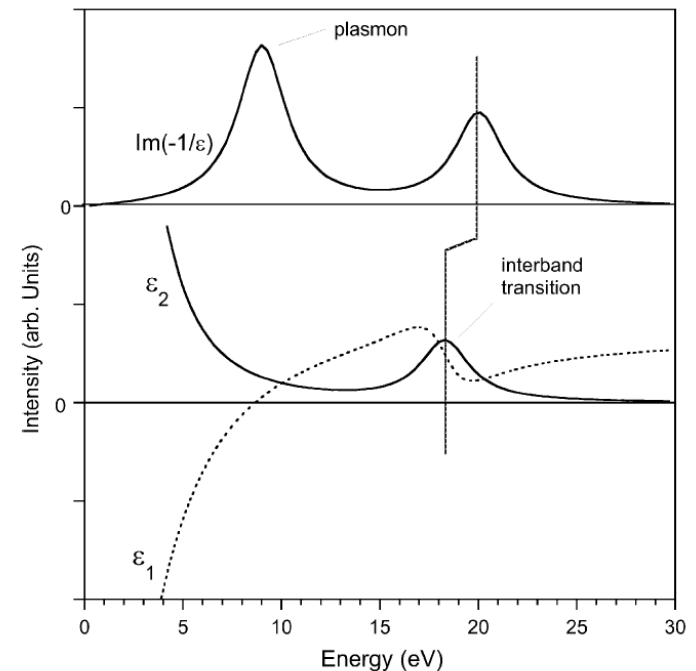
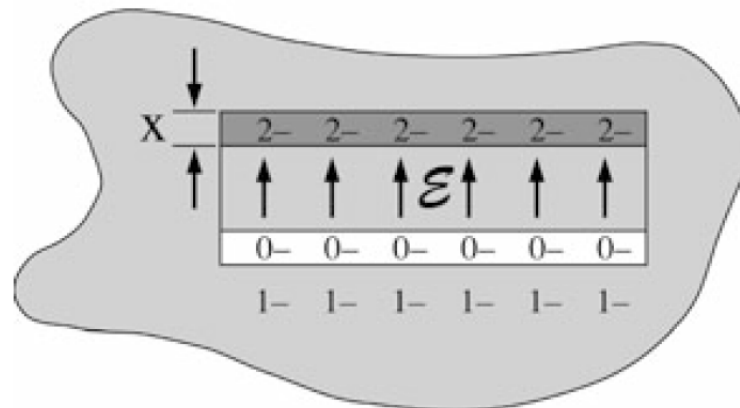


Fig. 6. Schematic of ε_1 , ε_2 and the loss-function calculated with Drude-Lorentz theory where there is a plasmon excitation and a single interband transition. There is a peak in the loss-function corresponding to the interband energy, but at a different transition to where it appears in ε_2 .

Fig. 5.7 Displacement of a slab of electric charge, leading to doubling of the charge density at the top of the slab over thickness x , and depletion of charge at the bottom. A wide, flat slab idealizes the problem as one dimensional



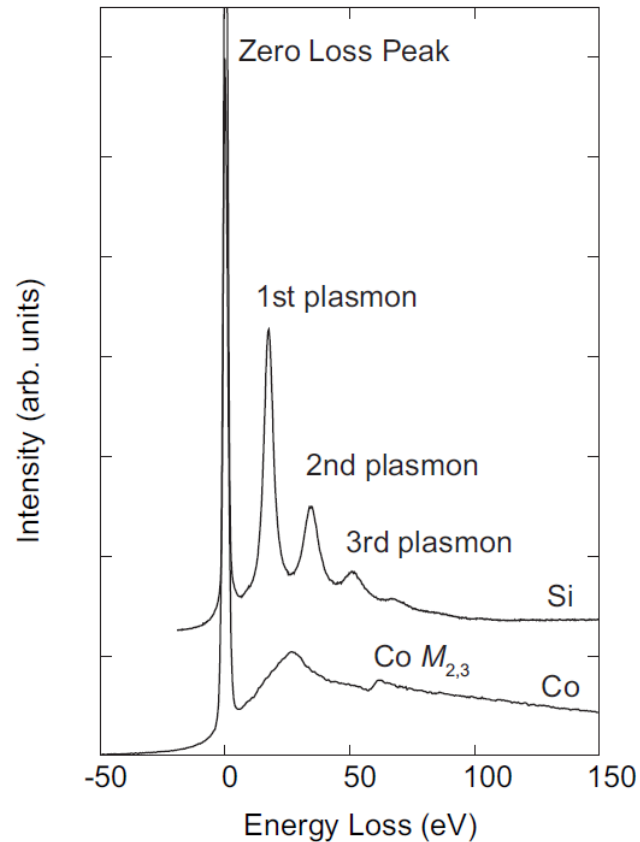


Figure 4.7: The low loss region of Si and Co. In the case of simple metals and semi-conductors, multiple, sharp plasmon peaks are usually observed in the low loss region, as is the case for Si seen in the figure. For more complex metals such as Co a single broad peak is observed. Also seen is the Co $M_{2,3}$ edge at approximately 60 eV.

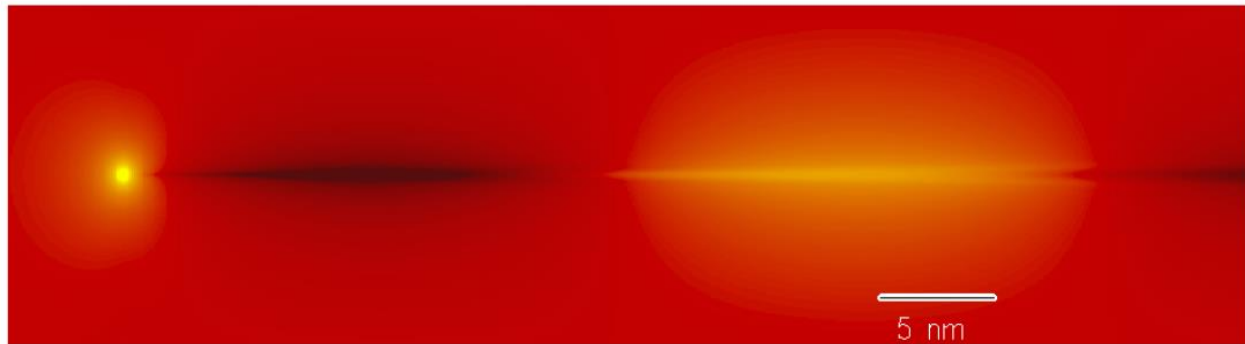
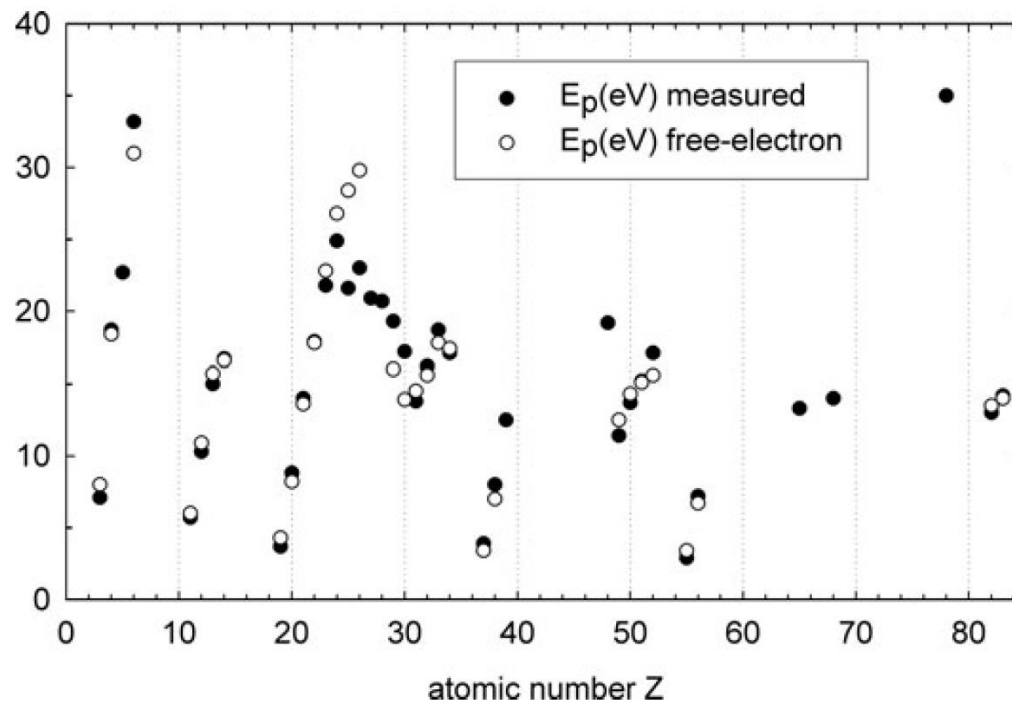


Figure 5. Plasmon wake of a 100 keV electron travelling through aluminium, calculated from the dielectric properties (P E Batson, personal communication). The electron is represented by the bright dot on the left; alternate dark and bright bands represent positive and negative regions of space charge that trail behind the electron.



$$\omega_p = \sqrt{\frac{ne^2}{m_0\epsilon_0}}$$

Fig. 3.12 Energy of the main valence-loss peak, as measured by EELS (*filled circles*) and as predicted by the free-electron formula, Eq. (3.41) with $m = m_0$ (*hollow circles*). Agreement is good except for transition metals and rare earths, where d- and f-electrons contribute to ionization edges with relatively low energy and high cross section

Table 5.1 Plasmon data for selected materials [5.5]

Material	E_p (calc.) (eV)	E_p (expt.) (eV)	ΔE_p (eV)	ϕ_{E_p} (mrad)	$\bar{\lambda}$ (nm)
Li	8.0	7.1	2.3	0.039	233
Be	18.4	18.7	4.8	0.102	102
Al	15.8	15.0	0.5	0.082	119
Si	16.6	16.5	3.7	0.090	115

Dielectric function, refractive index, speed of light

- The real part of the dielectric function gives the refractive index $n = \sqrt{\epsilon}$
- The refractive index gives the phase velocity of light in the material $c = c_0/n$.
- This is lower than the speed of light in vacuum

$$n_{Si}(\lambda \approx 600 \text{ nm}, E \approx 2 \text{ eV}) \approx 4$$

$$c_{Si} = \frac{c_0}{n_{Si}} \approx 0,25 c_0$$

$$v_e(200 \text{ kV}) \approx 0,7 c_0$$



Problems for next time

Exercise set 5: Low loss EELS

Exercise 1, Williams and Carter chapter 38

Do the following problems in the Williams and Carter textbooks:

- Q38.1-5
- Q38.8
- T38.2-4
- T38.9

Exercise 2

1. Make a plot of the phase velocity of light as a function of refractive indexes n between 1 and 10.
2. The critical acceleration voltage is defined as the voltage giving an electron velocity equal to the phase velocity of a material with refractive index n . Make a plot of the critical acceleration voltage as a function of n .