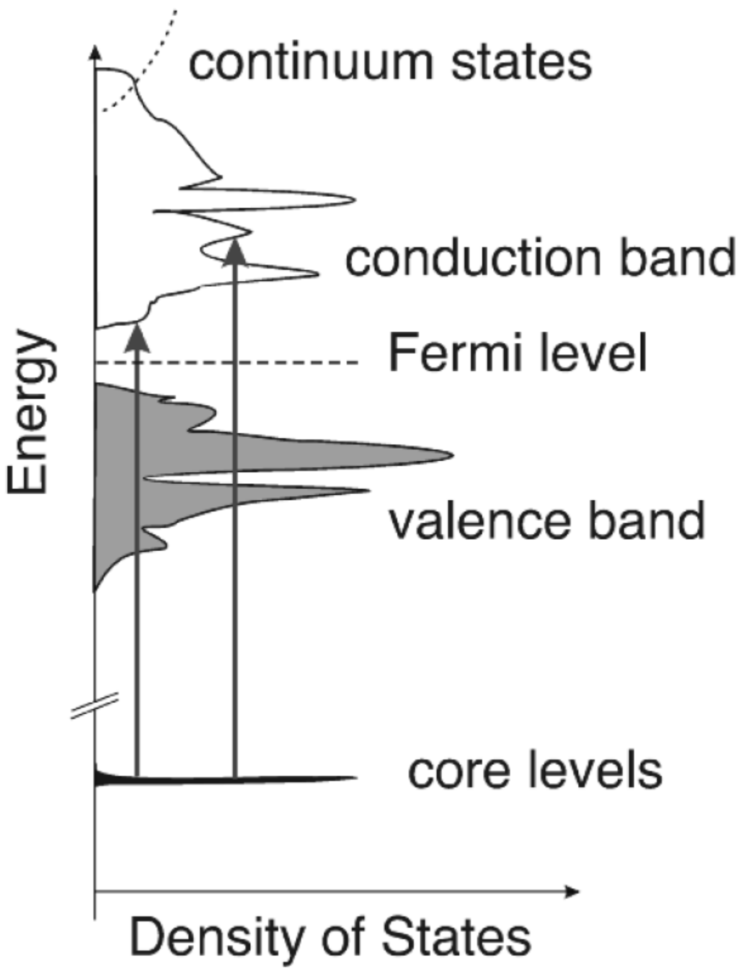
UiO : Department of Physics
University of Oslo

Low energy loss; electronic structure and dielectric properties pt 2

FYS5310/FYS9320
Lecture 8

09.03.2017

Recap from last time



- 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

$$Delta\ function \otimes cDOS = cDOS$$

- The spectrum reflects a scaled conduction band DOS

$$vDOS \otimes cDOS = ?$$

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

The EELS spectrum as a Joint Density of States

This is good for core losses:

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

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):

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

No dipole approximation?

The dielectric polarization of the material

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

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

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

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

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

The dielectric function in the Drude model

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

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

- Where ω_p is a harmonic oscilator resonance frequency given by

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

- τ is the scattering time/damping factor

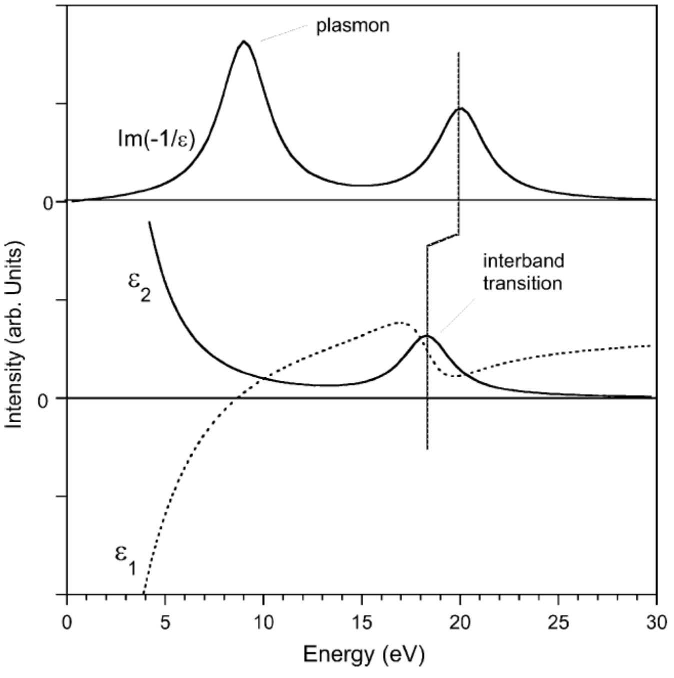


Fig. 6. Schematic of ε_1, ε_2 and the loss-function calculated with Drude–Lorentz theory where there is a plasmon excitation and a single interband transition. There is a peak in the loss-function corresponding to the interband energy, but at a different transition to where it appears in ε_2.

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

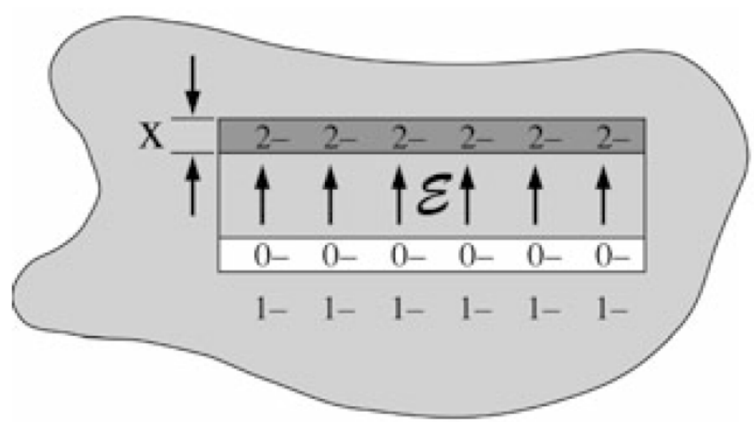


Table 5.1 Plasmon data for selected materials [5.5]

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

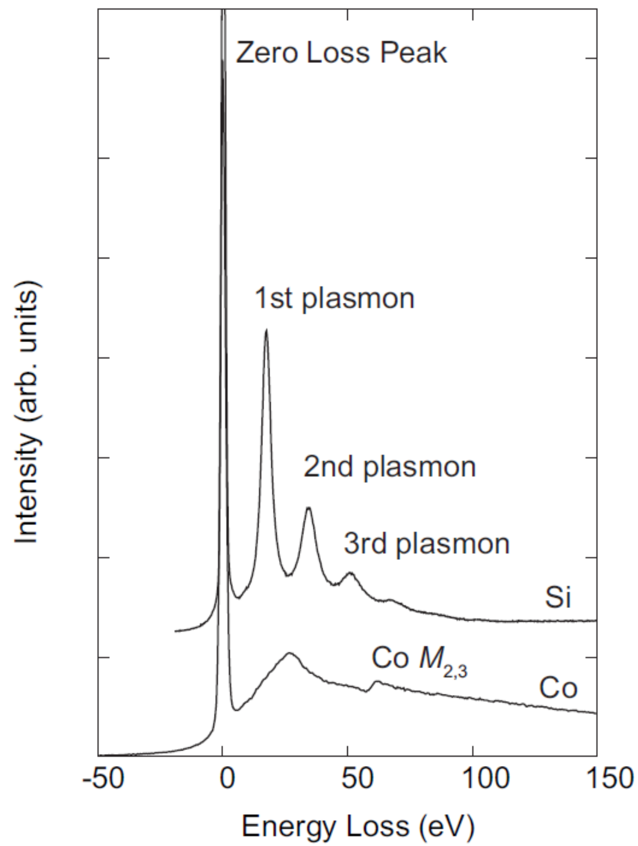
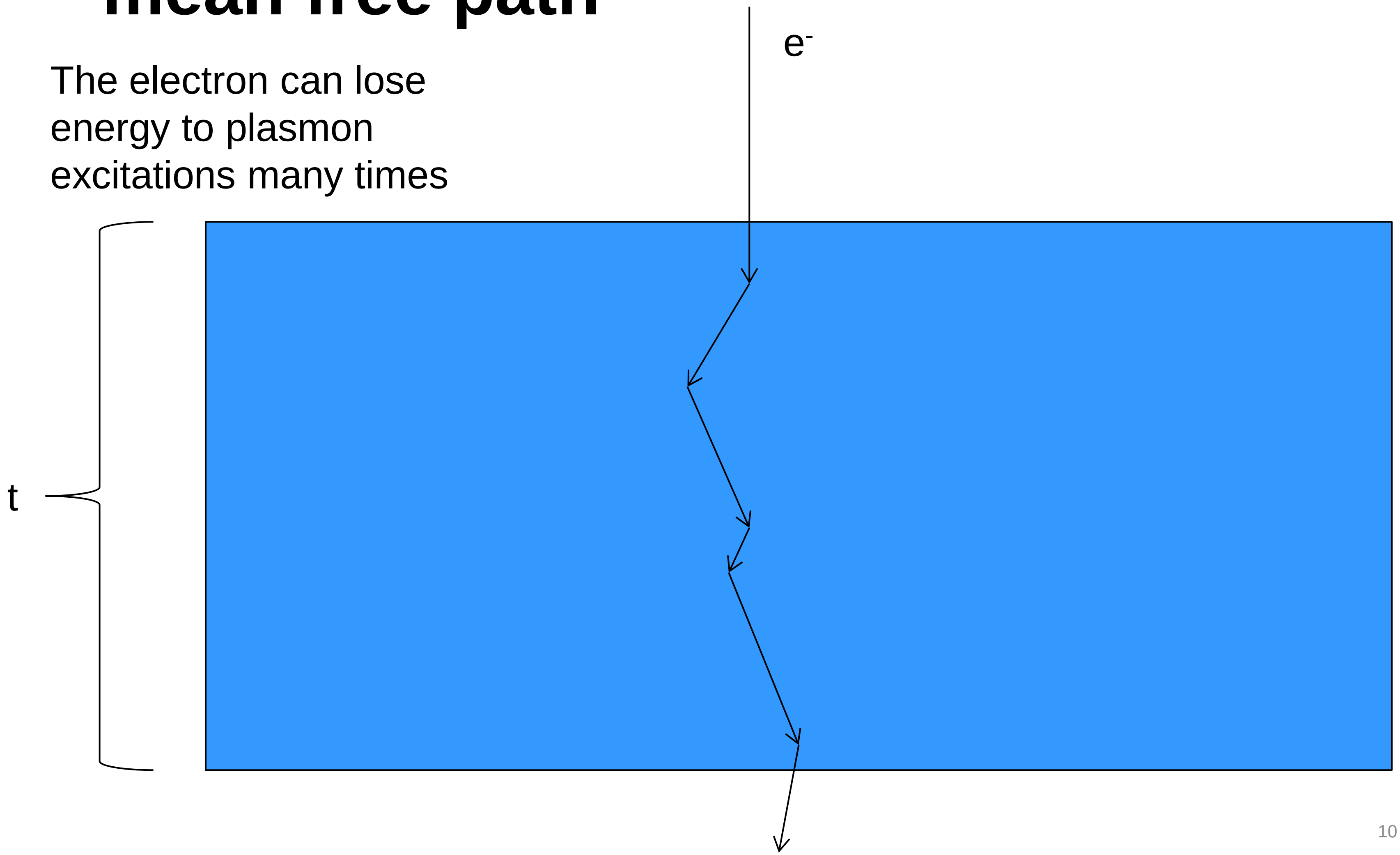


Figure 4.7: *The low loss region of Si and Co. In the case of simple metals and semi-conductors, multiple, sharp plasmon peaks are usually observed in the low loss region, as is the case for Si seen in the figure. For more complex metals such as Co a single broad peak is observed. Also seen is the Co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

Thickness measurements and the mean free path

The electron can lose energy to plasmon excitations many times

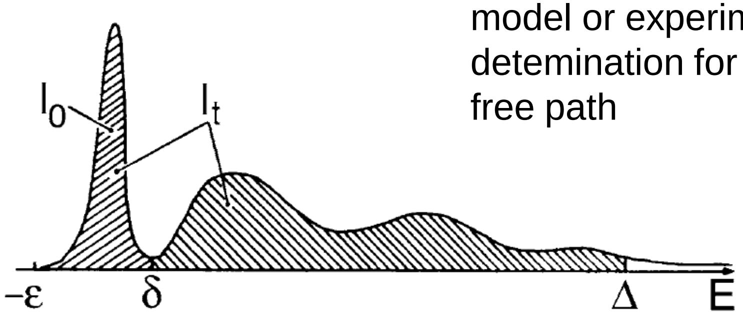


Thickness measurements and the mean free path

$$P_n = \frac{1}{n!}\left(\frac{t}{\bar{\bar{\lambda}}}\right)^n e^{-\frac{t}{\bar{\bar{\lambda}}}} = \frac{I_n}{I_t}$$

$$P_{n=0} = e^{-\frac{t}{\bar{\bar{\lambda}}}} = \frac{I_0}{I_t}$$

$$\frac{t}{\bar{\bar{\lambda}}} = \ln\left(\frac{I_t}{I_0}\right)$$



Absolute thickness determination is also possible, but need model or experimental detemination for mean free path

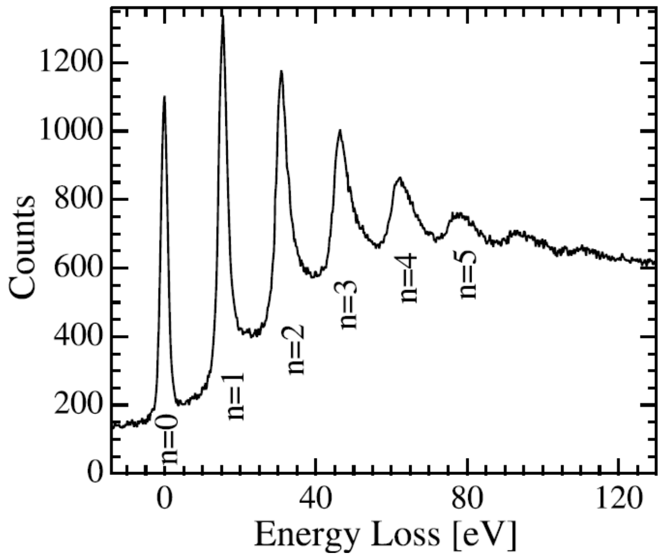


Fig. 5.8 Low-loss spectrum taken from a thick sample of ~120 nm Al metal on C using 120 keV electrons and $\beta = 100$ mrad. Plasmon peaks are visible at energies of $n \times 15$ eV, where n is the number of plasmons excited in the sample. After [5.4]

F&H

Dielectric function, refractive index, speed of light

- The real part of the dielectric fuction gives the refractive index $n=\sqrt{\varepsilon}$
- 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

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

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

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

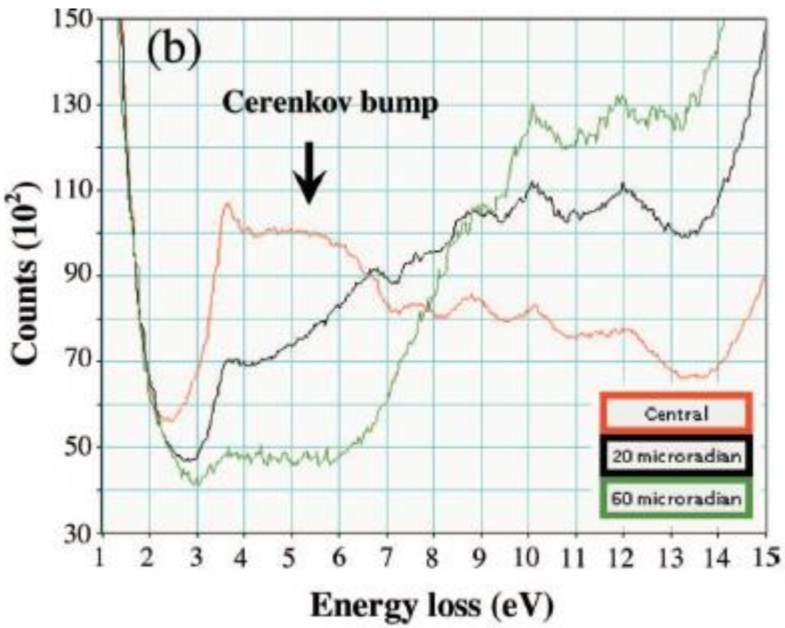
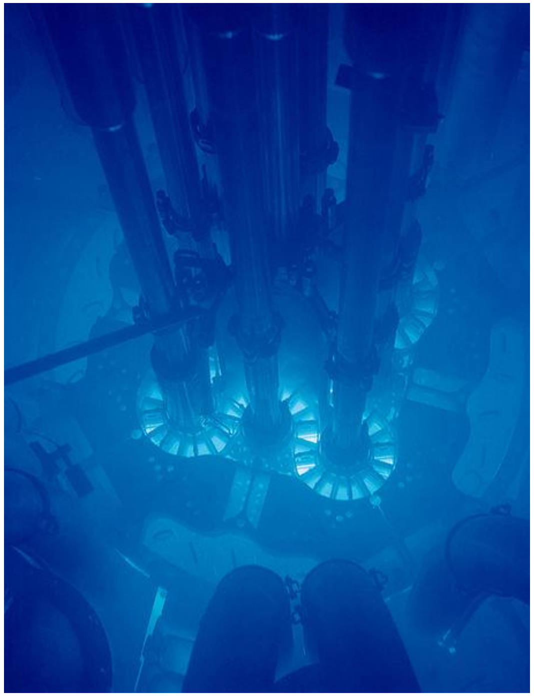


FIG. 3. (Color) (a) ω-q map of h-GaN at a thick region with strong Cerenkov losses and (b) line profiles extracted at different q values with a linewidth of about 5 μrad. The energy loss of Cerenkov radiation has a narrow angular distribution.

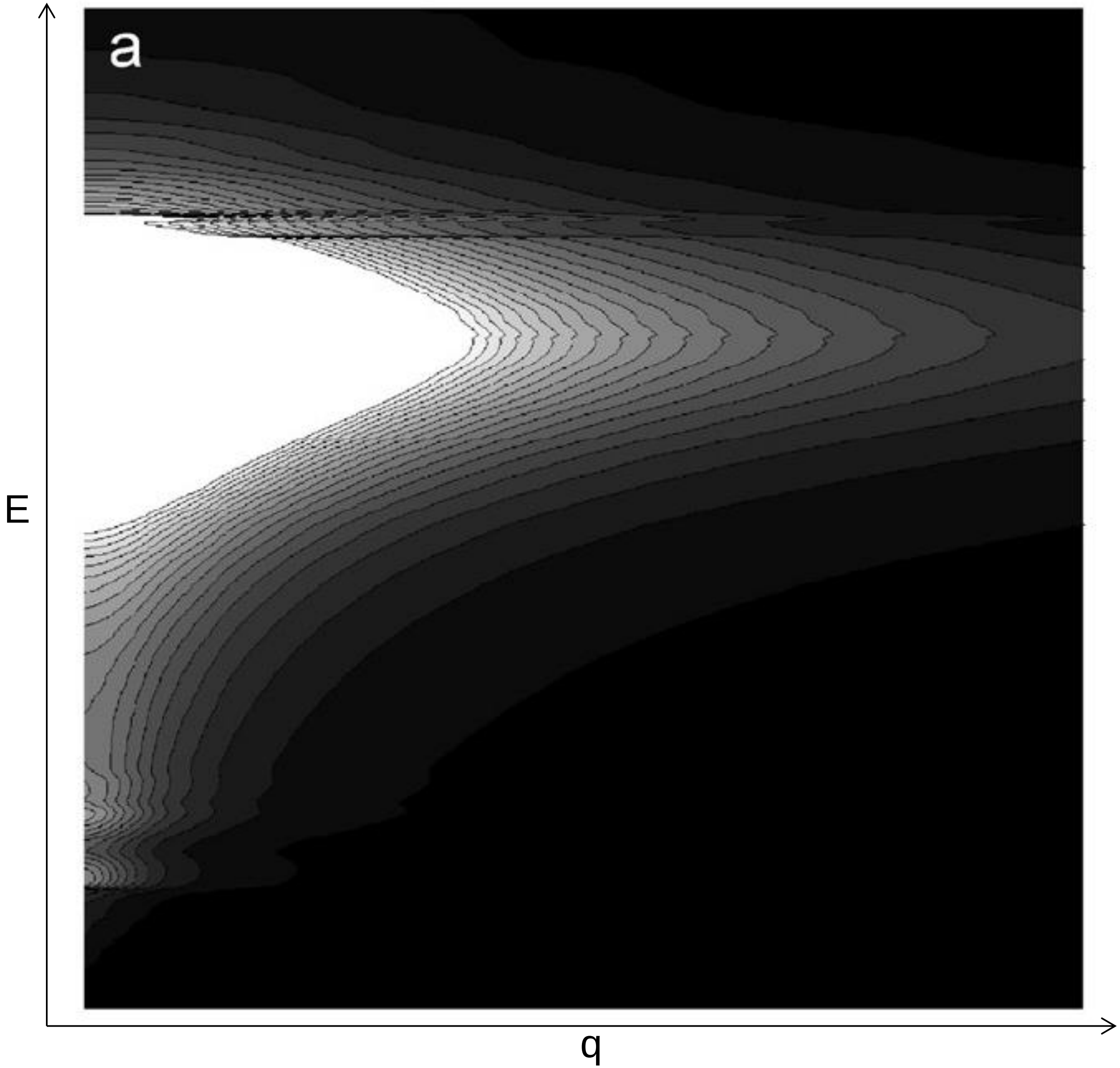


Erni & Browning, Ultramic (2008)

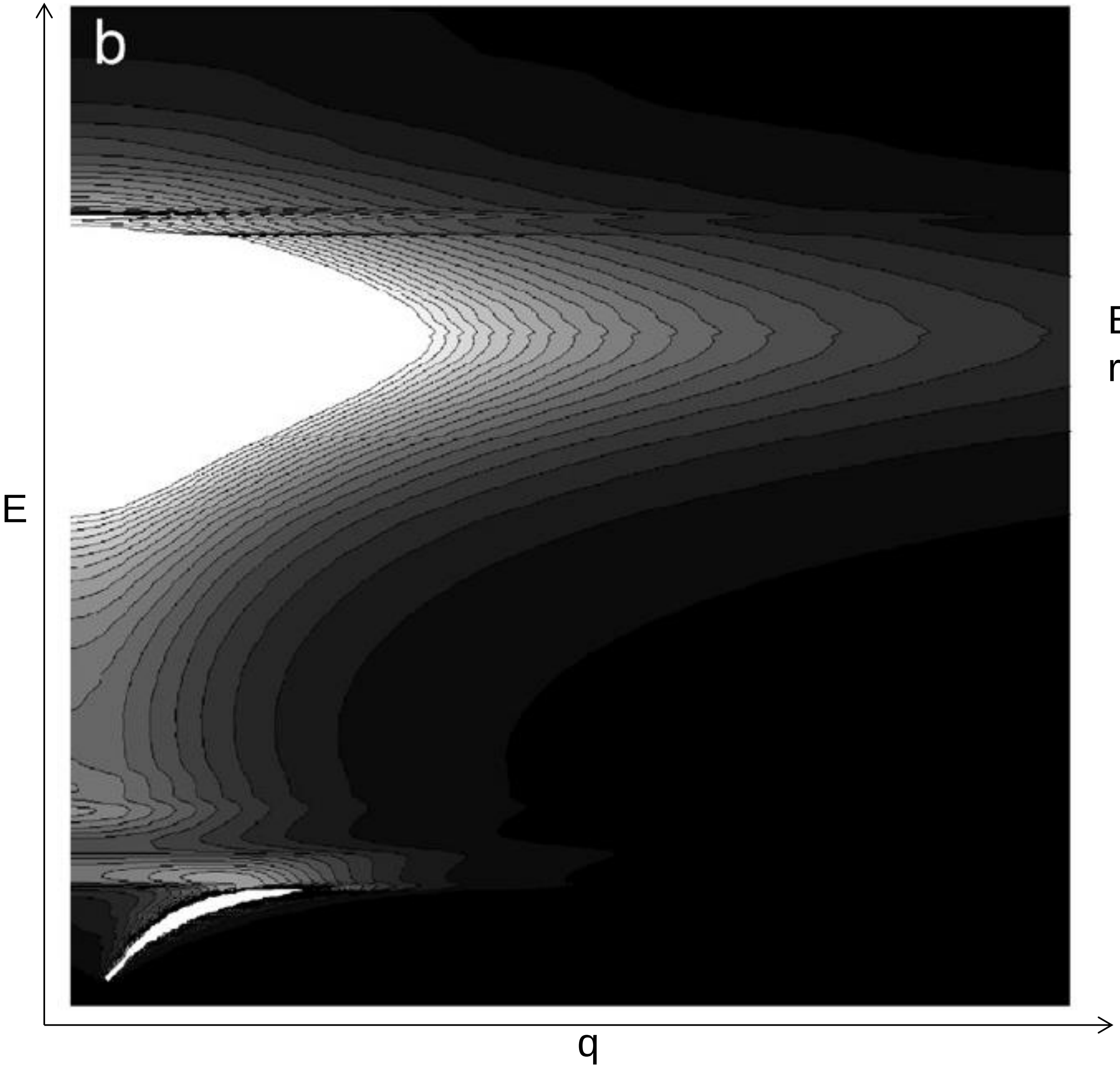
The Kröger equation

$$
\begin{aligned}
\frac{\partial^3 P(\vec{k}_\perp,\omega)}{\partial \Delta E \partial^2 \Omega} &= \frac{p_0^2}{\hbar^2}\frac{e^2}{\pi^2\hbar^2 v^2 \cos\alpha}\Im\left[\frac{1-\varepsilon\beta^2}{\varepsilon\phi^2}2a\right.\\
&-2\frac{(\varepsilon-\varepsilon_0)^2}{\phi_0^4\phi^4}\left\{\left(\frac{\sin^2(\kappa a/v_x)}{L^+}+\frac{\cos^2(\kappa a/v_x)}{L^-}\right)\frac{B^2}{\varepsilon\varepsilon_0}\right.\\
&-\left(\frac{\cos^2(\kappa a/v_x)\tan h(\lambda a)}{L^+}+\frac{\sin^2(\kappa a/v_x)\coth(\lambda a)}{L^-}\right)A^2\lambda\lambda_0\\
&+\left(\frac{1}{L^+}-\frac{1}{L^-}\right)\frac{\lambda_0}{\varepsilon_0}AB\sin\left(\frac{2\kappa a}{v_x}\right)\\
&+\left(\frac{\omega}{v}\right)^4\beta^6\sin^2(\alpha)\sin^2(\phi)\left[\left(\frac{\kappa}{v_x}\right)^2\left(\frac{\sin^2(\kappa a/v_x)}{M^+}+\frac{\cos^2(\kappa a/v_x)}{M^-}\right)\right.\\
&-\lambda\lambda_0\left(\frac{\cos^2(\kappa a/v_x)\tanh(\lambda a)}{M^+}+\frac{\sin^2(\kappa a/v_x)\coth(\lambda a)}{M^-}\right)\\
&\left.\left.\left.-\lambda_0\frac{\kappa}{v_x}\sin\left(\frac{2\kappa a}{v_x}\right)\left(\frac{1}{M^+}-\frac{1}{M^-}\right)\right]\right\}\right]
\end{aligned}
$$

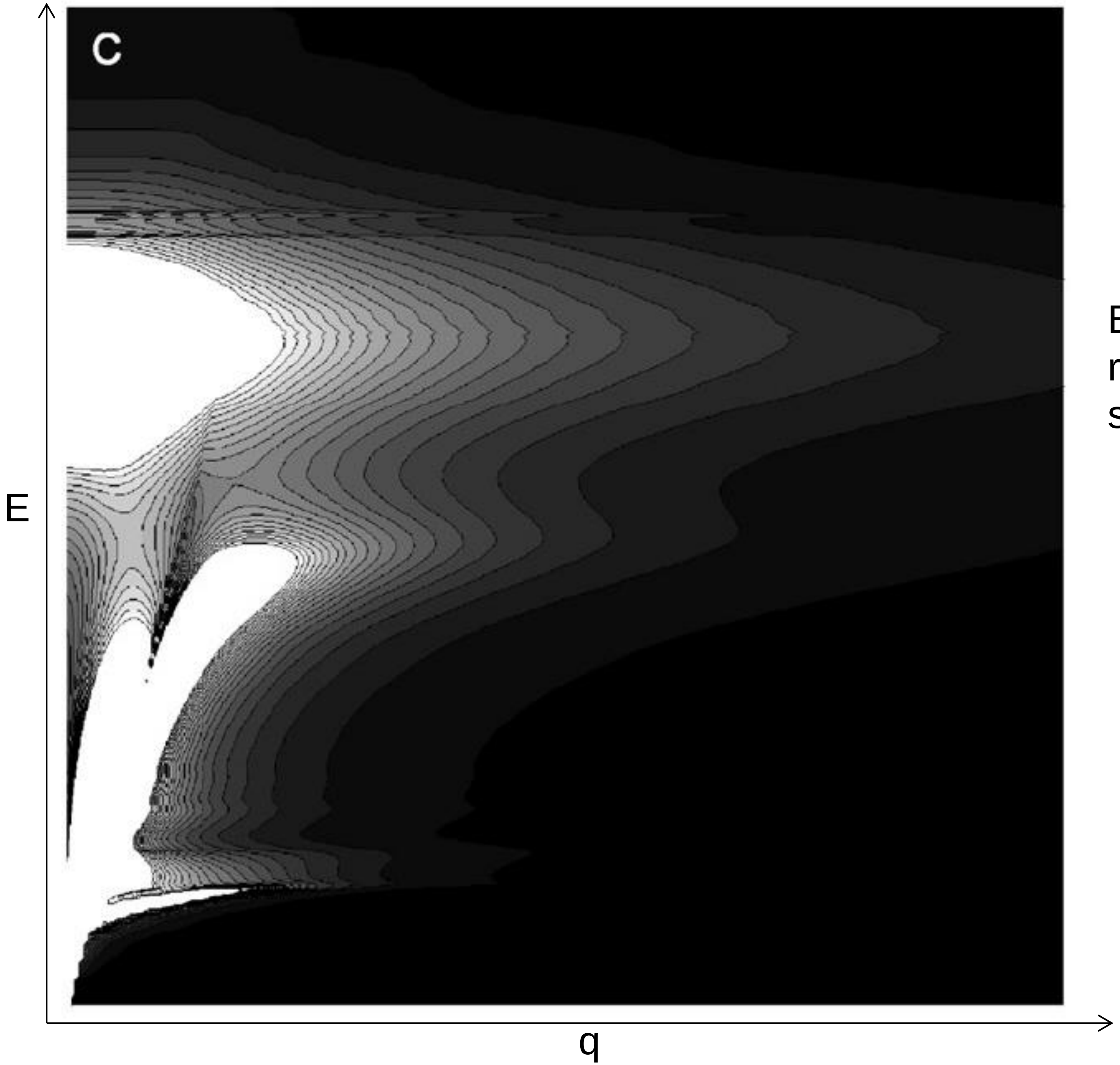
$$
I(E) = \frac{2I_0 t}{\pi a_0 m_0 v^2} Im\left(-\frac{1}{\varepsilon(E)}\right)\ln\left(1+\left[\left(\frac{\beta}{\Theta_E}\right)^2\right]\right)
$$



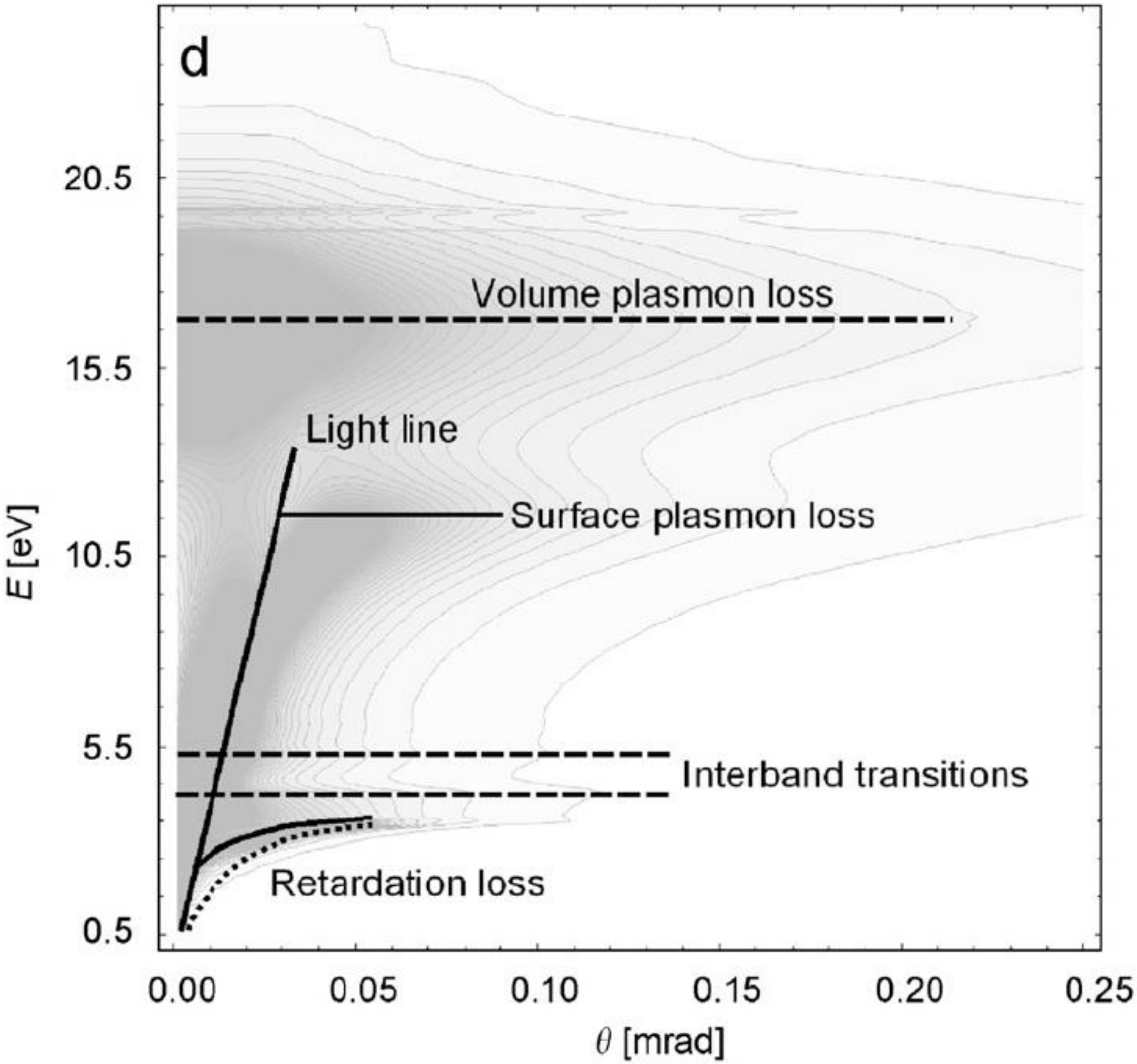
Only non-relativistic bulk effects



Bulk plus
relativistic effects



Bulk plus
relativistic plus
surface effects


d
Volume plasmon loss
Light line
Surface plasmon loss
Interband transitions
Retardation loss
20.5
15.5
10.5
5.5
0.5
E [eV]
0.00
0.05
0.10
0.15
0.20
0.25
θ [mrad]

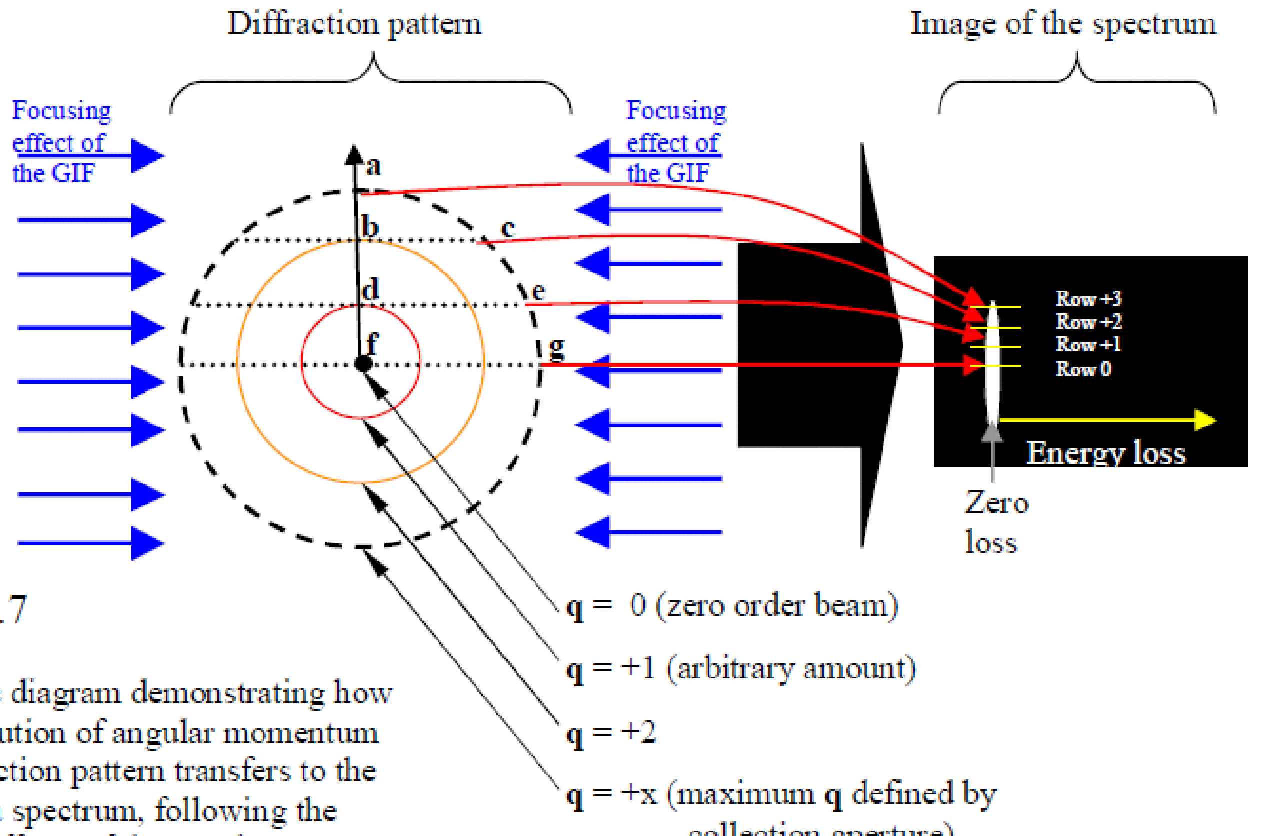


Figure 3.7

Schematic diagram demonstrating how the distribution of angular momentum in a diffraction pattern transfers to the image of a spectrum, following the focusing effects of the GIF lenses.

Row 0 (in the image of the spectrum) contains the momentum present between **f** and **g** (in the diffraction pattern), i.e. the integral from **q** = 0 to **q** = +x.
Row +1 contains the momentum present between **d** and **e**, i.e. the integral from **q** = +1 to **q** = +x.
Row +2 contains the momentum present between **b** and **c,** i.e. the integral from **q** = +2 to **q** = +x.
Row +3 contains the momentum present at **a,** i.e. **q** = +x.

H. R. Daniels, Phd thesis (2003)

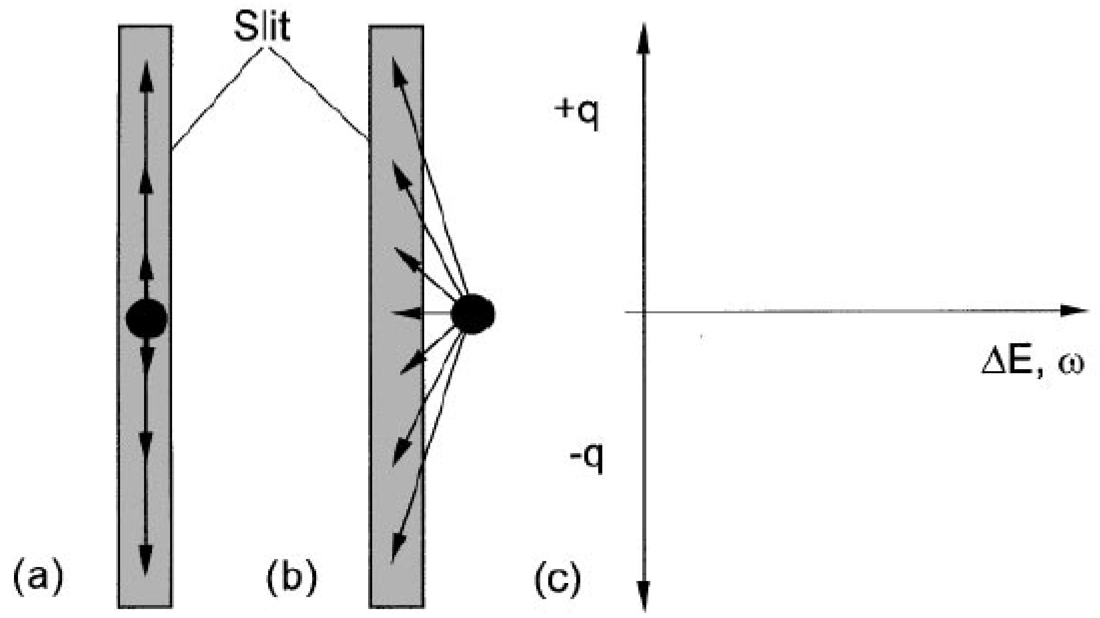
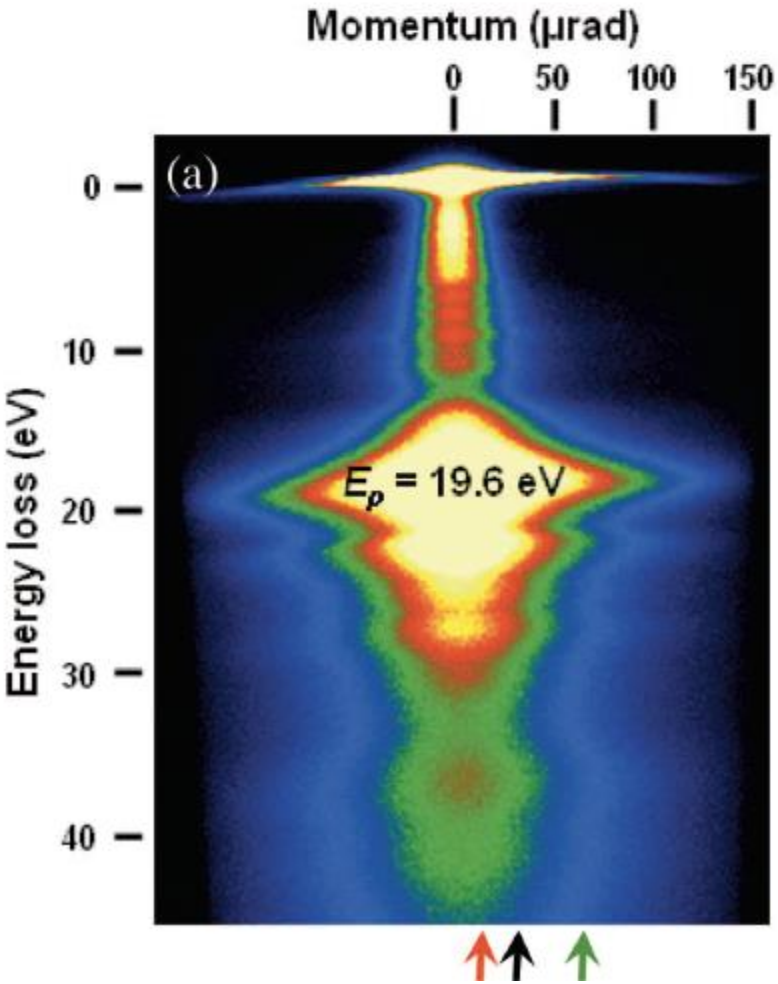
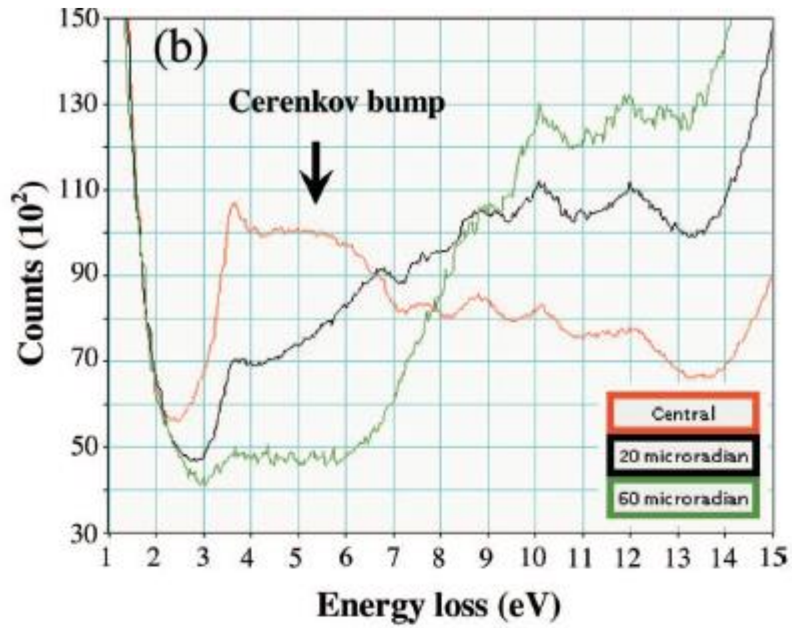


Fig. 3. Illustration of how the scattering vector is chosen by a narrow slit. In (a) the slit is placed symmetrically about the transmitted beam so that all the included scattering vectors are parallel to the slit axis. In (b) the slit is displaced slightly so that the included scattering vectors have a component of q perpendicular to the slit. This range of scattering is then integrated across the slit width and dispersed in energy to form the ω–q pattern as shown in (c).

Midgley, Ultramic. (1999)





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Problems for next time

1) Make a plot of the phase velocity of light as a function of refractive indexes *n* between 1 and 10.

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*

2) Make a plot of the critical acceleration voltage as a function of *n.*