First-principles Computational Material Research

Lecture Notes
Calculations on Optical Properties

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VASP Home Page

http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{eff}(\vec{r})\right]\psi_i(\vec{r}) = \varepsilon_i\psi_i(\vec{r}) \quad ; \quad \rho(\vec{r}) = \sum_i^{occ}\left|\psi_i(\vec{r})\right|^2$$

$$V_{eff}(\vec{r}) = V_{ext}(\vec{r}) + V_H(\vec{r}) + V_{xc}(\vec{r}) + V_{ps}(\vec{r})$$

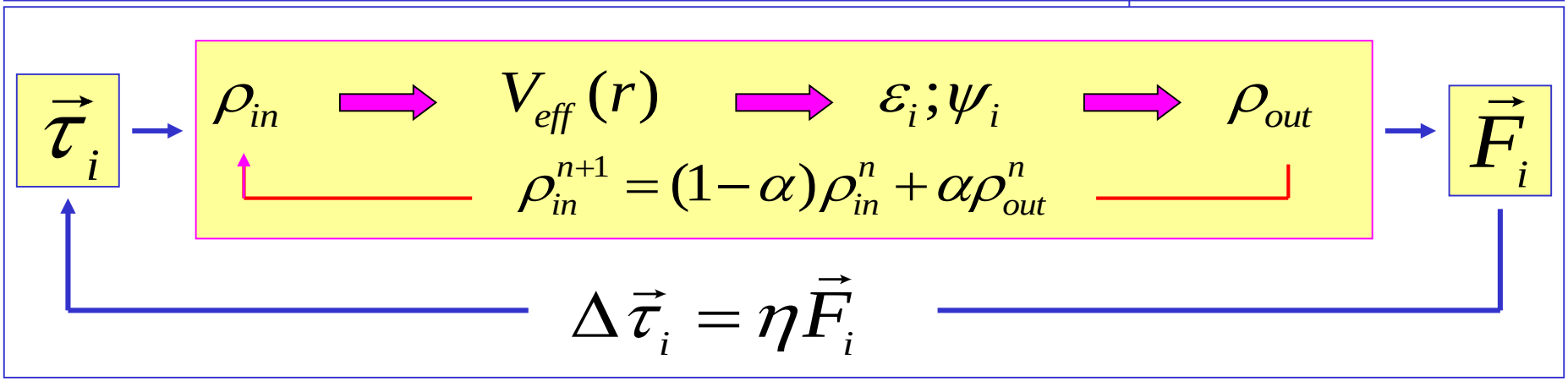
$$V_H(\vec{r}) = \int \frac{\rho(\vec{r})}{\left|\vec{r}-\vec{r}'\right|}d^3r \; ; \quad \boxed{V_{xc}(\vec{r}) = V_{xc}(\rho(\vec{r}))} \quad \textbf{LDA}$$

$$V_{eff}(\vec{r}+\vec{R}) = V_{eff}(\vec{r})$$

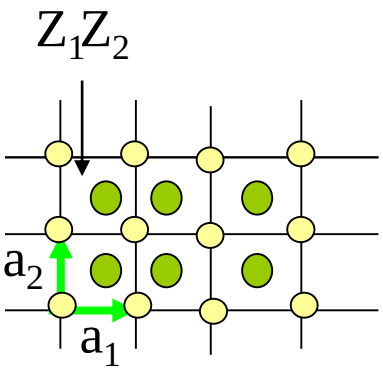
$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r})$$

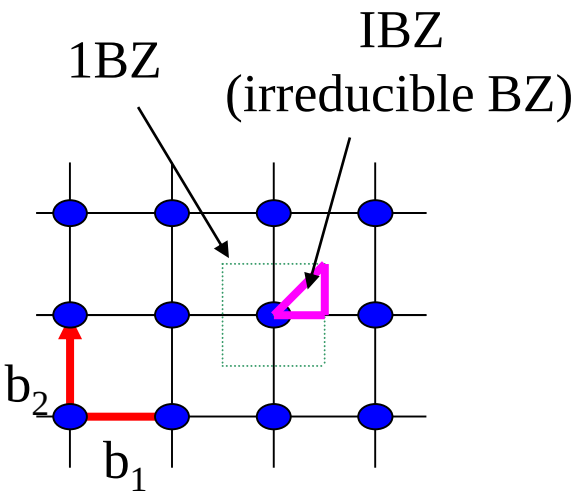
$$u_k(\vec{r}) = \sum_{G_n < G_{\max}} C_n e^{i\vec{G}_n\cdot\vec{r}}$$

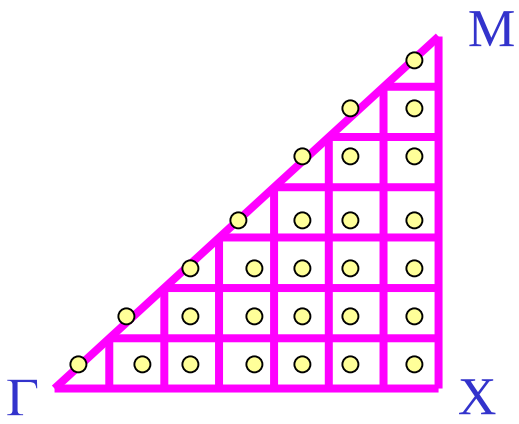
$$\underset{\sim}{H}(\vec{k})\underset{\sim}{C} - \lambda\underset{\sim}{S}\underset{\sim}{C} = 0$$



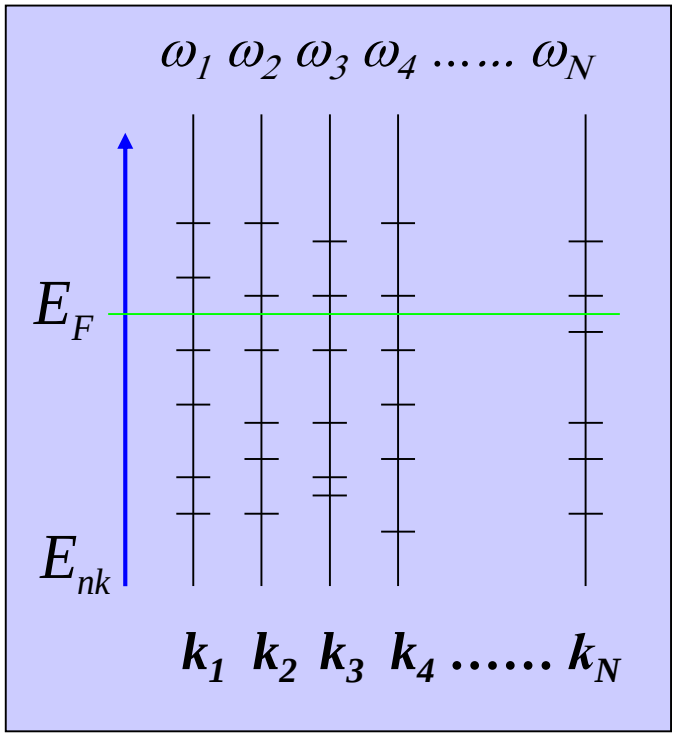
Example: 2 D







IBZ (irreducible BZ)



Weight of the k points:

$$\omega_k = \frac{2A_k}{\sum_k A_k}$$

$$\sum_n \sum_k \omega_k = Z_1 + Z_2$$

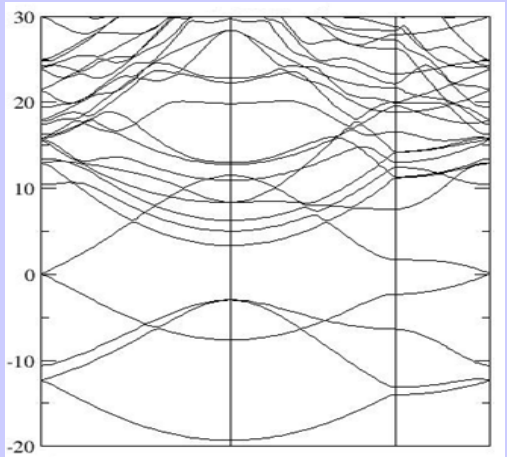
$$E_{nk} \le E_F$$

charge density

$$\rho(\vec{r}) = \sum_n \sum_k \omega_k \left|\psi_{nk}\right|^2$$

$$E_{nk} \le E_F$$

Band structure



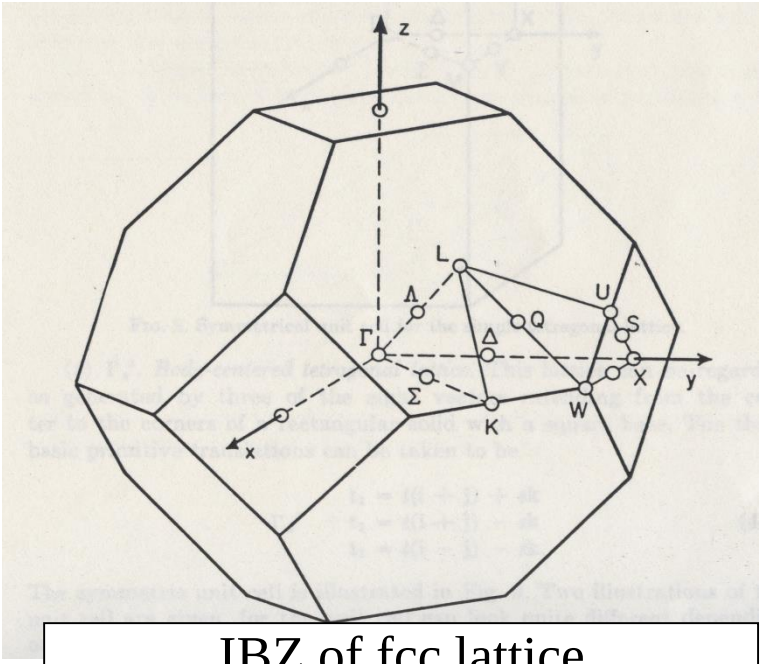
Example: 3 D

Copper (Cu) : fcc structure

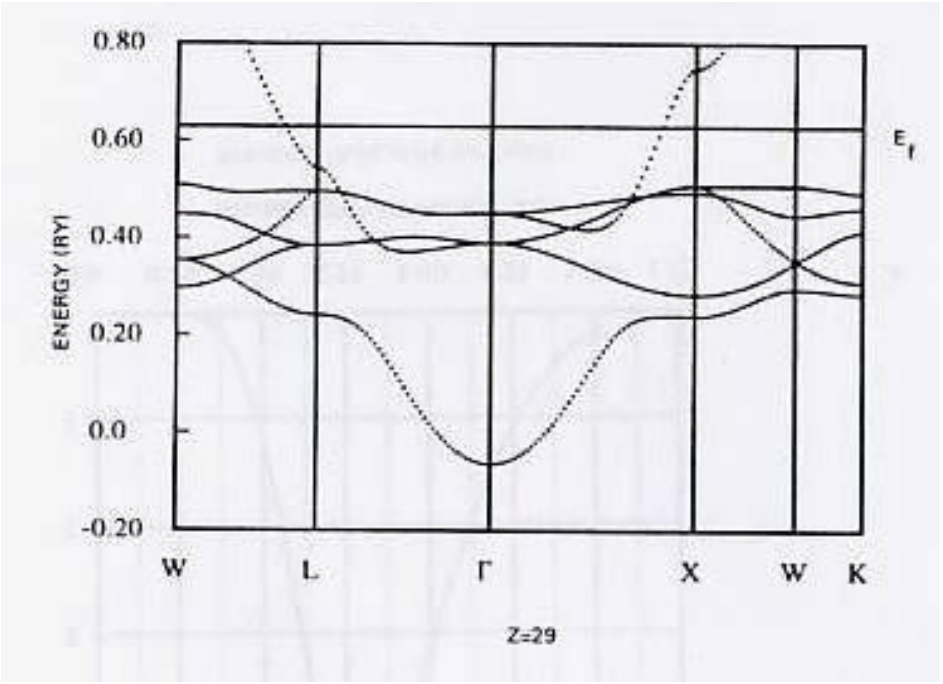
$$\vec{a}_1 = \frac{a}{2}(\vec{j} + \vec{k}) \qquad \vec{b}_1 = \frac{4\pi}{a}\frac{1}{2}(-\vec{i} + \vec{j} + \vec{k})$$

$$\vec{a}_2 = \frac{a}{2}(\vec{i} + \vec{k}) \qquad \vec{b}_2 = \frac{4\pi}{a}\frac{1}{2}(\vec{i} - \vec{j} + \vec{k})$$

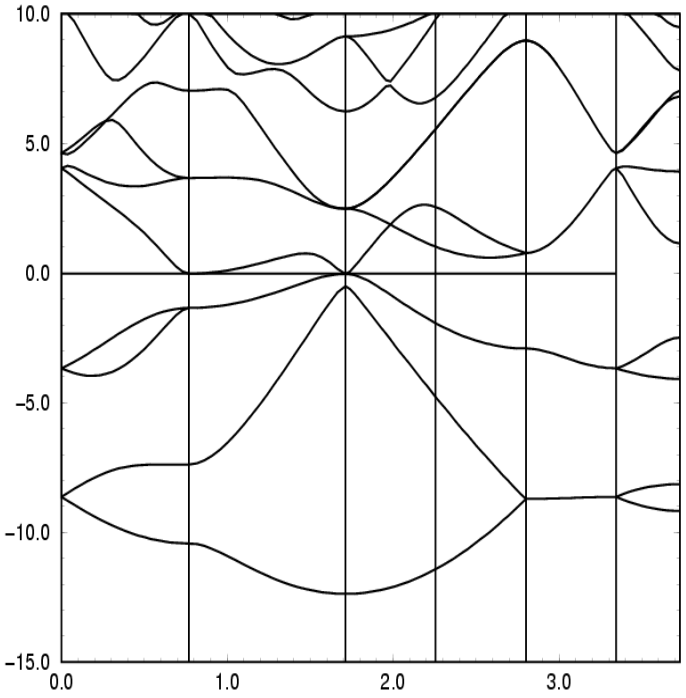
$$\vec{a}_3 = \frac{a}{2}(\vec{i} + \vec{j}) \qquad \vec{b}_3 = \frac{4\pi}{a}\frac{1}{2}(\vec{i} + \vec{j} - \vec{k})$$

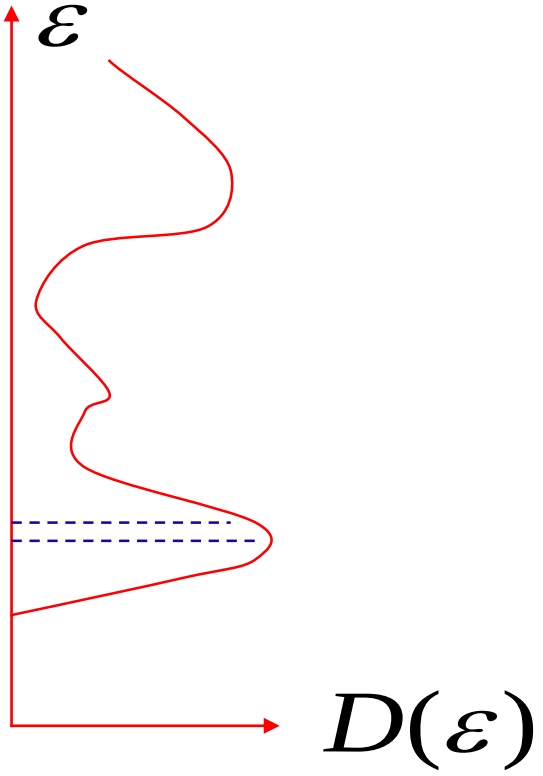


IBZ of fcc lattice



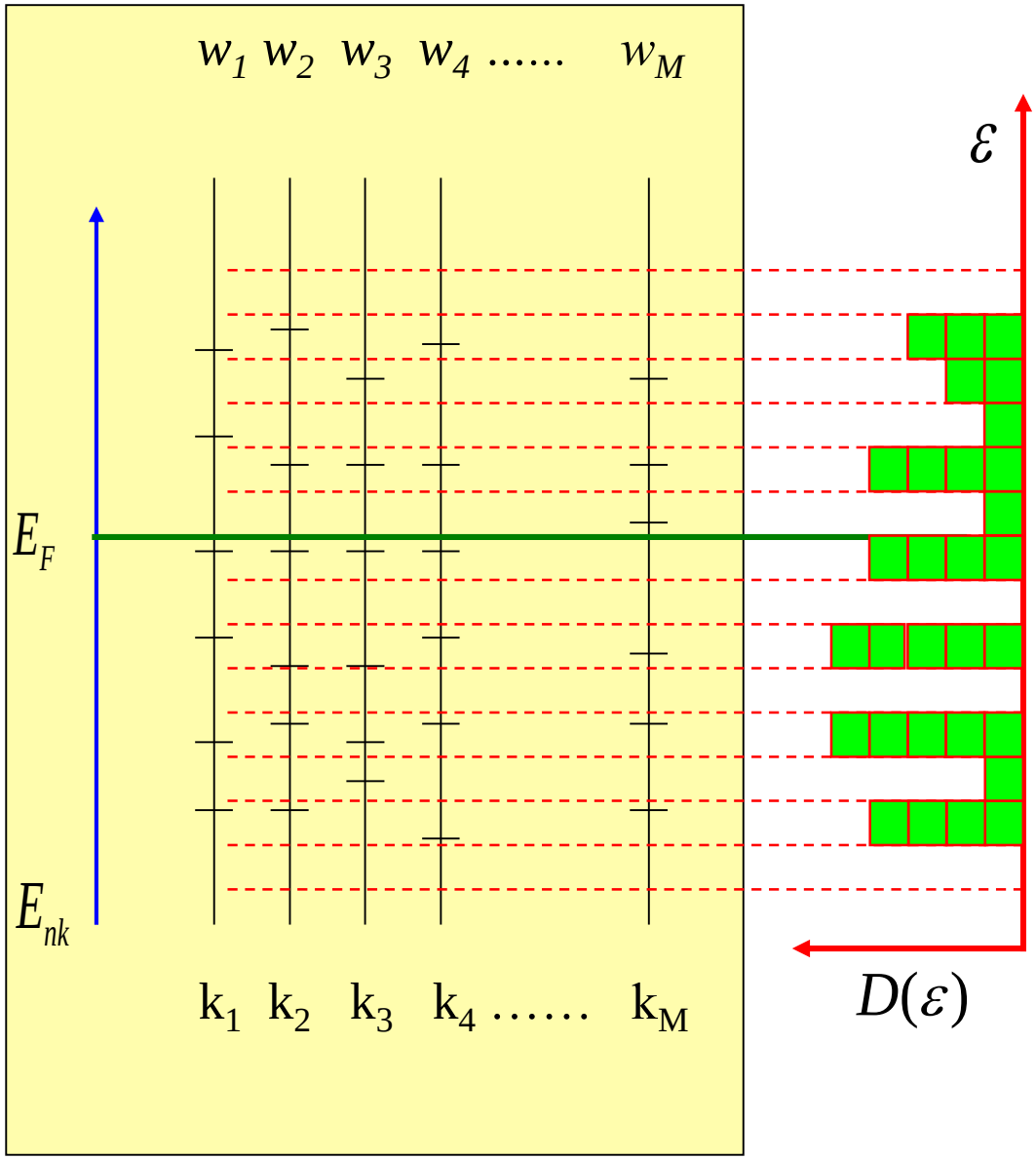
Density of states





$\Delta N = D(\varepsilon)\Delta\varepsilon$ *number of state from* ε *to* $\varepsilon + \Delta\varepsilon$

$D(\varepsilon)$: Density of states



$$D(\varepsilon_i)\Delta\varepsilon$$

Number of state within $\Delta\varepsilon$

$$\omega_k = \frac{2A_k}{\sum_k A_k}$$

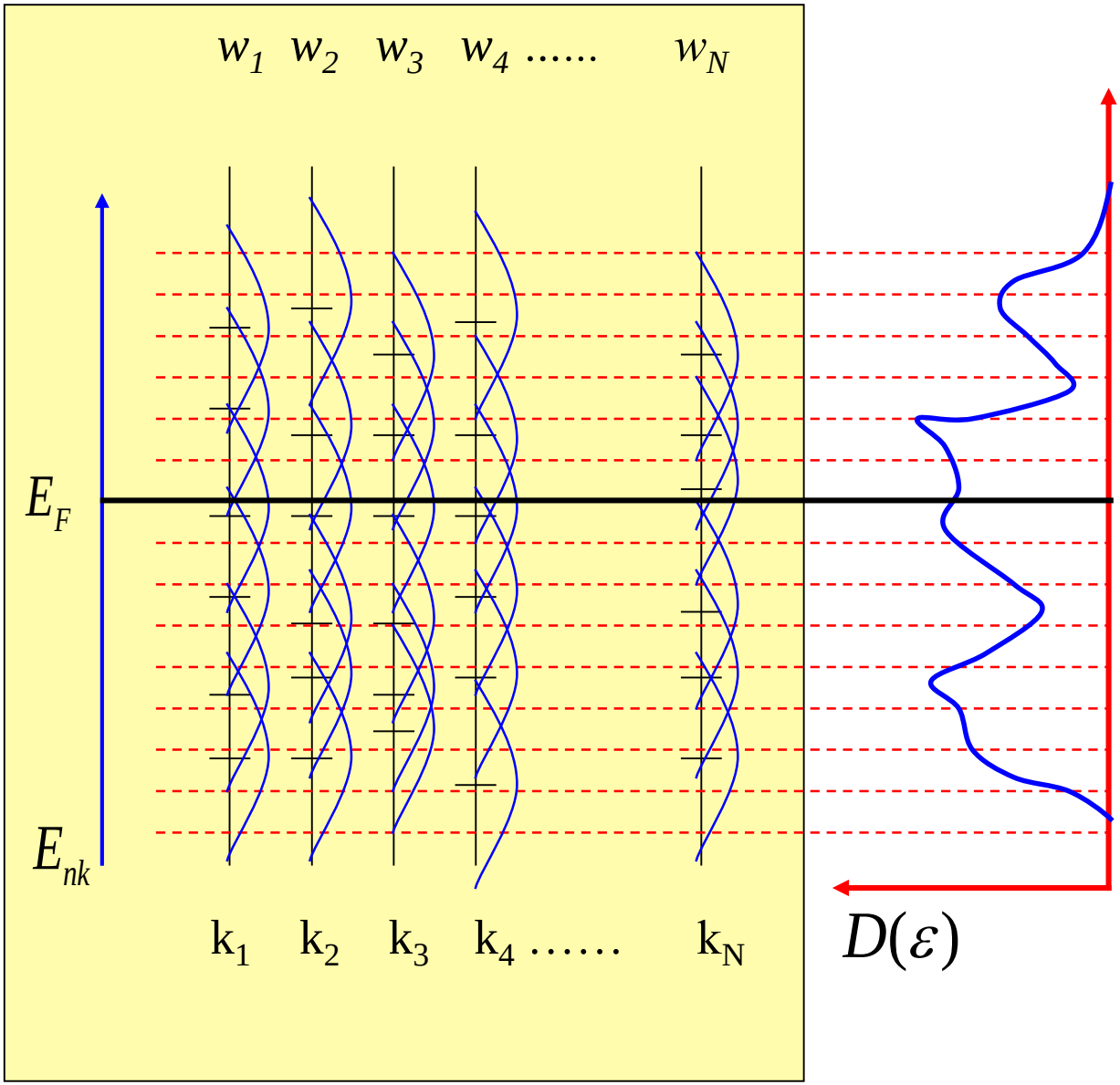
$$\sum_k \omega_k = 2$$

$$D(\varepsilon_i) = \frac{1}{\Delta\varepsilon}\sum_k \omega_k$$

$$N = \frac{1}{\Delta\varepsilon}\sum_k \omega_k f_k$$

where

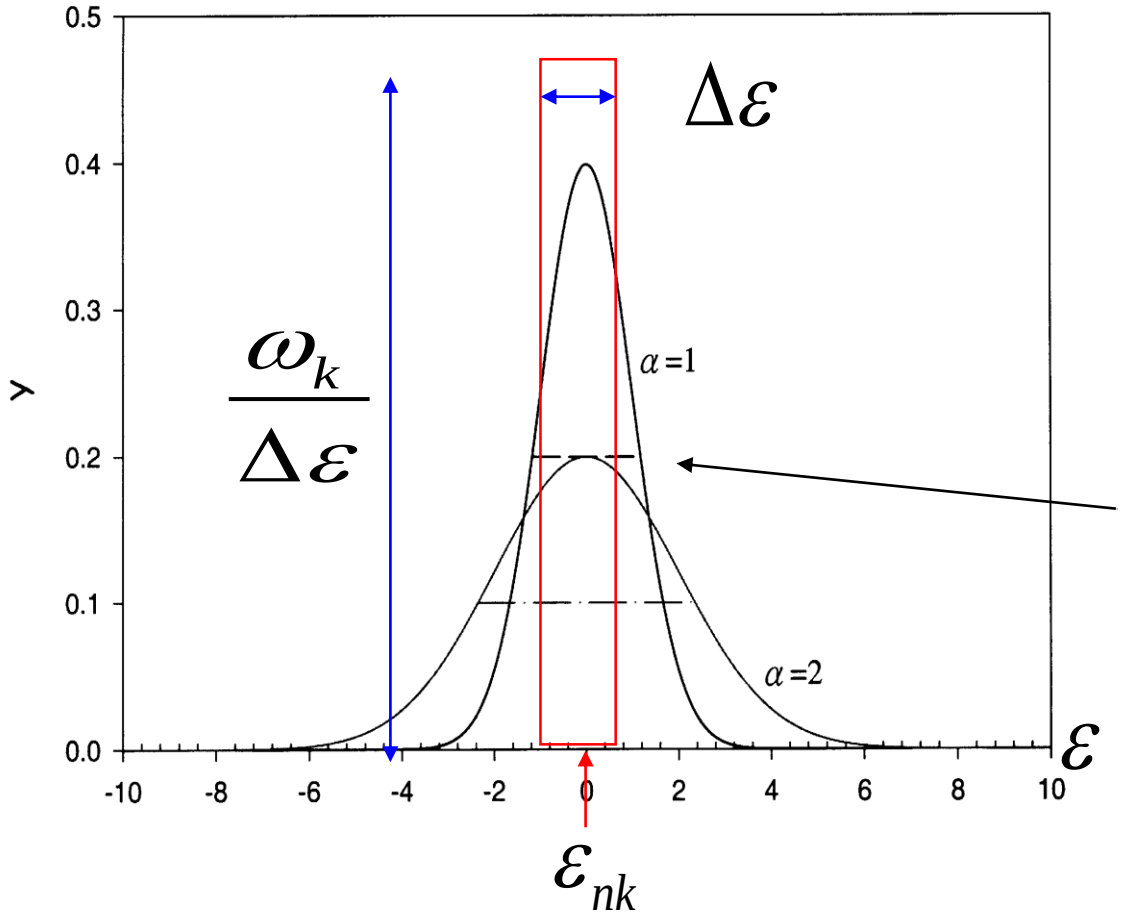
$$f_k = \begin{cases} 1 & occupied \\ 0 & otherwise \end{cases}$$



Smearing
(Gaussian)

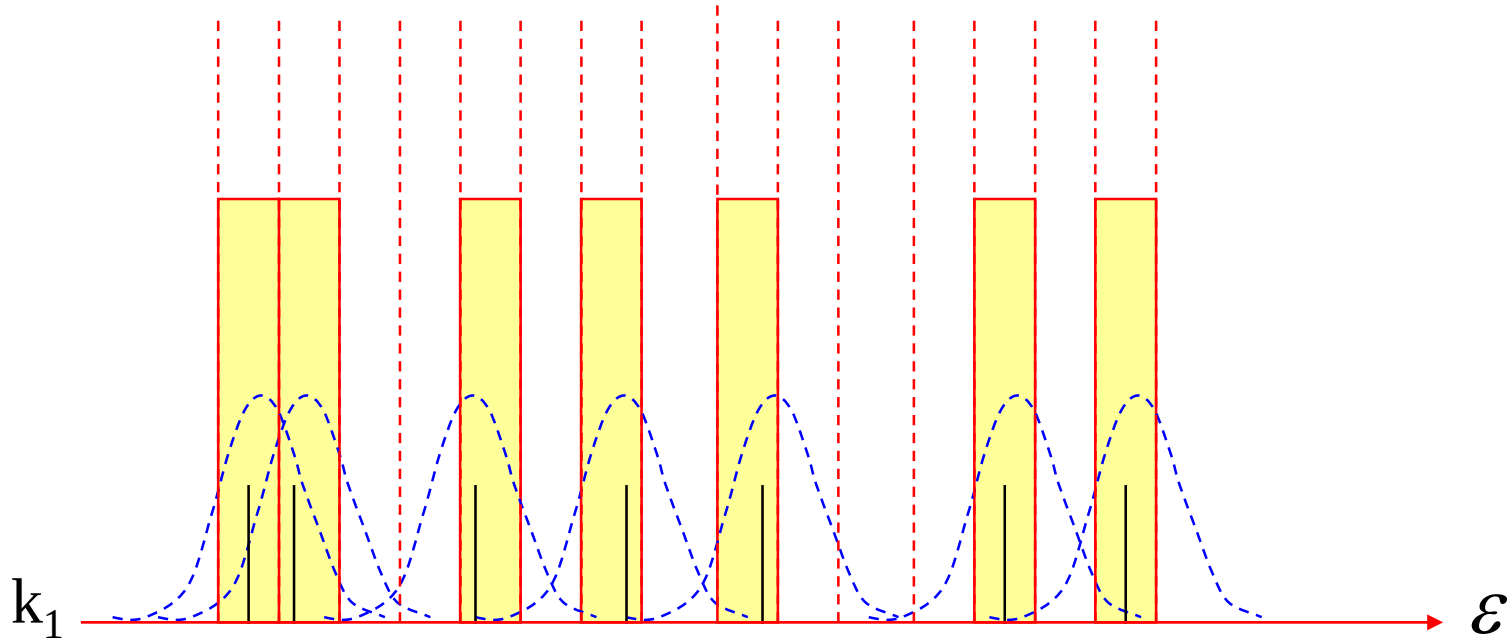
$$Ae^{-(\frac{\varepsilon-\varepsilon_i}{\sigma})^2}$$

$$\int_{\varepsilon<E_F} D(\varepsilon)d\varepsilon = N$$



They have the same area.

$$D_{nk}(\varepsilon) = \frac{\omega_k}{\sqrt{2\pi}\alpha} e^{-\frac{(\varepsilon-\varepsilon_{nk})^2}{2\alpha^2}}$$


k_1
ε

How to calculate the absorption spectrum of a crystal ?

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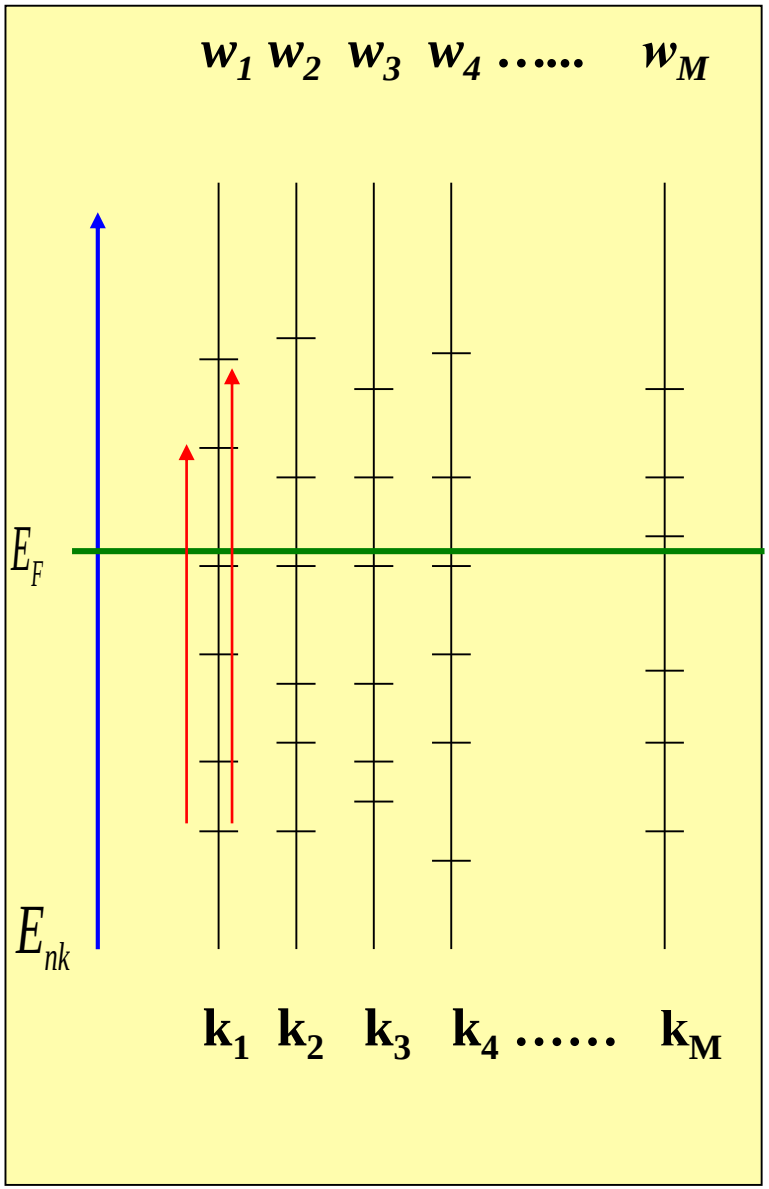


$$\psi(t=0)=\phi_{vi}$$

$$\mathrm{P_{cj}}(t)=\left|\left\langle \phi_{cj}\left|\psi(t)\right\rangle\right|^2=\left|c_{cj}(t)\right|^2$$

Transition probability per unit time:

$$\Gamma_{vi\to cj}=\frac{P_{vi,cj}(t)}{t}$$

Transition rate W :

$$W=\sum_{\substack{\text{valence}\\ \text{band}}}\sum_{\substack{\text{conduction}\\ \text{band}}}\sum_{\vec{k}} w_{\vec{k}}\Gamma_{vi\to cj}$$

Absorption Constant (α) :

$$\frac{\hbar\omega\times \text{Transition rate (W)}}{\text{Incident flux (I)}}$$

Time-Dependence Perturbation Theory

$$i\hbar\frac{\partial\psi(t)}{\partial t}=\left[H_0+\lambda V(t)\right]\ \psi(t) \quad ; \quad H_0\phi_n=E_n^0\phi_n \ ; \ \langle\phi_m|\phi_n\rangle=\delta_{mn}$$

$$\psi(t)=\sum_n c_n(t)\exp(-iE_n^0t/\hbar)\phi_n \qquad (if \quad V(t)=0 \quad \Rightarrow \quad C_n(t)=const.)$$

$$i\hbar\frac{\partial}{\partial t}\left[\sum_n c_n(t)\exp(-iE_n^0t/\hbar)\phi_n\right]=\left[H_0+\lambda V(t)\right]\left[\sum_n c_n(t)\exp(-iE_n^0t/\hbar)\phi_n\right]$$

$$\sum_n\left[i\hbar\frac{dc_n(t)}{dt}+E_n^0c_n(t)\right]\exp(-iE_n^0t/\hbar)\ \phi_n=\sum_n\left[E_n^0+\lambda V(t)\right]c_n(t)\exp(-iE_n^0t/\hbar)\ \phi_n$$

$$i\hbar\sum_n\frac{dc_n(t)}{dt}\exp(-iE_n^0t/\hbar)\phi_n=\lambda\sum_n c_n(t)V(t)\exp(-iE_n^0t/\hbar)\ \phi_n \quad .....(1)$$

$$\langle\phi_m|\exp(iE_m^0t/\hbar)\times(1)$$

$$i\hbar\frac{dc_m(t)}{dt}=\lambda\sum_n c_n(t)\exp\left[i(E_m^0-E_n^0)t/\hbar\right]\langle\phi_m|V(t)|\phi_n\rangle$$

$$i\hbar \frac{dc_m(t)}{dt} = \lambda \sum_n c_n(t) \exp\left[i(E_m^0 - E_n^0)t / \hbar \right] \langle \phi_m | V(t) | \phi_n \rangle$$

$$initial\ condition\ \text{at t} = 0 : \psi(\text{t} = 0) = \phi_{\text{k}} \rightarrow c_n(0) = \delta_{nk}$$

We want to find $C_n(t)$

$$for\ \text{m} \neq \text{k}$$

$$i\hbar \frac{dc_m(t)}{dt} = \lambda \exp\left[i(E_m^0 - E_k^0)t / \hbar \right] \langle \phi_m | V(t) | \phi_k \rangle$$

$$c_m(t) = \frac{\lambda}{i\hbar} \int_0^t dt' \exp\left[i(E_m^0 - E_k^0)t' / \hbar \right] \langle \phi_m | V(t') | \phi_k \rangle$$

$$\text{the probability } \text{P}_{\text{n}}(t) = \left| \langle \phi_n | \psi(t) \rangle \right|^2 = \left| c_n(t) \right|^2$$

Absorption of Light

$$H = \frac{\left[\vec{p} + e\vec{A}(\vec{r},t)\right]^2}{2m} + V(\vec{r})$$

(1) Choose Coulomb gauge $\quad \vec{\nabla} \cdot \vec{A} = 0$

$$\left[\vec{p}, \vec{A}\right] = 0 \Rightarrow \vec{p} \cdot \vec{A} = \vec{A} \cdot \vec{p}$$

(2) Neglect A^2 term $\Rightarrow$ $\lambda V(t) = \frac{e}{m} \vec{A} \cdot \vec{P}$

$$\vec{A}(\vec{r},t) = A_0 \vec{\varepsilon} \cos(\vec{k} \cdot \vec{r} - \omega t)$$

$$= \frac{1}{2} A_0 \vec{\varepsilon} \exp(i\vec{k} \cdot \vec{r}) \exp(-i\omega t) + c.c.$$

$$c_n(t) = \frac{eA_0}{2m} \langle \phi_n | e^{i\vec{k}\cdot\vec{r}} \vec{\varepsilon} \cdot \vec{p} | \phi_k \rangle \int_0^t dt' e^{i(E_n^0 - E_k^0 - \hbar\omega)t'/\hbar}$$

$$+ \frac{eA_0}{2m} \langle \phi_n | e^{-i\vec{k}\cdot\vec{r}} \vec{\varepsilon} \cdot \vec{p} | \phi_k \rangle \int_0^t dt' e^{i(E_n^0 - E_k^0 + \hbar\omega)t'/\hbar}$$

$$\left|\int_0^t dt' e^{i(E_n^0 - E_k^0 \pm \hbar\omega)t'/\hbar}\right|^2 = \left|\int_0^t dt' e^{i\Omega t'}\right|^2 = \left|\frac{2}{\Omega} e^{i\Omega t/2} \sin\frac{\Omega t}{2}\right|^2 = \frac{4}{\Omega^2}\sin^2\frac{\Omega t}{2}$$

where $\Omega = \dfrac{E_n^0 - E_k^0 \pm \hbar\omega}{\hbar}$

$$\int_{-\infty}^{\infty} f(\Omega)\frac{4}{\Omega^2}\sin^2\frac{\Omega t}{2}\,d\Omega$$

$$\doteq f(0)\int_{-\infty}^{\infty} d\Omega\,\frac{4}{\Omega^2}\sin^2\frac{\Omega t}{2}$$

$$= 2tf(0)\int_{-\infty}^{\infty} dy\,\frac{1}{y^2}\sin^2 y$$

$$= 2\pi t f(0)$$

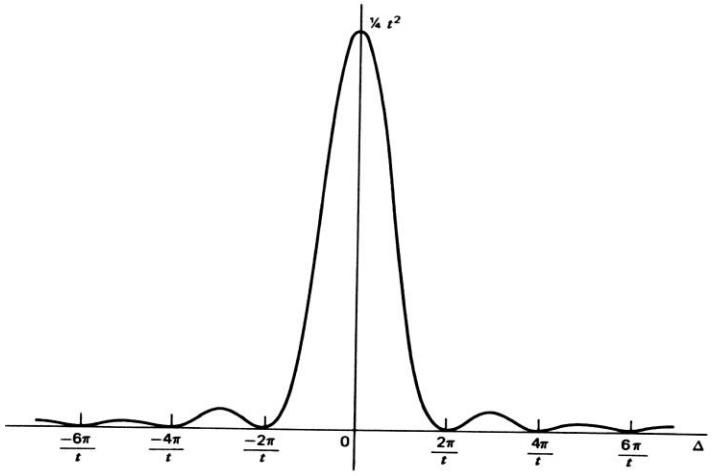


Figure 21-1. Plot of the function $1/\Delta^2 \sin^2 t\Delta/2$ versus Δ.

$$f(\Omega) = \frac{1}{\Omega^2}\sin^2\frac{\Omega t}{2} = \frac{1}{4}t^2\left[\frac{\sin^2 \Omega t/2}{\left(\Omega t/2\right)^2}\right]$$

For large t

$$\frac{4}{\Omega^2}\sin^2\frac{\Omega t}{2} \to 2\pi t\delta(\Omega) = 2\pi t\hbar\delta(E_n^0 - E_k^0 \pm \hbar\omega)$$

$$P_n(t) = \left|C_n(t)\right|^2$$

$$= \frac{2\pi}{\hbar} t \left(\frac{eA_0}{m}\right)^2 \left|\left\langle \phi_n \left| \exp(\pm i\vec{k}\cdot\vec{r})\vec{\varepsilon}\cdot\vec{p} \right| \phi_k \right\rangle\right|^2 \delta(E_n^0 - E_k^0 \pm \hbar\omega)$$

Optical properties : energy of photon 0.1 eV – 20 eV ; $\exp(\pm i\vec{k}\bullet\vec{r}) \sim 1$

Transition probability per unit time:

$$\Gamma_{k\to n} = \frac{2\pi}{\hbar}\left(\frac{eA_0}{m}\right)^2 \left|\left\langle \phi_n \left| \vec{\varepsilon}\cdot\vec{p} \right| \phi_k \right\rangle\right|^2 \delta(E_n^0 - E_k^o \pm \hbar\omega)$$

For absorption process :

$$\Gamma_{k\to n} = \frac{2\pi}{\hbar}\left(\frac{eA_0}{m}\right)^2 \left|\left\langle \phi_n \left| \vec{\varepsilon}\cdot\vec{p} \right| \phi_k \right\rangle\right|^2 \delta(E_n^0 - E_k^o - \hbar\omega)$$

Transition rate W : $\vec{M}_{cv} = \left\langle \phi_c \mid \vec{p} \mid \phi_v \right\rangle$

$$W(\omega) = \frac{2\pi}{\hbar}\left(\frac{eA_0}{m}\right)^2 \frac{V}{(2\pi)^3} \sum_v \sum_c \int_{Bz} d^3k \left|\vec{\varepsilon}\cdot\overrightarrow{M_{cv}}(\vec{k})\right|^2 \delta\left[E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega\right]$$

Absorption constant (α) = $\dfrac{\hbar\omega \times \text{Transition rate (W)}}{\text{Incident flux (I)}}$

$$I = v\bar{u} = \frac{c}{n}\frac{1}{2}\varepsilon\omega^2 A_0{}^2 = \frac{1}{2}nc\varepsilon_0\omega^2 A_0{}^2$$

$$\alpha(\omega) = \frac{4\pi e^2}{m^2 nc\varepsilon_0\omega}\frac{V}{(2\pi)^3}\sum_v\sum_c\int_{Bz} d^3k\left|\vec{\varepsilon}\cdot\overrightarrow{M_{cv}}(\vec{k})\right|^2\delta\left[E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega\right]$$

$$G_{cv}(\omega) = \frac{V}{(2\pi)^3}\int_{Bz} d^3k\,\delta\left[E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega\right]$$

Joint Density of States

$$= \frac{V}{(2\pi)^3}\int_{Bz}\frac{dS_E}{\vec{\nabla}_{\vec{k}}\left[E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega\right]} = \sum\nolimits_{T_i} G^i_{cv}(\omega)$$

$$\alpha(\omega) = \frac{4\pi e^2}{m^2 nc\varepsilon_0\omega}\sum_{T_i}\sum_v\sum_c\left|\vec{\varepsilon}\cdot\overrightarrow{M_{cv}}(\vec{k})\right|^2 G^i{}_{cv}(\omega)$$

Calculation of Dielectric Constant

$$\nabla^2\vec{E}-\frac{\mu\varepsilon}{c^2}\frac{\partial^2\vec{E}}{\partial t^2}=0 \qquad assume \qquad \mu=1$$

(Jackson P297)

$$\vec{E}=\vec{E}_0e^{i(kz-\omega t)} \quad ; \quad k^2=\varepsilon\frac{\omega^2}{c^2}$$

$$\vec{E}=\vec{E}_0e^{i(k_1z-\omega t)-\frac{1}{2}\alpha z}$$

$$I\sim E^2\sim I_0e^{-\alpha z}$$

$$\varepsilon=\varepsilon_1+i\varepsilon_2$$

$$k=k_1+i\frac{\alpha}{2}$$

$$\Rightarrow \begin{cases} k_1^{\,2}-\dfrac{\alpha^2}{4}=\dfrac{\omega^2}{c^2}\varepsilon_1 \\ k_1\alpha=\dfrac{\omega^2}{c^2}\varepsilon_2 \end{cases}$$

$$\alpha=\sqrt{2}\frac{\omega}{c}\left[-\varepsilon_1\pm\sqrt{\varepsilon_1^2+\varepsilon_2^2}\right]^{1/2}$$

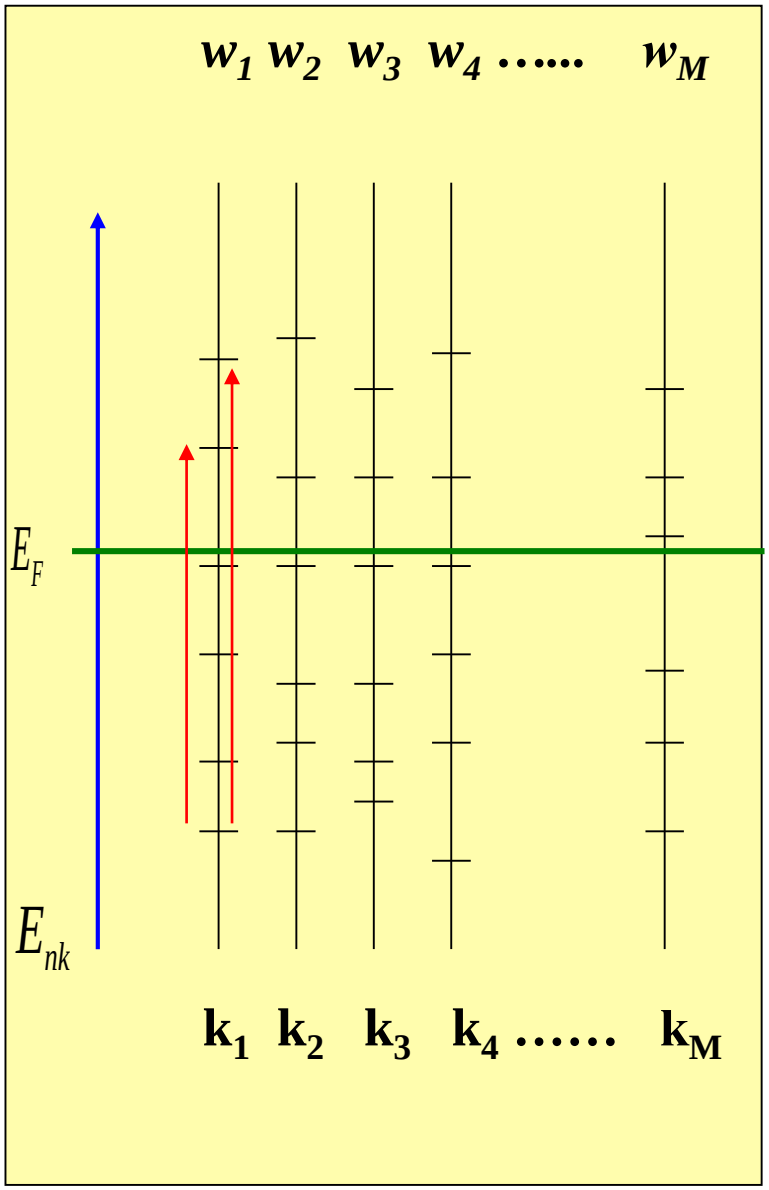
$$\alpha=\frac{\omega^2}{c^2k_1}\varepsilon_2=\frac{\omega}{nc}\varepsilon_2$$

$$\varepsilon_2(\omega)=\frac{4\pi e^2}{m^2\omega^2}\sum_v\sum_c\left|\vec{\varepsilon}\bullet\overrightarrow{M_{cv}}(\vec{k})\right|^2G_{cv}(\hbar\omega)$$

Kramers-Kronig relations

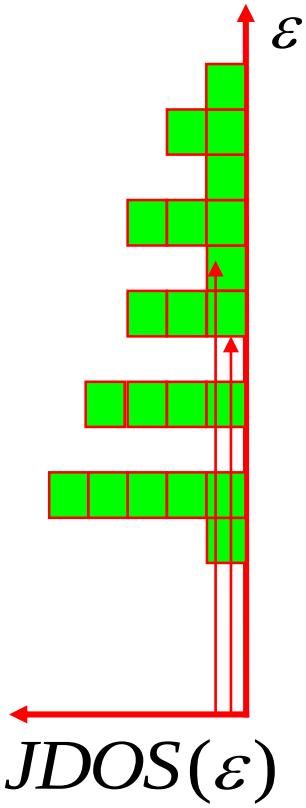
$$\varepsilon_1(\omega)=1+\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{\varepsilon_2(\omega')-1}{\omega'-\omega}d\omega'$$

Joint Density of State



$$G_{cv}(\omega) = \frac{V}{(2\pi)^3} \int_{Bz} d^3k \delta\left[E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega \right]$$

$$\varepsilon_2(\omega) = \frac{4\pi e^2}{m^2\omega^2} \sum_v \sum_c \left| \vec{\varepsilon} \cdot \overrightarrow{M_{cv}}(\vec{k}) \right|^2 G_{cv}(\hbar\omega)$$



$$\vec{M}_{cv} = \left\langle \phi_c \mid \vec{p} \mid \phi_v \right\rangle$$

The fermi dirac function

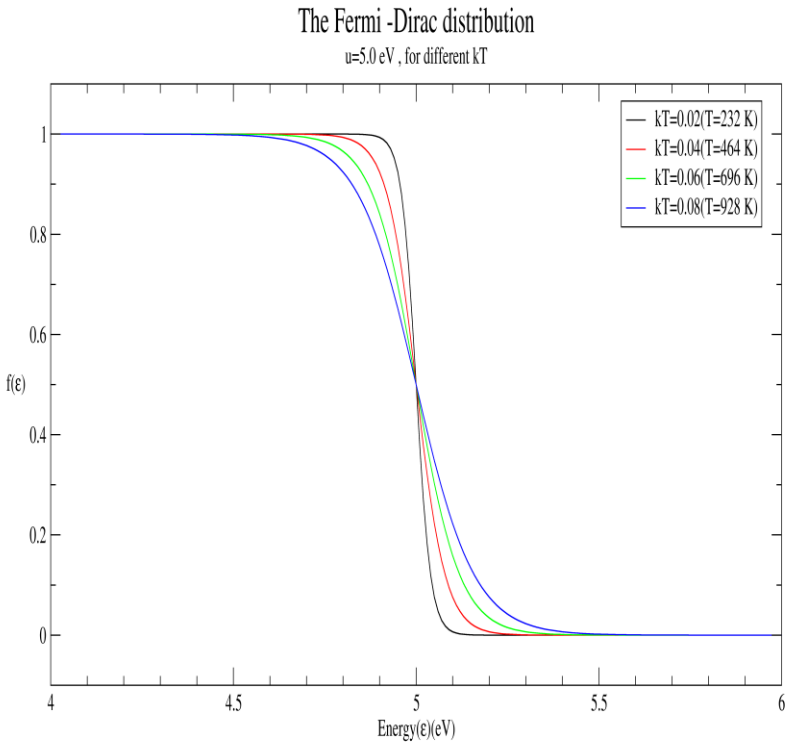
$$f(\varepsilon) = \frac{1}{1 + e^{(\varepsilon - \mu)/kT}}$$

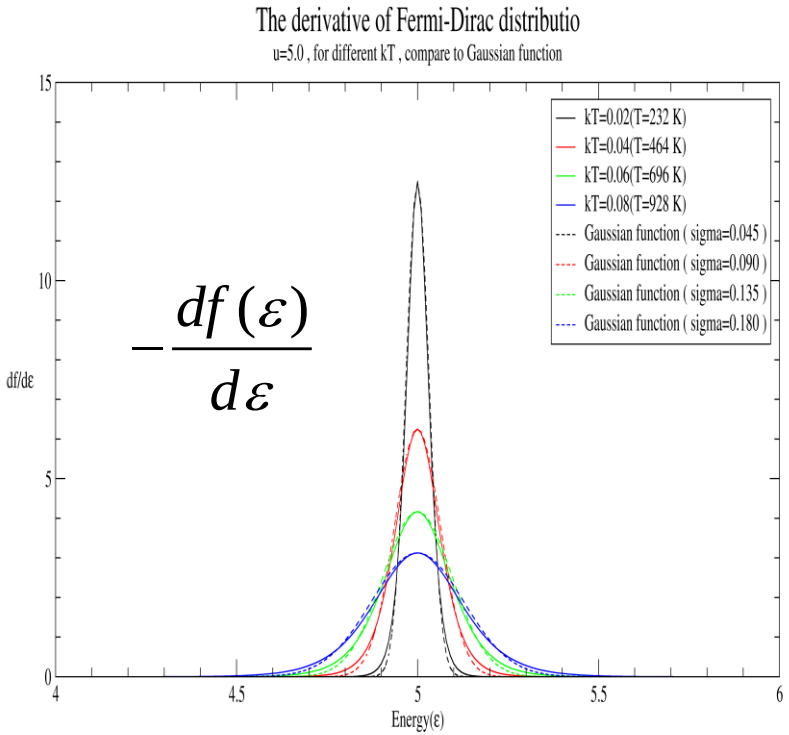
At T = 0

$$-\frac{df(\varepsilon)}{d\varepsilon} = \delta(\varepsilon - \mu)$$

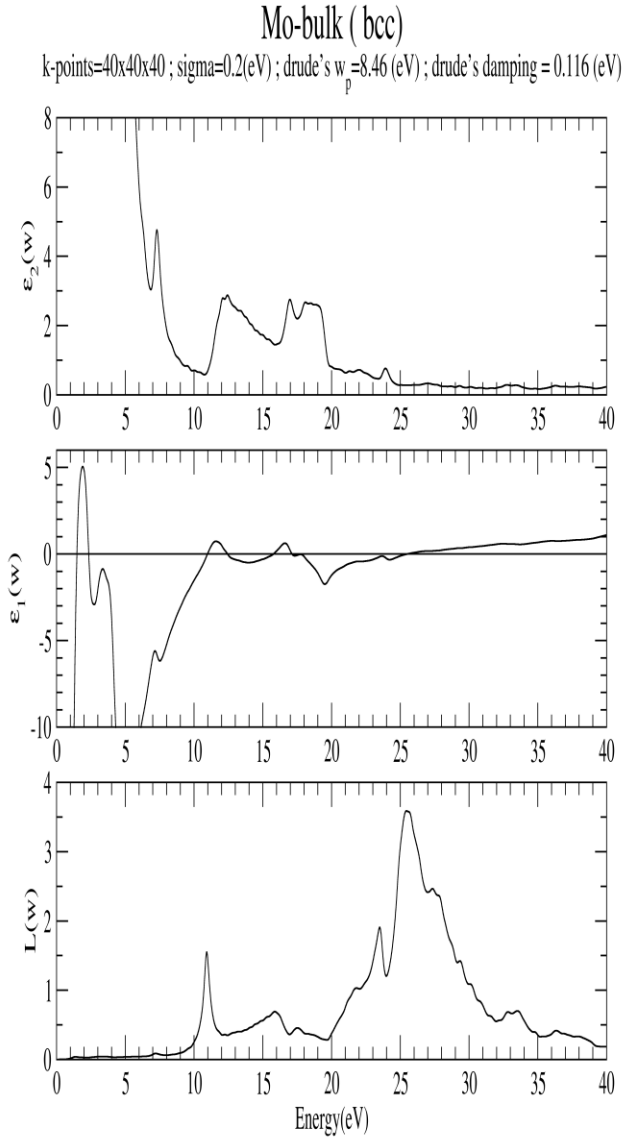
For small T, it behaves like Gaussian function

$$f(\varepsilon) = \frac{1}{\alpha\sqrt{\pi}} e^{-(\frac{\varepsilon-\mu}{\alpha})^2}$$





$$\varepsilon_2^{\text{int } ra}(\omega) = \frac{4\pi e^2}{m^2\omega^2} \sum_{nk} \left| \vec{\varepsilon} \cdot \overrightarrow{M_{nn}}(\vec{k}) \right|^2 \left(-\frac{\partial f_0}{\partial \varepsilon} \right)_{\varepsilon_{nk}} D_n(\hbar\omega)$$



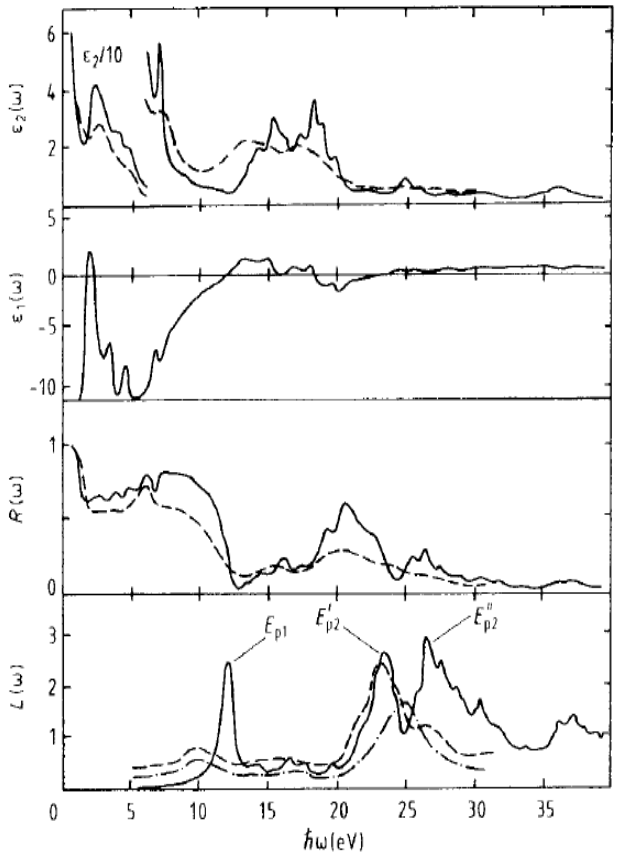
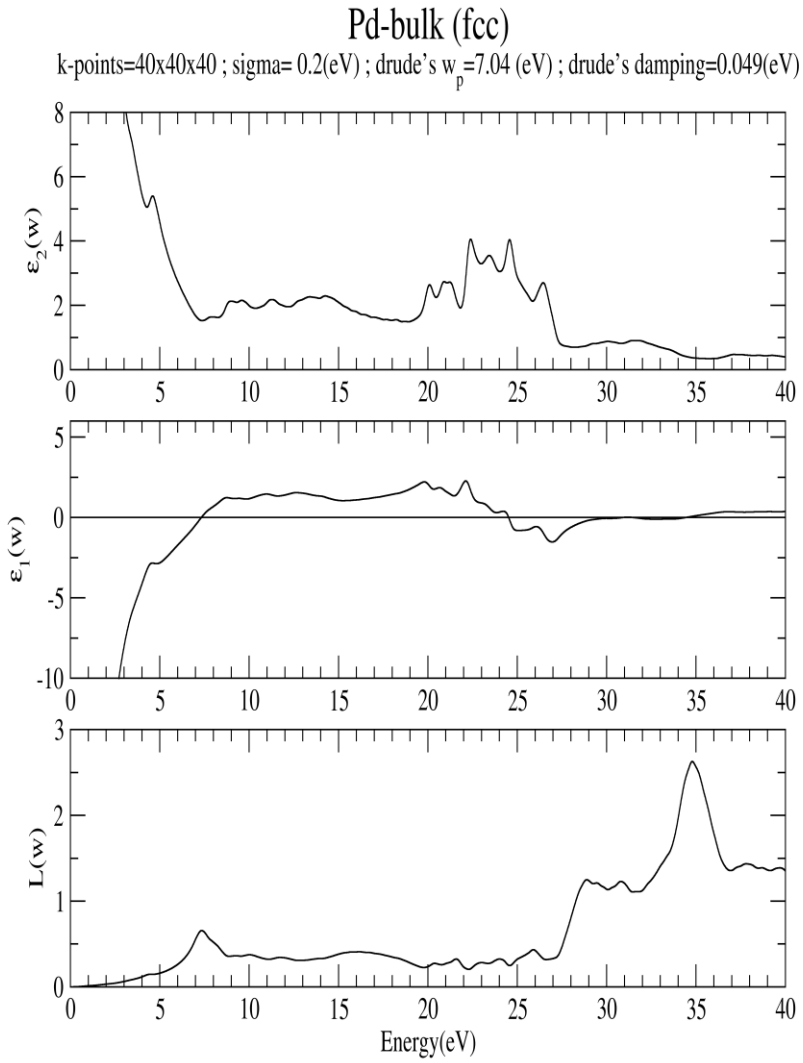


Figure 6. Optical properties of molybdenum: full curves, calculations; broken curves, measurements (from Mayevskii *et al* 1981); chain curve, measurements of $L(\omega)$ (from Weaver *et al* 1974) (arbitrary units).

J.Phys.F:Met.Phys.18(1988) 833-849



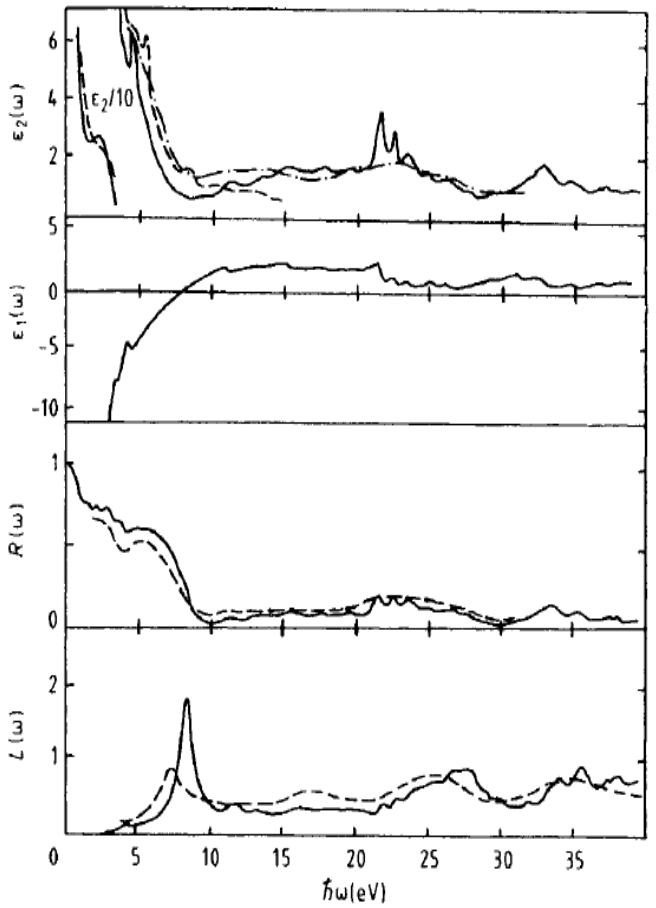


Figure 4. Optical properties of palladium: full curves, calculations; broken curves, measurements of $\varepsilon_2(\omega)$ (from Weaver 1973), $R(\omega)$ (from Vehse *et al* 1970) and $L(\omega)$ (from Daniels 1969); chain curve, measurements of $\varepsilon_2(\omega)$ (from Vehse *et al* 1970) (arbitrary units).

J.Phys.F:Met.Phys.18(1988) 833-849

Step by Step Tutorial

Calculations on Optical Properties

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$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{eff}(\vec{r})\right]\psi_i(\vec{r}) = \varepsilon_i\psi_i(\vec{r}) \quad ; \quad \rho(\vec{r}) = \sum_i^{occ}\left|\psi_i(\vec{r})\right|^2$$

$$V_{eff}(\vec{r}) = V_{ext}(\vec{r}) + V_H(\vec{r}) + V_{xc}(\vec{r}) + V_{ps}(\vec{r})$$

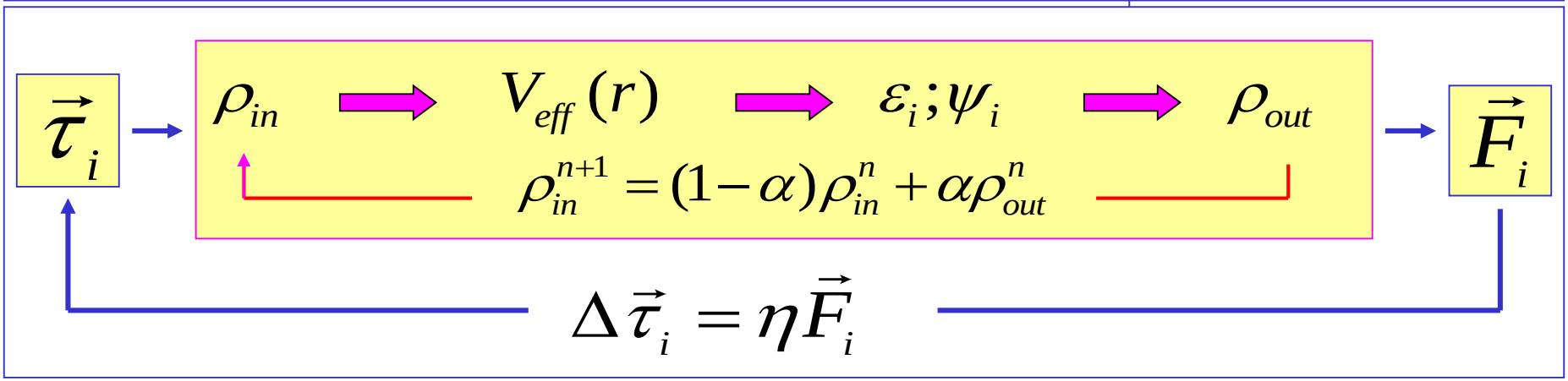
$$V_H(\vec{r}) = \int \frac{\rho(\vec{r})}{\left|\vec{r}-\vec{r}'\right|}d^3r \; ; \quad \boxed{V_{xc}(\vec{r}) = V_{xc}(\rho(\vec{r})) \quad \textbf{LDA}}$$

$$V_{eff}(\vec{r}+\vec{R}) = V_{eff}(\vec{r})$$

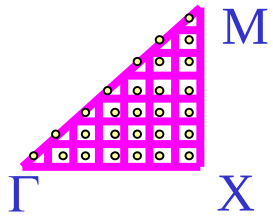
$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u(\vec{r})$$

$$u_k(\vec{r}) = \sum_{G_n < G_{\max}} C_n e^{i\vec{G}_n\cdot\vec{r}}$$

$$\underset{\sim}{H}(\vec{k})\underset{\sim}{C} - \lambda\underset{\sim}{S}\underset{\sim}{C} = 0$$



Structure of the system ($\boldsymbol{R}$, $\boldsymbol{\tau}$) : **POSCAR**
Pseudopotential of the atoms : **POTCAR**
Number of K- points in the IBZ : **KPOINTS**

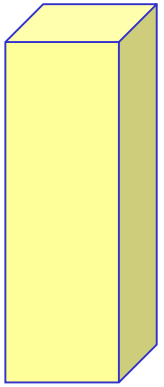


$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{G_n < G_{\max}} C_n e^{i\vec{G}_n\cdot\vec{r}}$$

$$\rho(\vec{r}) = \sum_{\vec{G}} \rho(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$

$$V(\vec{r}) = \sum_{\vec{G}} V(\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$

INCAR



G_{max}, NGX, NGY, NGZ

NGX,NGY,NGZ **:** controls the number of grid-points in the FFT-mesh into the direction of the three lattice-vectors**.**

Break condition for electronic SC-loop and ionic relaxation loop.
Max. number of electronic step and ionic step.
How the ions are updated and moved (conjugate-gradient method).
How the partial occupancies $\boldsymbol{f_{nk}}$ are set for each wavefunction.

VASP

INPUT FILES

POSCAR
POTCAR
KPOINTS
INCAR

OUTPUT FILES

OUTCAR
OSZICAR
CONTCAR
CHGCAR
WAVECAR
EIGENVAL
PROCAR
MME
MME2

Stop VASP during the program execution

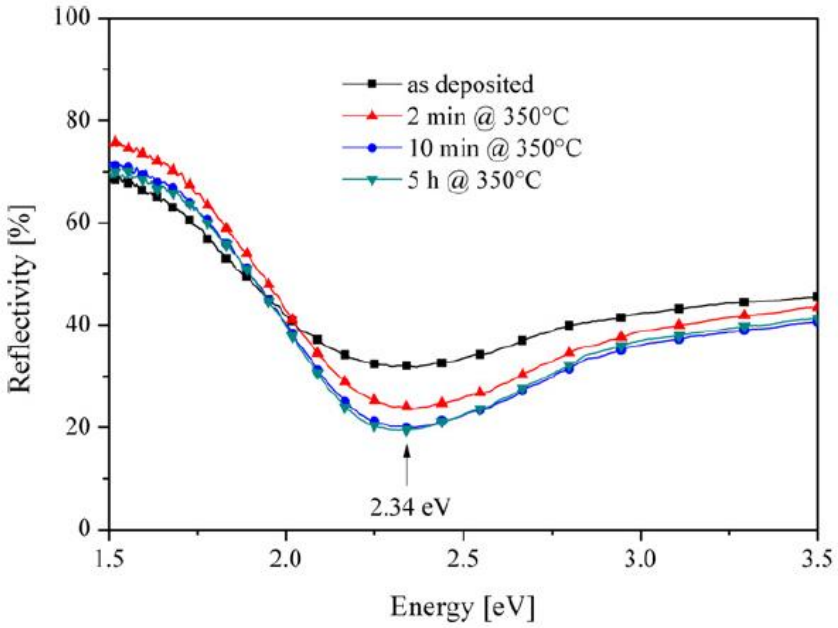
STOPCAR

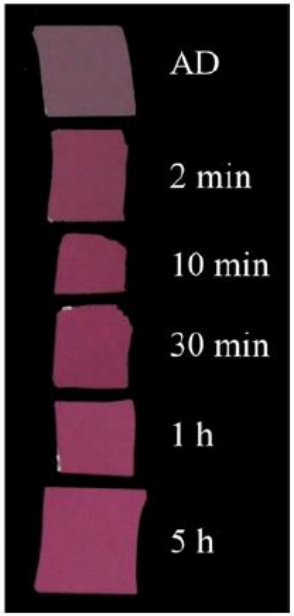
LSTOP = .TRUE. **(Ionic step)**
LABORT = .TRUE. **(Electronic step)**

VASP will check the existence of STOPCAR
for every electronic step and ionic step.
Print out WAVECAR and CHGCAR before stop.

vsub_opitcs name
bkill jobid

The unusual purple color in $AuAl_2$





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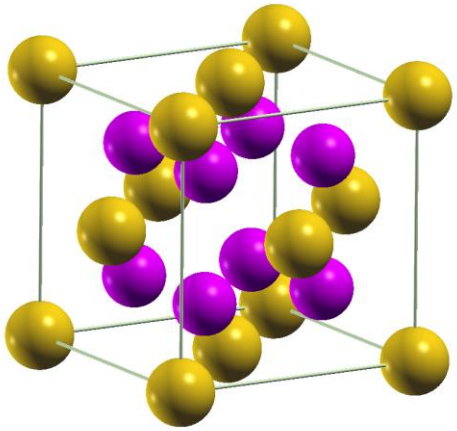
Lattice structure of $AuAl_2$



Fluorite structure

A = Au

B = Al, Ga

POSCAR

```
AuAl2
6.500000
0.000000 0.500000 0.500000
0.500000 0.000000 0.500000
0.500000 0.500000 0.000000
1 2
Direct
0.000000 0.000000 0.000000
0.250000 0.250000 0.250000
0.750000 0.750000 0.750000
```

Set up the environment in optics calculaiton

```
cd
cp /home/s11gyg00/cp-1218.sh  .
./cp-1218.sh
```

How to run optics

1. Calculate the lattice constant of AuAl2

cdw
cd Hands-on-1218
Hands-on-1218> ls
1-Au 2-W 3-AuAl2 4-AuGa2 5-AuAl2-results
cd 3-AuAl2
mkdir 1-stress
mkdir 2-optics
cd 1-stress
cat ~/pot/POTCAR.Au.LDA > POTCAR
cat ~/pot/POTCAR.Al.LDA >> POTCAR
vi INCAR / POSCAR / KPOINTS
1-stress> ls
1-stress> vsub_optics 3-stress
JOBID = 7344 JOB=3-stress
This script is for running a single VASP job
…….
How manyf CPUs do you want to run your job?
1cpu, 4cpu, 8cpu, 12cpu, 24cpu, 48cpu, 96cpu, 192cpu? [1cpu]
12cpu
If more than 48 cpus were selected, specify the number of cores per node:
6, 12, 24, or 48?
(Enter)
Job <544761> is submitted to queue <12cpu>j

INCAR

```
System=AuAl2
PREC=high
ISIF=3
IBRION=2
NSW=100
EDIFF=0.000001
EDIFFG = -0.01
RWIGS=1.503 1.402
```

KPOINTS

```
10x10x10
0
Monkhorst
10 10 10
0 0 0
```

POSCAR

```
AuAl2
6.500000
0.000000 0.500000 0.500000
0.500000 0.000000 0.500000
0.500000 0.500000 0.000000
1 2
Direct
0.000000 0.000000 0.000000
0.250000 0.250000 0.250000
0.750000 0.750000 0.750000
```

2. Calculate the matrix element of AuAl2

1-stress> cd ../2-optics
2-optics> mkdir 10k
2-optics> cd 10k
cp ../../1-stress/CONTCAR POSCAR
cp ../../1-stress/POTCAR .
cp ../../1-stress/INCAR .
cp ../../1-stress/KPOINTS .
cp ../../1-stress/CHGCAR .

```
System=AuAl2 with spin-orbit coupling
RWIGS=1.503 1.402
NPAR=1
ISMEAR=0
SIGMA = 0.2
MAGMOM=0 0 0.000001 0 0 0.000001 0 0 0.000001
LSORBIT=.TRUE.
SAXIS=0 0 1
GGA_COMPAT=.FALSE.
LOPTICS=.TRUE.
NBANDS=60
```

```
System=AuAl2
RWIGS=1.503 1.402
NPAR=1
ISMEAR=0
SIGMA = 0.2
LOPTICS=.TRUE.
NBANDS=30
```

```
10X10x10
0
Monkhorst
10 10 10
0 0 0
```

```
AuAl2
  6.50000
    0.0000000000000000   0.4583121851601681   0.4583121851601681
    0.4583121851601681   0.0000000000000000   0.4583121851601681
    0.4583121851601681   0.4583121851601681  -0.0000000000000000
   Au   Al
    1    2
Direct
  0.0000000000000000 -0.0000000000000000  0.0000000000000000
  0.2500000000000000  0.2500000000000000  0.2500000000000000
  0.7500000000000000  0.7500000000000000  0.7500000000000000

  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
  0.00000000E+00  0.00000000E+00  0.00000000E+00
```

2-optics> ls
CHGCAR INCAR KPOINTS POSCAR POTCAR
2-optics> vsub_optics optics

3. Calculate the optical properties of AuAl2

2-optics > ls (only important output are shown in the following)

MME OUTCAR_EPSIM.dat PROCAR WAVEDER
MME2 OUTCAR_EPSRE.dat OPTIC STRUC

s11gyg00@alps6:/work/s11gyg00/Hands-on-1218/3-AuAl2/2-optics> **grep fermi OU***

OUTCAR: ISMEAR = 0; SIGMA = 0.20 broadening in eV -4-tet -1-fermi 0-gaus

OUTCAR: E-fermi : **7.8818** XC(G=0): -10.8076 alpha+bet :-13.7653

2-optics > optics.sh AuAl2

2-optics > cd optics

optics> ls

AuAl2.mme AuAl2.mme2 AuAl2.opticin AuAl2.procar AuAl2.strucin opticpack.def

```
2, 1                    ! intra (1/2 no/yes), imme (1/2)
2, 2, 0.1               ! islot,ikk,kkshift (for interband transition)
2, 0.07, 0              ! idrude,drude_damping,wpshift (not use for intra =1 )
1, 7.8818, 1, 1, 0, 0   ! ival,ef,imetal,ispin,iso,itr
0.0, 20.0, 0.02, 0.2, 30 ! emin,erange,de,sigma,nbcal0
1                       ! isci
0.0                     ! eshift
3                       ! itot
1                       ! icom(1~itot 1:xx, 2:yy 3:zz)
2
3
```

AuAl2.opticin

optics> optics-2017.x

AuAl2.opticin


```
2, 1                        ! intra (1/2 no/yes), imme (1/2)
2, 2, 0.1                   ! islot,ikk,kkshift (for interband transition)
2, 0.07, 0                  ! idrude,drude_damping,wpshift (not use for intra =1 )
1, 7.8818, 1, 1, 0, 0       ! ival,ef,imetal,ispin,iso,itr
0.0, 20.0, 0.02, 0.2, 30    ! emin,erange,de,sigma,nbcal0
1                           ! isci
0.0                         ! eshift
3                           ! itot
1                           ! icom(1~itot 1:xx, 2:yy 3:zz)
2
3
```

For intraband transitions

idrude=1 (formula from exciting code) :

$$\varepsilon_{ab,a=b}=\delta_{aa}+\frac{4\pi i\sigma(\omega)}{\omega+i\eta(\omega)}=1-\frac{\omega_p^2}{(\omega+i\eta(\omega))^2}=1-\frac{\omega_p^2(\omega^2-\eta^2)}{(\omega^2+\eta^2)^2}+i\left(\frac{2\omega_p^2\omega\eta}{(\omega^2+\eta^2)^2}\right)$$

Where η is sigma , the Gaussian smear factor .

(Don't use the damping term)

idrude= else (formula from drude-model (**default**)) :

$$\varepsilon_{ab,a=b}=\varepsilon_1(\omega)+i\varepsilon_2(\omega)=1-\frac{\omega_p^2}{\omega^2+i\Gamma\omega}=\left(1-\frac{\omega_p^2}{\omega^2+\Gamma^2}\right)+i\frac{\omega_p^2\Gamma}{\omega(\omega^2+\Gamma^2)}$$

where Γ is the damping term (unit in eV)

wpshift : Shift the calculated plasma energy (unit in eV),

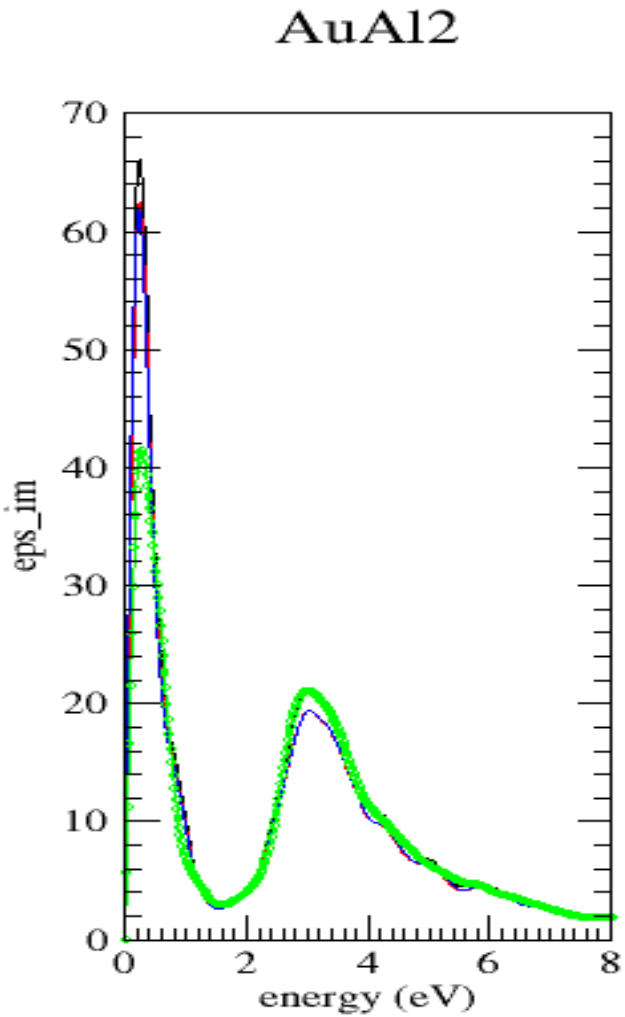
intra : 1= false, otherwise = true (include the intraband transition)
imme: 1-read mme file(case.mme), otherwise-read mme2 file (case.mme2 : vasp's mme)
ifstatic : if calculate static value only (default = 0)
islot : 1 is closed , other : open
ikk : 1 is closed , other : open
kkshift : useful for ikk ≠ 1 (default : 0.1)
ival : number of valence bands (not used for metal)
ef : fermi energy (eV) (not used for a non-metal)
imetal: 1 for metal , otherwise for a non-metal)
ispin: 1 or 2 (2 for spin-polarized)
iso: 1 for spin-orbit coupling (default=0)
itr: 1 without symmetry (default = 0)
emin: minimum energy
erange: maximum energy=emin+erange
de: △energy
sigma: Gaussian smear factor (unit in eV)
nbcal0: number of bands to be considered , could be determined by mme file
(equal to NBANDS from INCAR)
isci: 0 – do not use
1 – native form , only shift energy
2 – also renormalize momentum matrix
(default : 1)
eshift: energy shift (default : 0.0)
itot: 1~6
1 – xx 2 – yy 3—zz 4—yz(zy) 5—zx(xz) 6—xy(yx)
icom: icom=icom(itot)

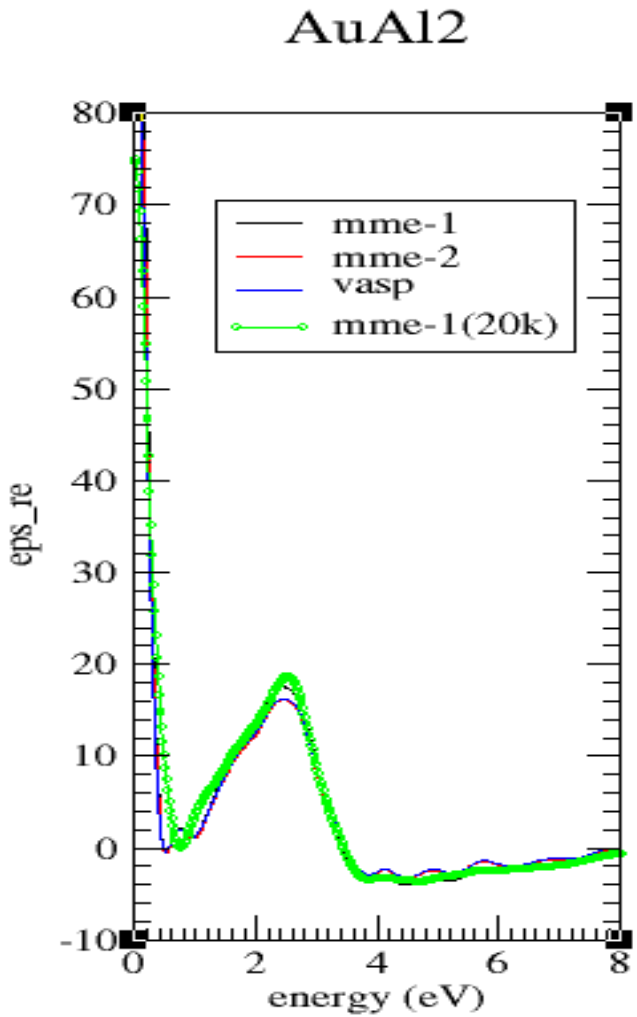
output of optics-2017.x

AuAl2.opticout	AuAl2.jdos	AuAl2.alpha1
AuAl2.epsre_intra	AuAl2.epsim_intra	
AuAl2.epsre_inter	AuAl2.epsim_inter	
AuAl2.epsre	AuAl2.epsim	AuAl2.epsabs
AuAl2.refrare	AuAl2.refraim	
AuAl2.sigre	AuAl2.sigim	
AuAl2.eels_intra	AuAl2.eels_inter	AuAl2.eels
AuAl2.wplas		

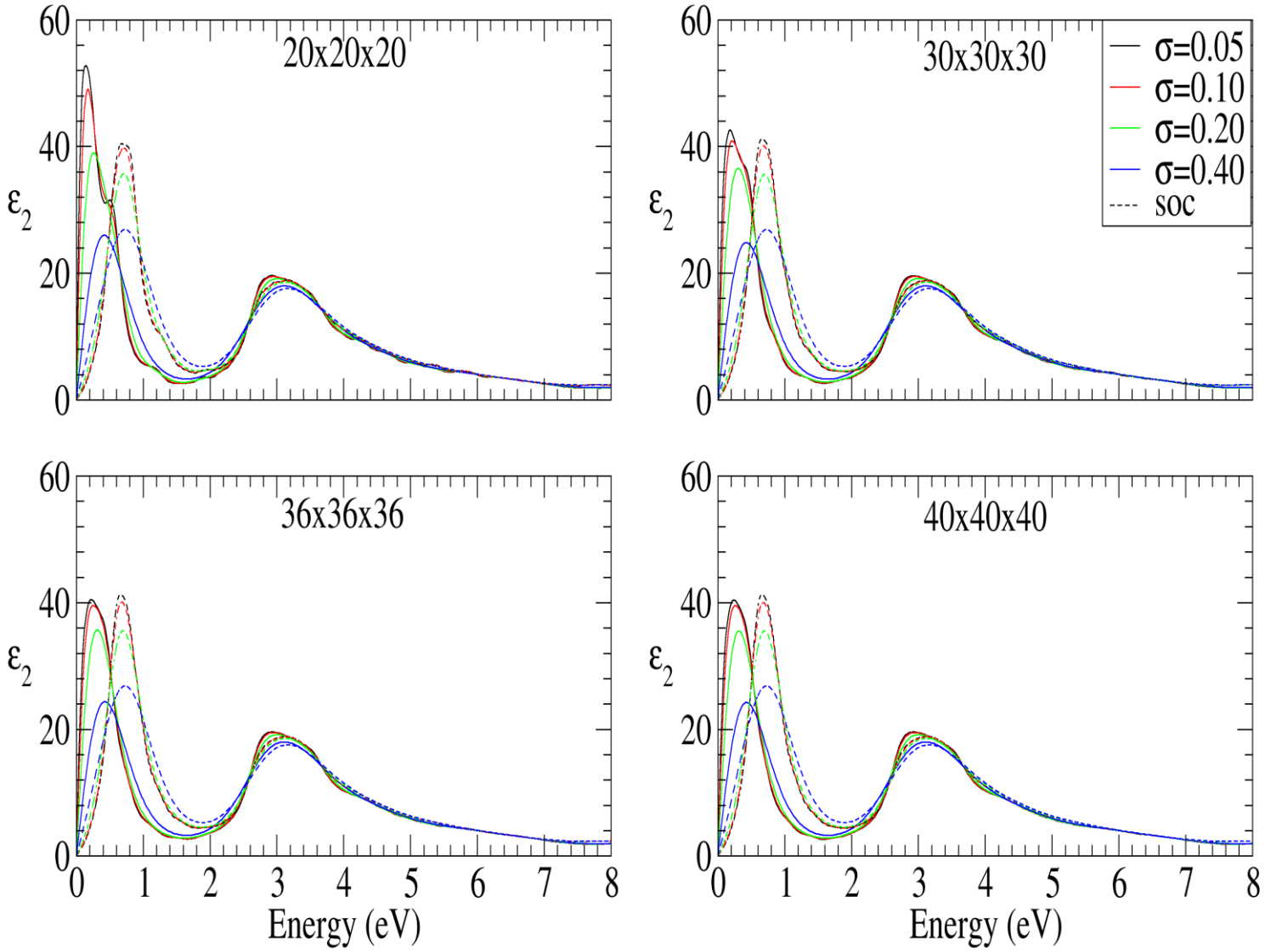
optics.sh name

```
mkdir optics
cd optics
cp ../MME $1.mme
cp ../MME2 $1.mme2
cp ../STRUC $1.strucin
cp ../PROCAR $1.procar
cp ~/bin/X.opticin $1.opticin
cat >opticpack.def<<!
$1
!
```

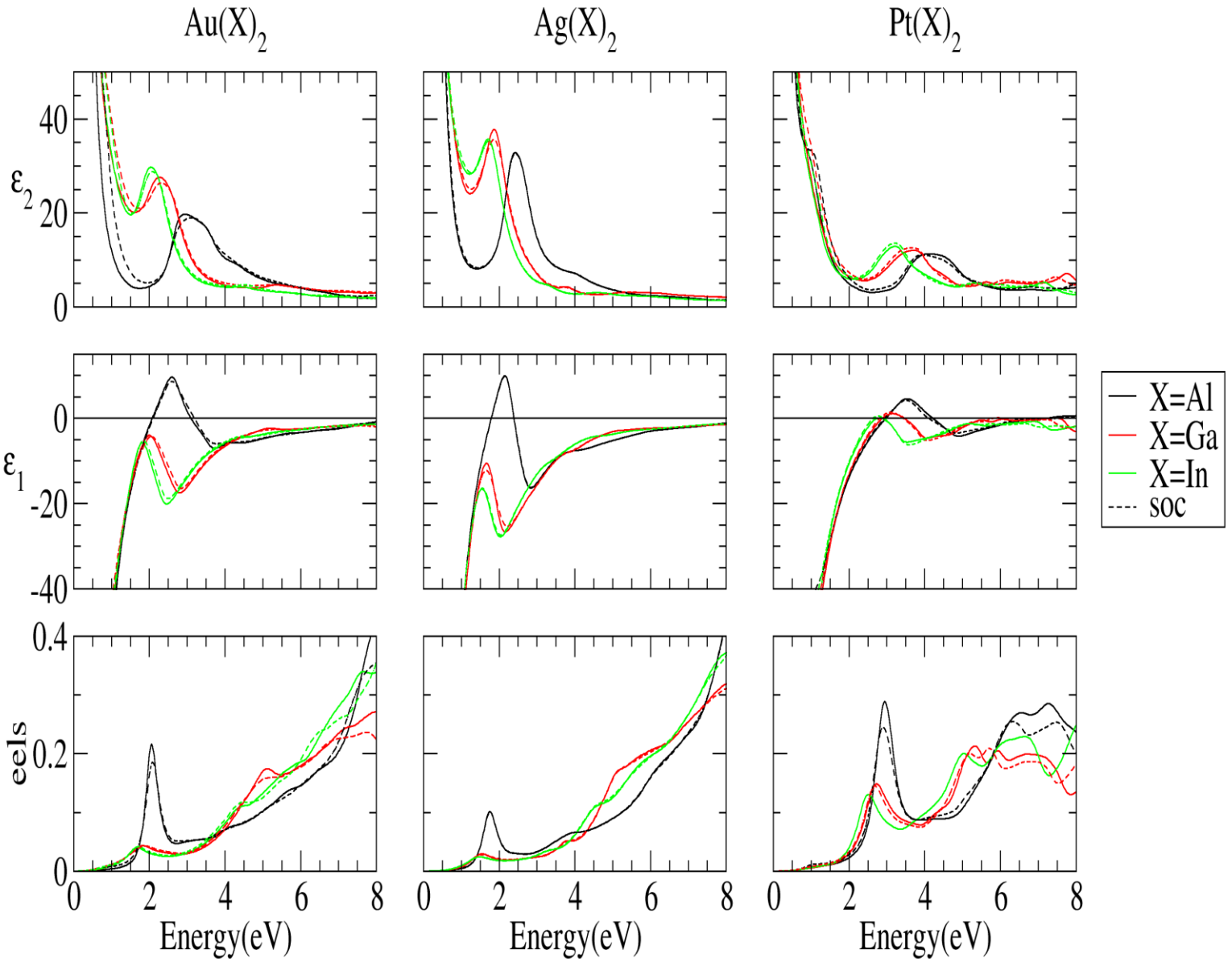




interband contribution only



interband contribution only



interband + intraband

Homework in Optics Properties

1. **Find the joint density of states, dielectric function, energy loss function and absorption constant of Au and W (see example) . Find the spin-orbit interaction effect and strain effect on the optical properties. (- 4%, -2%, 0%, 2%, 4%)**

2. **Find the joint density of states, dielectric function, energy loss function and absorption constant of $AuAl_2$ and $AuGa_2$. Find the spin-orbit interaction effect and strain effect on the optical properties. (- 4%, -2%, 0%, 2%, 4%)**

END