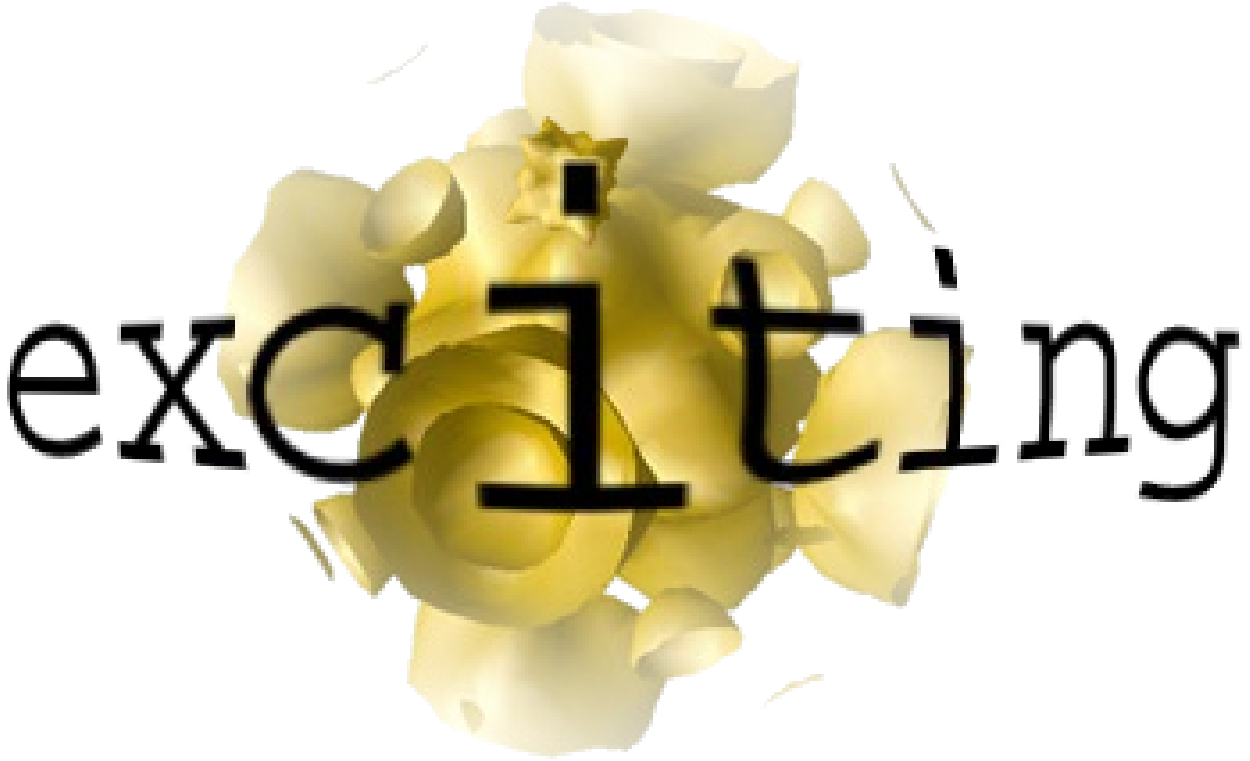
http://exciting-code.org



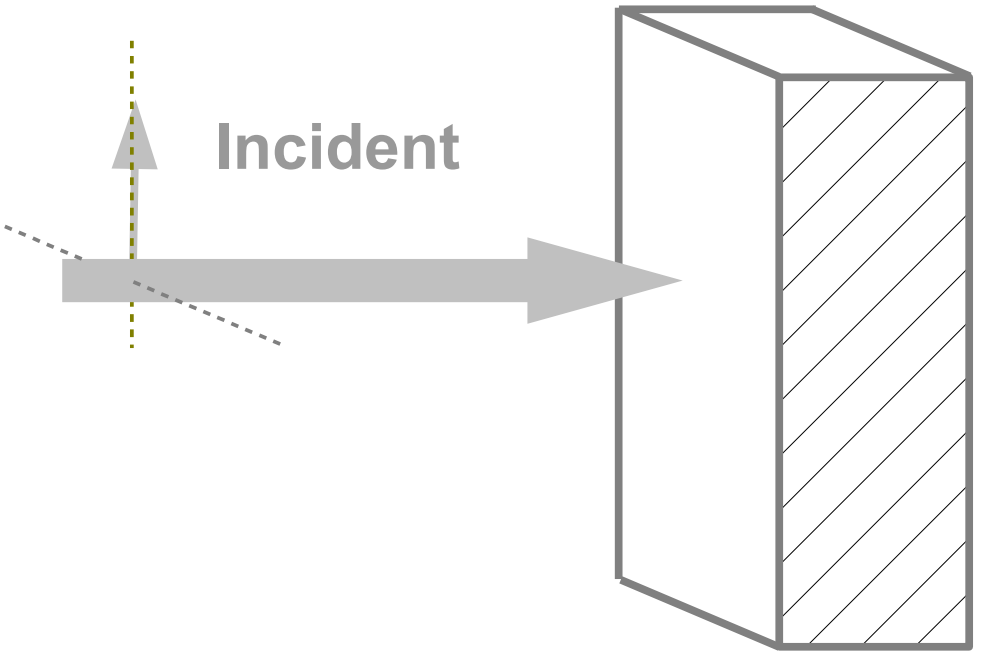
Magneto optical Kerr effect in **exciting**

Santiago Rigamonti
Humboldt Universität zu Berlin

exciting Workshop, 7 August 2014, Berlin

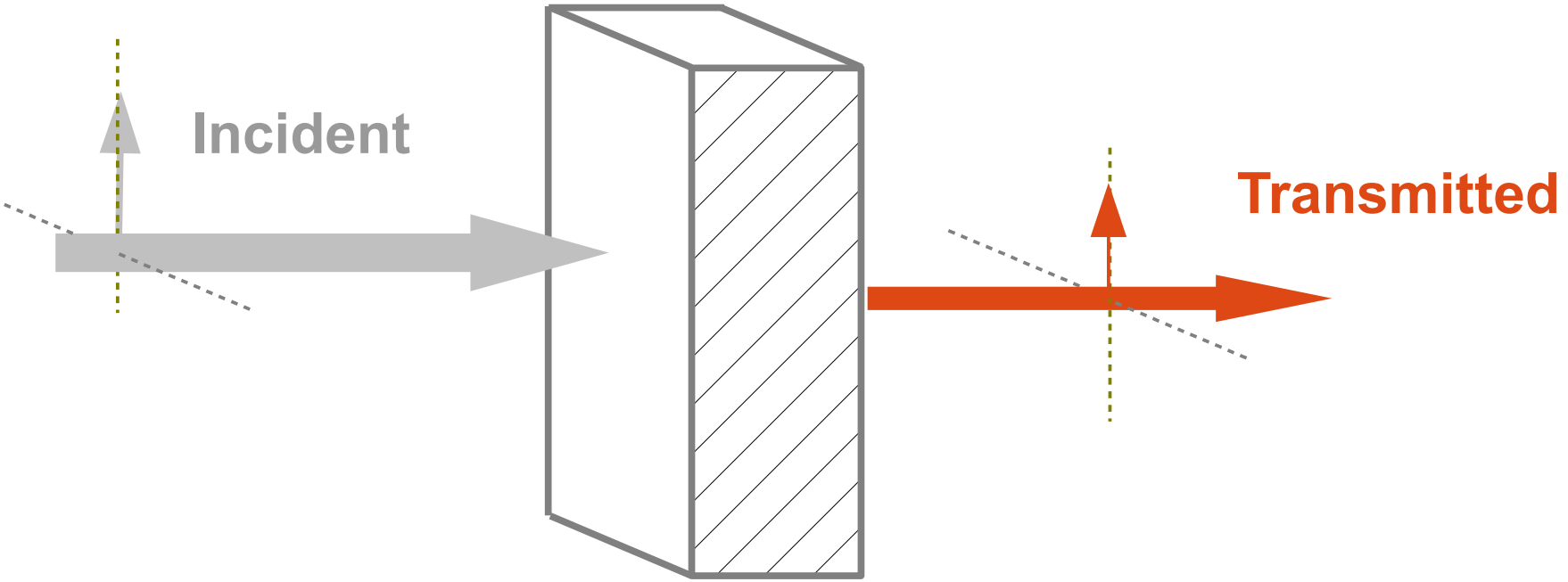
MOKE in a nutshell

Kerr and **Faraday** effects



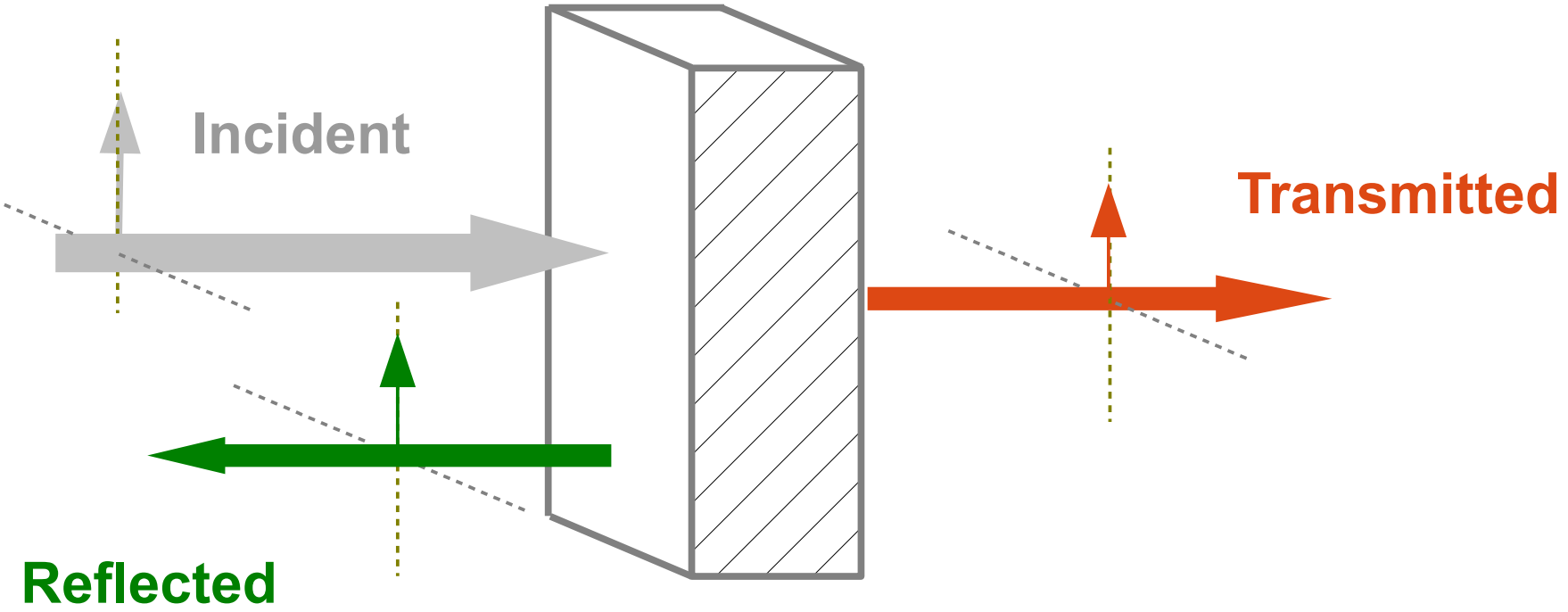
MOKE in a nutshell

Kerr and **Faraday** effects



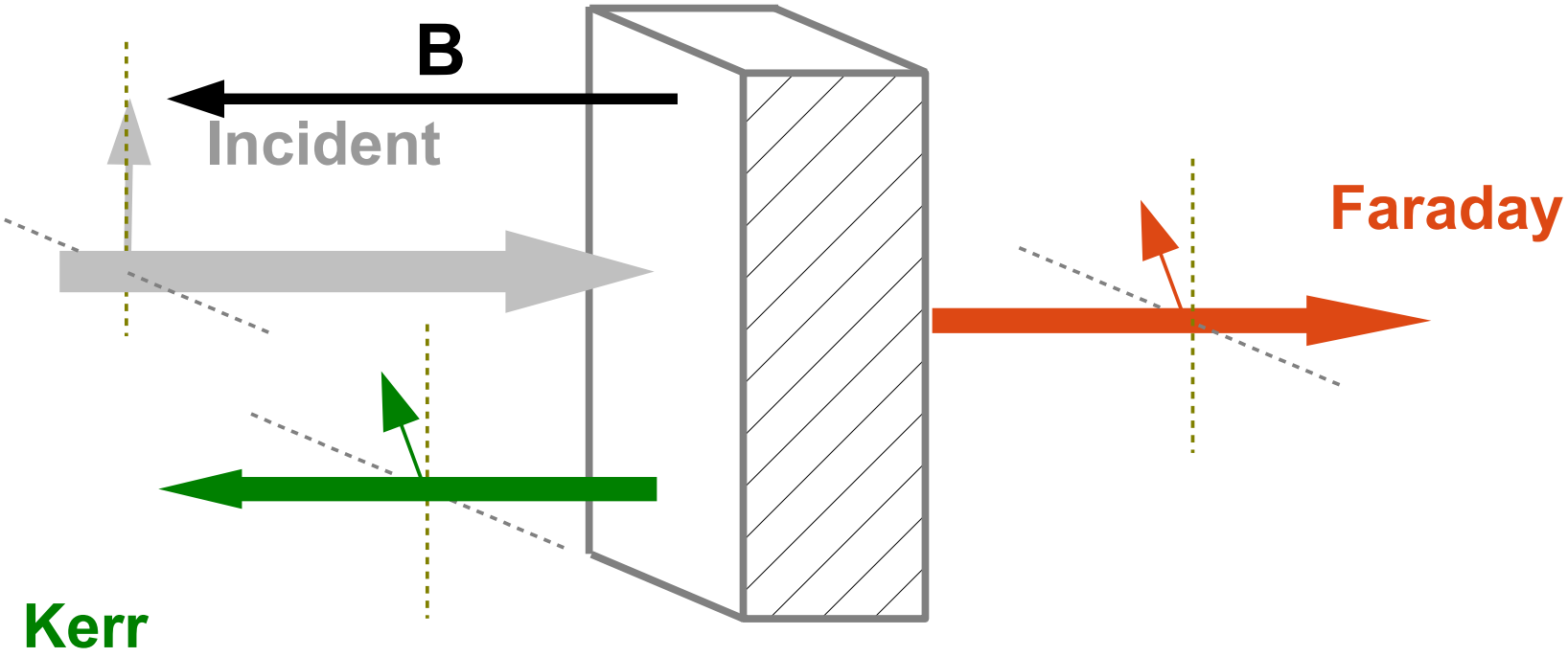
MOKE in a nutshell

Kerr and **Faraday** effects



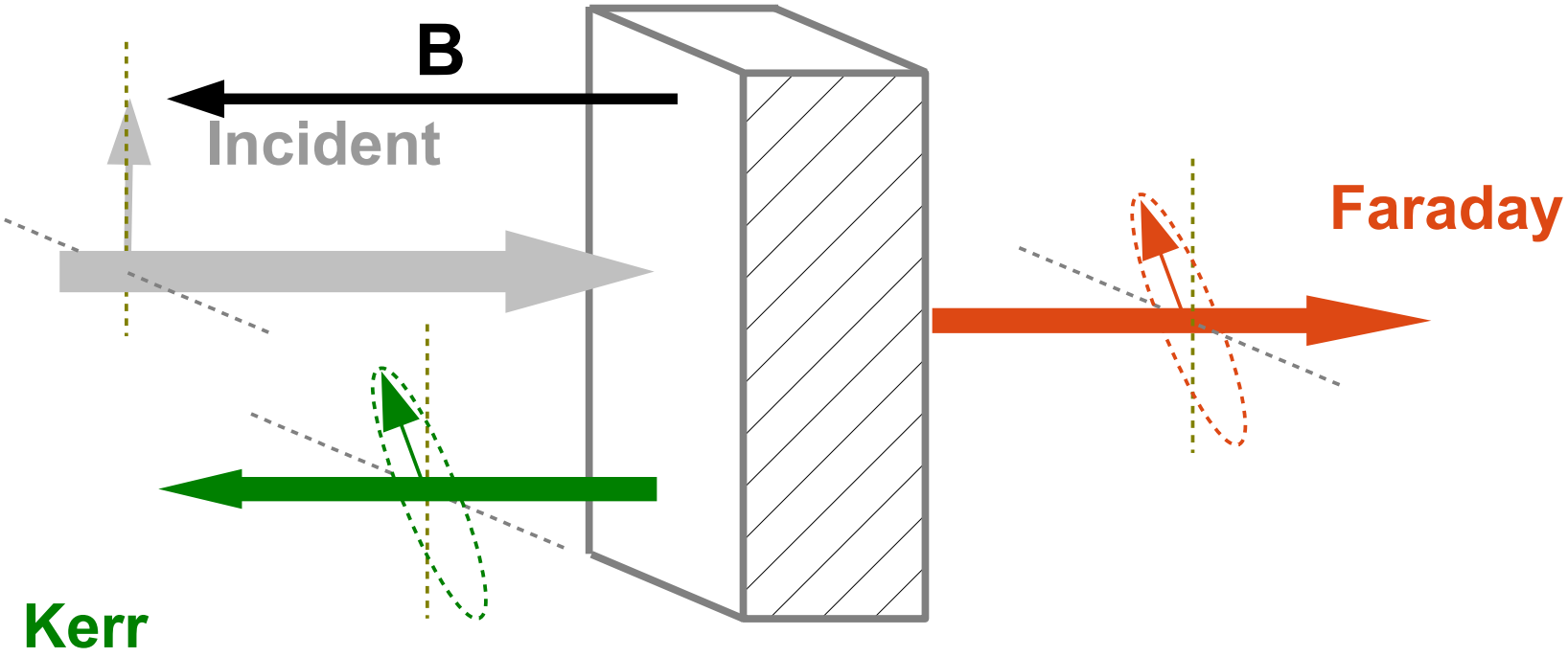
MOKE in a nutshell

Kerr and **Faraday** effects



MOKE in a nutshell

Kerr and **Faraday** effects



MOKE in a nutshell

Key quantity: dielectric tensor

$$\varepsilon_{\alpha\beta} \qquad \alpha,\ \beta = x,\ y,\ z$$

MOKE in a nutshell

Key quantity: dielectric tensor

$$\varepsilon_{\alpha\beta} \qquad \alpha, \beta = x, y, z$$

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix}$$

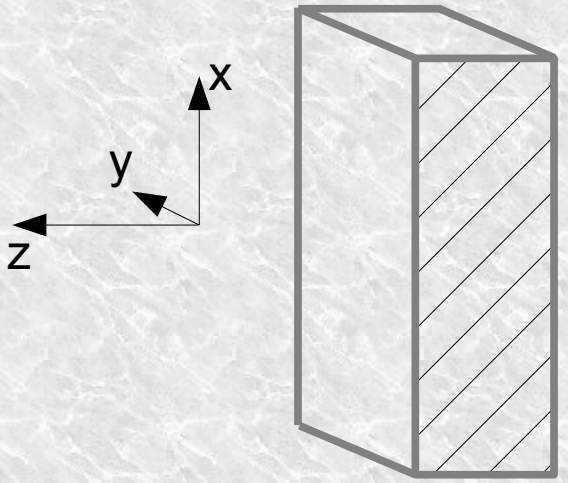
MOKE in a nutshell

Key quantity: dielectric tensor

$$\varepsilon_{\alpha\beta} \qquad \alpha,\ \beta = x,\ y,\ z$$

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{xx} \end{pmatrix}$$



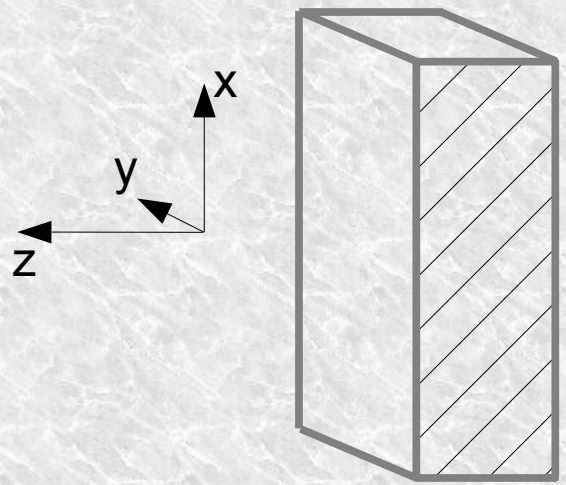
MOKE in a nutshell

Key quantity: dielectric tensor

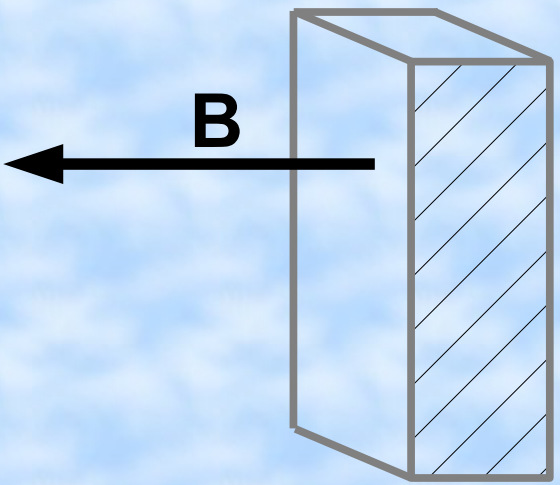
$$\varepsilon_{\alpha\beta} \qquad \alpha, \beta = x, y, z$$

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{xx} \end{pmatrix}$$



$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$



MOKE in a nutshell

Key quantity: dielectric tensor

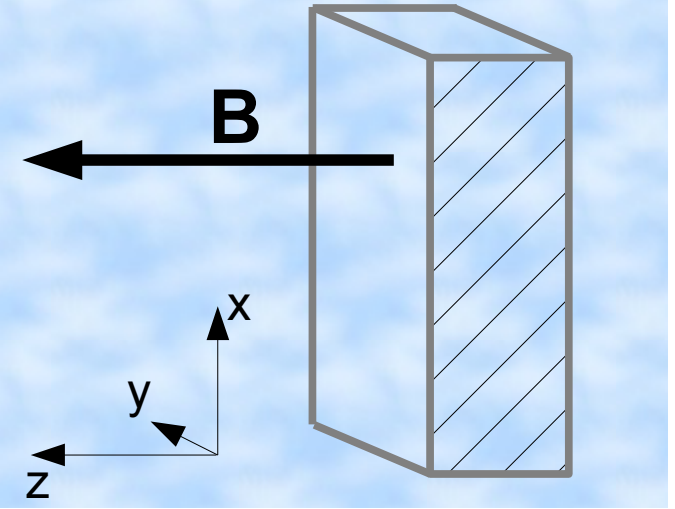
$$\varepsilon_{\alpha\beta} \qquad \alpha,\, \beta = x,\, y,\, z$$

Simple example: induced current

$$\varepsilon^{-1} = \begin{pmatrix} \varepsilon_{xx} & -\varepsilon_{xy} \\ \varepsilon_{xy} & \varepsilon_{xx} \end{pmatrix} \frac{1}{\varepsilon_{xx}^2 + \varepsilon_{xy}^2} \qquad D \propto \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$J = \frac{\omega}{4\pi i}(1 - \varepsilon^{-1})D$$

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$



MOKE in a nutshell

Key quantity: dielectric tensor

$$\varepsilon_{\alpha\beta} \qquad \alpha,\ \beta = x,\ y,\ z$$

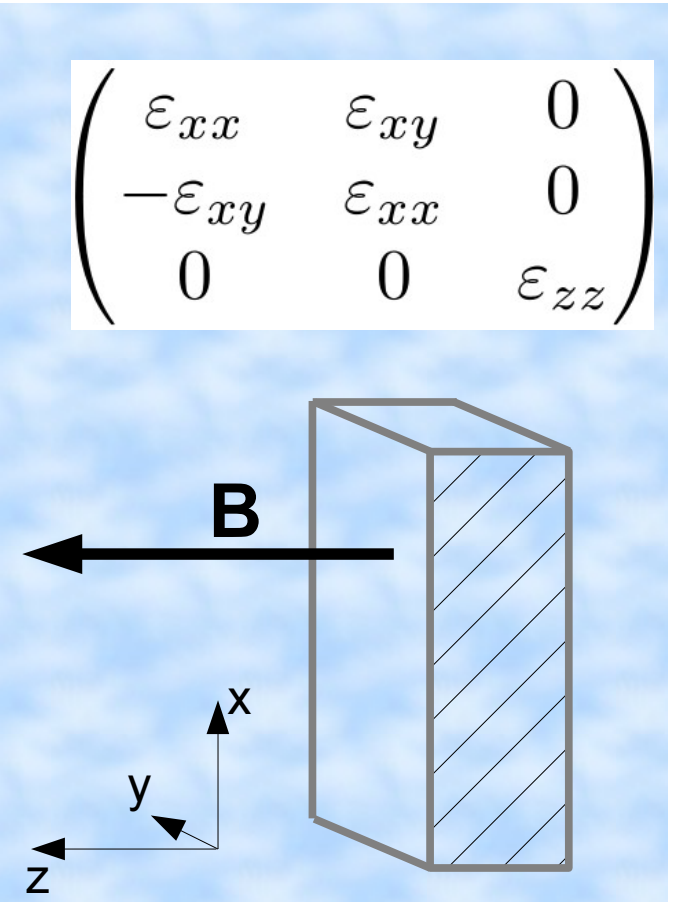
Simple example: induced current

$$\varepsilon^{-1} = \begin{pmatrix} \varepsilon_{xx} & -\varepsilon_{xy} \\ \varepsilon_{xy} & \varepsilon_{xx} \end{pmatrix} \frac{1}{\varepsilon_{xx}^2 + \varepsilon_{xy}^2}$$

$$D \propto \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$J = \frac{\omega}{4\pi i}(1 - \varepsilon^{-1})D$$

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$



MOKE in a nutshell

Key quantity: dielectric tensor

$$\varepsilon_{\alpha\beta} \qquad \alpha,\ \beta = x,\ y,\ z$$

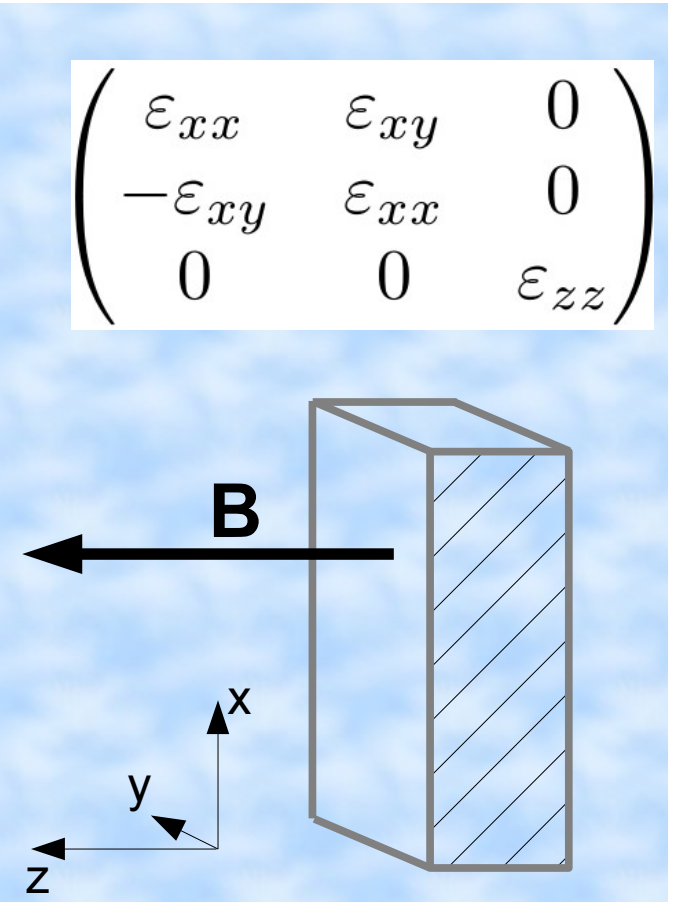
Simple example: induced current

$$\varepsilon^{-1} = \begin{pmatrix} \varepsilon_{xx} & -\varepsilon_{xy} \\ \varepsilon_{xy} & \varepsilon_{xx} \end{pmatrix} \frac{1}{\varepsilon_{xx}^2 + \varepsilon_{xy}^2} \qquad D \propto \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$J = \frac{\omega}{4\pi i}(1 - \varepsilon^{-1})D$$

$$J \propto \begin{pmatrix} 1 - \varepsilon_{xx} \\ \varepsilon_{xy} \end{pmatrix} \qquad \Psi_J \approx \frac{-\varepsilon_{xy}}{\varepsilon_{xx} - 1}$$

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$



MOKE in a nutshell

Key quantity: dielectric tensor

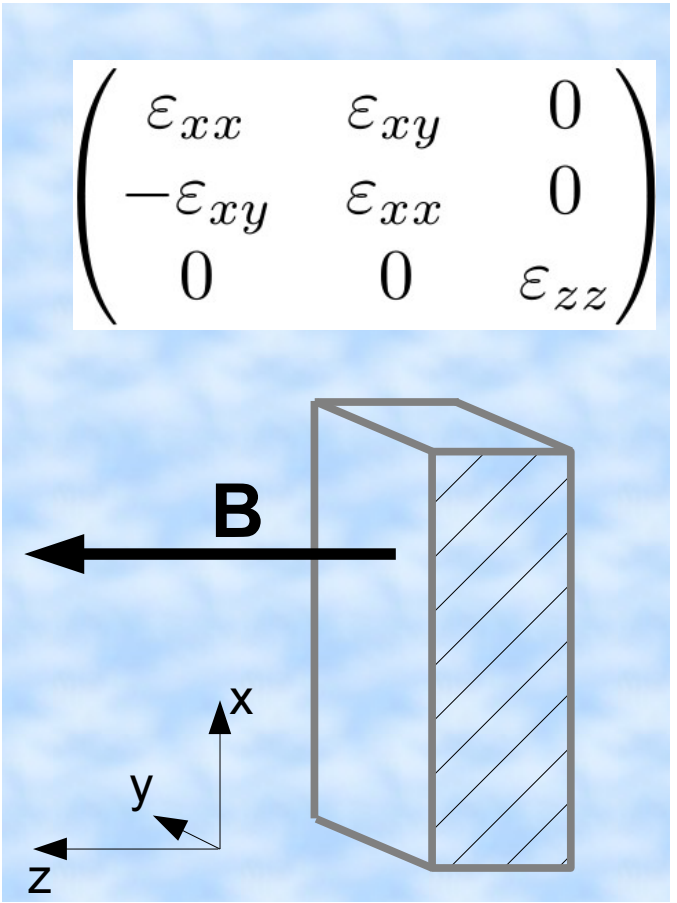
$$\varepsilon_{\alpha\beta} \qquad \alpha,\, \beta = x,\, y,\, z$$

Reflected light: **Kerr angle**

$$D \propto \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\Psi_K \approx \frac{-\varepsilon_{xy}}{(\varepsilon_{xx}-1)\sqrt{\varepsilon_{xx}}}$$

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$



Relation to TDDFT

General case

$$\mathbf{D} = \varepsilon \mathbf{E}$$

Relation to TDDFT

General case

$$\mathbf{D} = \varepsilon \mathbf{E}$$

Longitudinal fields → $\mathbf{D} = \mathbf{q} V_e \quad , \quad \mathbf{E} = \mathbf{q} V_t$

$$V_e = \hat{q}_\alpha \varepsilon_{\alpha\beta} \hat{q}_\beta V_t$$

Relation to TDDFT

General case

$$\mathbf{D} = \varepsilon \mathbf{E}$$

Longitudinal fields → $\mathbf{D} = \mathbf{q} V_e \quad , \quad \mathbf{E} = \mathbf{q} V_t$

$$V_e = \hat{q}_\alpha \varepsilon_{\alpha\beta} \hat{q}_\beta V_t$$

TDDFT(IP-RPA) → $V_e = \hat{q}_\alpha \left(\delta_{\alpha\beta} - v \, \chi^0_{\alpha\beta} \right) \hat{q}_\beta V_t$

Relation to TDDFT

General case

$$\mathbf{D} = \varepsilon \mathbf{E}$$

Longitudinal fields → $\mathbf{D} = \mathbf{q} V_e \quad , \quad \mathbf{E} = \mathbf{q} V_t$

$$V_e = \hat{q}_\alpha \varepsilon_{\alpha\beta} \hat{q}_\beta V_t$$

=

TDDFT(IP-RPA) → $$V_e = \hat{q}_\alpha \left(\delta_{\alpha\beta} - v\, \chi^0_{\alpha\beta} \right) \hat{q}_\beta V_t$$

Relation to TDDFT

General case

$$\mathbf{D} = \varepsilon \mathbf{E}$$

Longitudinal fields → $\mathbf{D} = \mathbf{q} V_e \quad , \quad \mathbf{E} = \mathbf{q} V_t$

$$V_e = \hat{q}_\alpha \varepsilon_{\alpha\beta} \hat{q}_\beta V_t$$

$$\stackrel{?}{=}$$

TDDFT(IP-RPA) → $V_e = \hat{q}_\alpha \left(\delta_{\alpha\beta} - v\, \chi^0_{\alpha\beta} \right) \hat{q}_\beta V_t$

Relation to TDDFT

General case

$$\mathbf{D} = \varepsilon \mathbf{E}$$

Longitudinal fields → $\mathbf{D} = \mathbf{q} V_e \quad , \quad \mathbf{E} = \mathbf{q} V_t$

$$V_e = \hat{q}_\alpha \varepsilon_{\alpha\beta} \hat{q}_\beta V_t$$

$$\hat{q}_\alpha A_{\alpha\beta} \hat{q}_\beta = 0 \quad ?$$

TDDFT(IP-RPA) → $V_e = \hat{q}_\alpha \left(\delta_{\alpha\beta} - v \chi^0_{\alpha\beta} \right) \hat{q}_\beta V_t$

Relation to TDDFT

General case

$$\mathbf{D} = \varepsilon \mathbf{E}$$

Longitudinal fields → $\mathbf{D} = \mathbf{q} V_e \quad , \quad \mathbf{E} = \mathbf{q} V_t$

$$V_e = \hat{q}_\alpha \varepsilon_{\alpha\beta} \hat{q}_\beta V_t$$

$$\hat{q}_\alpha A_{\alpha\beta} \hat{q}_\beta = 0$$

TDDFT(IP-RPA) → $V_e = \hat{q}_\alpha \left(\delta_{\alpha\beta} - v \, \chi^0_{\alpha\beta} \right) \hat{q}_\beta V_t$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - v \, \chi^0_{\alpha\beta} + A_{\alpha\beta}$$

Dielectric tensor determined to within an arbitrary antisymmetric matrix in TDDFT(work with J. Sofo on summer 2013)

Relation to TDDFT

General case

$$\mathbf{D} = \varepsilon \mathbf{E}$$

Longitudinal fields → $\mathbf{D} = \mathbf{q} V_e \quad , \quad \mathbf{E} = \mathbf{q} V_t$

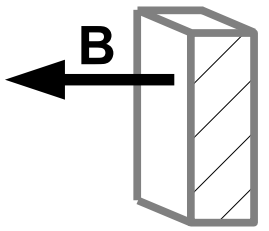
$$V_e = \hat{q}_\alpha \boxed{\varepsilon_{\alpha\beta}} \hat{q}_\beta V_t$$

$$\overset{?}{=} \hat{q}_\alpha A_{\alpha\beta} \hat{q}_\beta = 0$$

TDDFT(IP-RPA) → $V_e = \hat{q}_\alpha \boxed{\left(\delta_{\alpha\beta} - v\,\chi^0_{\alpha\beta}\right)} \hat{q}_\beta V_t$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - v\,\chi^0_{\alpha\beta} + A_{\alpha\beta}$$

$$\begin{pmatrix} \varepsilon_{xx} & \boxed{\varepsilon_{xy}} & 0 \\ \boxed{-\varepsilon_{xy}} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$



But... MOKE effect is due to the antisymmetric part of the matrix

Relation to TDDFT

Alternative: current-current response

$$\mathbf{J} = \frac{e}{c}\chi_{jj}\mathbf{A}$$

Relation to TDDFT

Alternative: current-current response

$$\mathbf{J} = \frac{e}{c}\chi_{jj}\mathbf{A}$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\frac{n}{m}\delta_{\alpha\beta} + \chi^{p}_{jj}(\omega)\right]$$

Relation to TDDFT

Alternative: current-current response

$$\mathbf{J} = \frac{e}{c}\chi_{jj}\mathbf{A}$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\frac{n}{m}\delta_{\alpha\beta} + \chi^{p}_{jj}(\omega)\right]$$

diamagnetic paramagnetic

Relation to TDDFT

Alternative: current-current response

$$\mathbf{J} = \frac{e}{c}\chi_{jj}\mathbf{A}$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\frac{n}{m}\delta_{\alpha\beta} + \chi^{p}_{jj}(\omega)\right]$$

diamagnetic paramagnetic

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\left(\chi^{(0)}_{jj} + \frac{n}{m}\delta_{\alpha\beta}\right) + \omega\chi^{(1)}_{jj}(\omega) + \omega^2\chi^{(2)}_{jj}(\omega)\right]$$

Relation to TDDFT

Alternative: current-current response

$$\mathbf{J} = \frac{e}{c}\chi_{jj}\mathbf{A}$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\frac{n}{m}\delta_{\alpha\beta} + \chi^{p}_{jj}(\omega)\right]$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\underbrace{\left(\chi^{(0)}_{jj} + \frac{n}{m}\delta_{\alpha\beta}\right)}_{\text{Drude}} + \underbrace{\omega\chi^{(1)}_{jj}(\omega)}_{\substack{\text{Anomalous}\\ \text{Hall}\\ \text{Conductivity}}} + \underbrace{\omega^2\chi^{(2)}_{jj}(\omega)}_{\text{Interband}}\right]$$

Relation to TDDFT

Alternative: current-current response

$$\varepsilon_{\alpha\beta}^{\text{Drude}} \approx \frac{1}{\omega}\frac{\omega_p^2}{\omega + i\omega_\tau}$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\underbrace{\left(\chi_{jj}^{(0)} + \frac{n}{m}\delta_{\alpha\beta}\right)}_{\text{Drude}} + \underbrace{\omega\chi_{jj}^{(1)}(\omega)}_{\substack{\text{Anomalous}\\ \text{Hall}\\ \text{Conductivity}}} + \underbrace{\omega^2\chi_{jj}^{(2)}(\omega)}_{\text{Interband}}\right]$$

Relation to TDDFT

Alternative: current-current response

$$\varepsilon_{\alpha\beta}^{\text{Drude}} \approx \frac{1}{\omega}\frac{\omega_p^2}{\omega + i\omega_\tau}$$

$$\varepsilon_{\alpha\beta}^{\text{AHC}} = -\frac{4\pi}{\omega}\chi_{jj}^{(1)}(\omega) \longrightarrow \begin{pmatrix} \varepsilon_{xx} & \boxed{\varepsilon_{xy}} & 0 \\ \boxed{-\varepsilon_{xy}} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\underbrace{\left(\chi_{jj}^{(0)} + \frac{n}{m}\delta_{\alpha\beta}\right)}_{\text{Drude}} + \underbrace{\omega\chi_{jj}^{(1)}(\omega)}_{\substack{\text{Anomalous} \\ \text{Hall} \\ \text{Conductivity}}} + \underbrace{\omega^2\chi_{jj}^{(2)}(\omega)}_{\text{Interband}}\right]$$

Relation to TDDFT

Alternative: current-current response

$$\varepsilon_{\alpha\beta}^{\text{Drude}} \approx \frac{1}{\omega}\frac{\omega_p^2}{\omega + i\omega_\tau}$$

$$\varepsilon_{\alpha\beta}^{\text{AHC}} = -\frac{4\pi}{\omega}\chi_{jj}^{(1)}(\omega) \longrightarrow \begin{pmatrix} \varepsilon_{xx} & \boxed{\varepsilon_{xy}} & 0 \\ \boxed{-\varepsilon_{xy}} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

$$\varepsilon_{\alpha\beta}^{\text{inter}} = \delta_{\alpha\beta} - 4\pi\chi_{jj}^{(2)}(\omega) = \delta_{\alpha\beta} - v\,\chi^0_{\alpha\beta} \longrightarrow \text{TDDFT(IP-RPA)}$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \frac{4\pi}{\omega^2}\left[\underbrace{\left(\chi_{jj}^{(0)} + \frac{n}{m}\delta_{\alpha\beta}\right)}_{\text{Drude}} + \underbrace{\omega\chi_{jj}^{(1)}(\omega)}_{\substack{\text{Anomalous} \\ \text{Hall} \\ \text{Conductivity}}} + \underbrace{\omega^2\chi_{jj}^{(2)}(\omega)}_{\text{Interband}}\right]$$

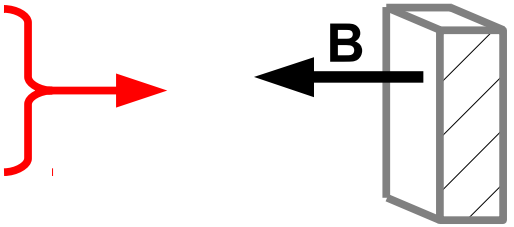
Phys. Rev. B. **86**, 125139 (2012). D. Sangalli, A. Marini, A. Debernardi

Input parameters

```
<groundstate
   do="skip"
   xctype="LDA_PW"
   rgkmax="7.0"
   epsengy="1.0d-4">

   <spin
      reducebf="0.5"
      spinorb="true"/>

</groundstate>
```

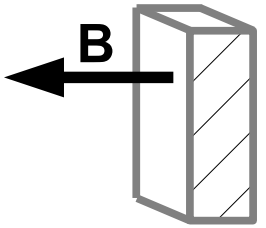
Input parameters

```
<groundstate
   do="skip"
   xctype="LDA_PW"
   rgkmax="7.0"
   epsengy="1.0d-4">

   <spin
      reducebf="0.5"
      spinorb="true"/>

</groundstate>
```



Input parameters

```
<groundstate
   do="skip"
   xctype="LDA_PW"
   rgkmax="7.0"
   epsengy="1.0d-4">

   <spin
      reducebf="0.5"
      spinorb="true" />

</groundstate>
```



Input parameters

```
<xs
   xstype="TDDFT"
   ngridk="8 8 8"
   vkloff="0.097 0.273 0.493"
   dfoffdiag="true"
   dogroundstate="fromscratch"
   maxscl="200"
   bfieldc="0.0 0.0 -2.0"
   broad="0.02"
   tevout="true">

   <tddft
       fxctype="RPA"
       drude="0.18 0.001"
       ahc="true"/>

   <qpointset>
      <qpoint> 0.0 0.0 0.0 </qpoint>
   </qpointset>

   <energywindow
      intv="0.00 0.32" points="150"/>

</xs>
```

Input parameters

```
<xs
   xstype="TDDFT"
   ngridk="8 8 8"
   vkloff="0.097 0.273 0.493"
   dfoffdiag="true"
   dogroundstate="fromscratch"
   maxscl="200"
   bfieldc="0.0 0.0 -2.0"
   broad="0.02"
   tevout="true">

   <tddft
       fxctype="RPA"
       drude="0.18 0.001"
       ahc="true"/>

   <qpointset>
      <qpoint> 0.0 0.0 0.0 </qpoint>
   </qpointset>

   <energywindow
      intv="0.00 0.32" points="150"/>

</xs>
```

Input parameters

```
<xs
   xstype="TDDFT"
   ngridk="8 8 8"
   vkloff="0.097 0.273 0.493"
   dfoffdiag="true"
   dogroundstate="fromscratch"
   maxscl="200"
   bfieldc="0.0 0.0 -2.0"
   broad="0.02"
   tevout="true">

   <tddft
       fxctype="RPA"
       drude="0.18 0.001"
       ahc="true"/>

   <qpointset>
      <qpoint> 0.0 0.0 0.0 </qpoint>
   </qpointset>

   <energywindow
      intv="0.00 0.32" points="150"/>

</xs>
```

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

Input parameters

```
<xs
   xstype="TDDFT"
   ngridk="8 8 8"
   vkloff="0.097 0.273 0.493"
   dfoffdiag="true"
   dogroundstate="fromscratch"
   maxscl="200"
   bfieldc="0.0 0.0 -2.0"
   broad="0.02"
   tevout="true">

   <tddft
      fxctype="RPA"
      drude="0.18 0.001"
      ahc="true"/>

   <qpointset>
      <qpoint> 0.0 0.0 0.0 </qpoint>
   </qpointset>

   <energywindow
      intv="0.00 0.32" points="150"/>

</xs>
```

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

Input parameters

```
<xs
   xstype="TDDFT"
   ngridk="8 8 8"
   vkloff="0.097 0.273 0.493"
   dfoffdiag="true"
   dogroundstate="fromscratch"
   maxscl="200"
   bfieldc="0.0 0.0 -2.0"
   broad="0.02"
   tevout="true">

   <tddft
      fxctype="RPA"
      drude="0.18 0.001"
      ahc="true"/>

   <qpointset>
      <qpoint> 0.0 0.0 0.0 </qpoint>
   </qpointset>

   <energywindow
      intv="0.00 0.32" points="150"/>

</xs>
```

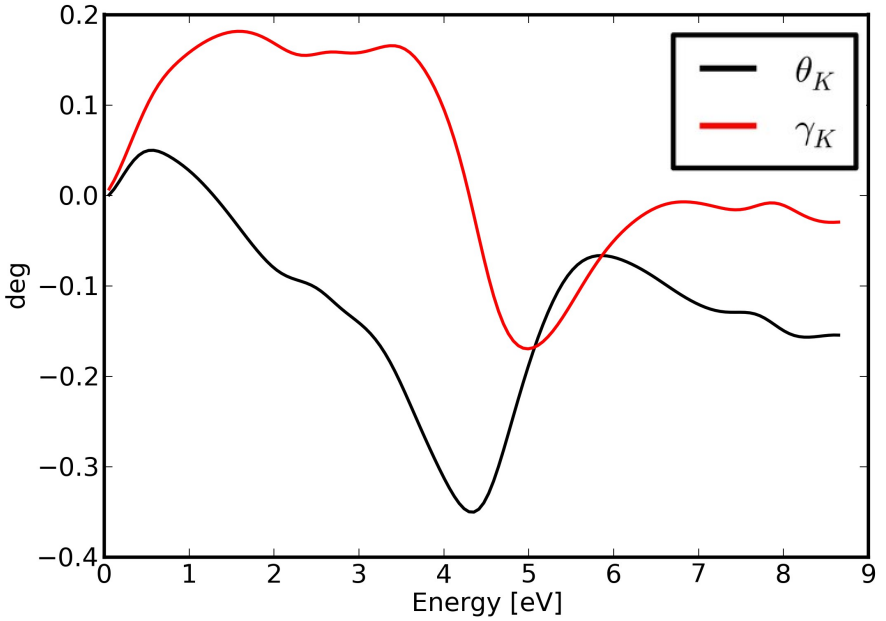
$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}$$

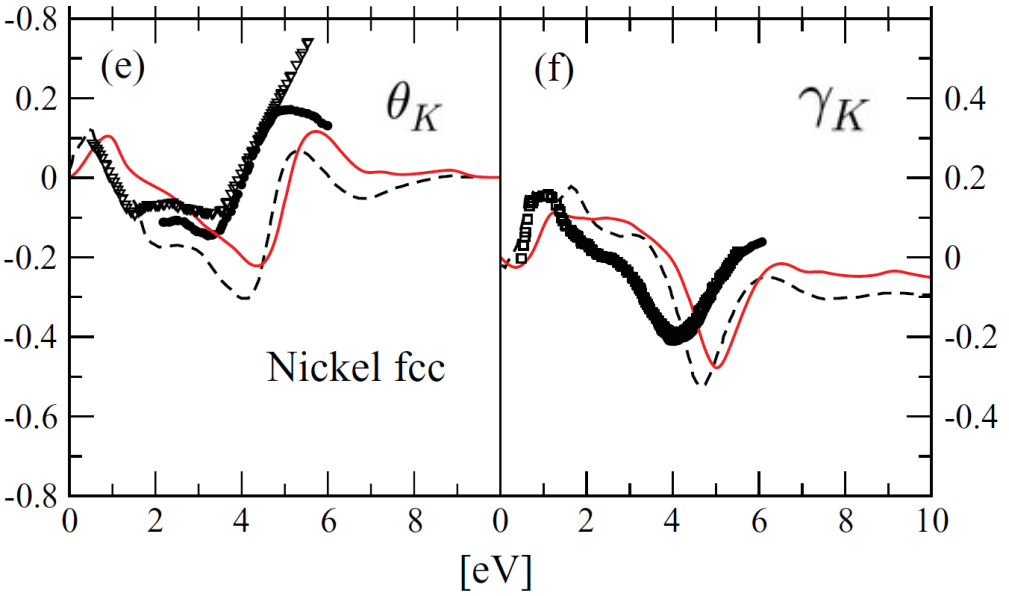
$$\varepsilon_{\alpha\beta}^{\text{Drude}} \approx \frac{1}{\omega} \frac{\omega_p^2}{\omega + i\omega_\tau}$$

The case of Nickel

```
<xs
   xstype="TDDFT"
   ngridk="8 8 8"
   vkloff="0.097 0.273 0.493"
   dfoffdiag="true"
   dogroundstate="fromscratch"
   maxscl="200"
   bfieldc="0.0 0.0 -2.0"
   broad="0.02"
         fxctype="RPA"
         drude="0.18 0.001"
         ahc="true"/>

   <qpointset>
      <qpoint> 0.0 0.0 0.0 </qpoint>
   </qpointset>

   <energywindow
      intv="0.00 0.32" points="150"/>

</xs>
```

$$\Psi_K = \theta_K(\omega) + i\gamma_K(\omega) \approx \frac{-\varepsilon_{xy}}{(\varepsilon_{xx}-1)\sqrt{\varepsilon_{xx}}}$$





Phys. Rev. B. **86**, 125139 (2012). D. Sangalli, A. Marini, A. Debernardi

Thanks!