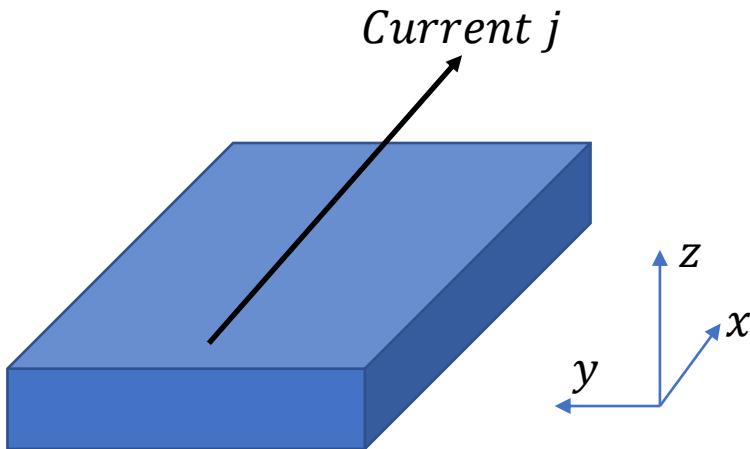


# Crystalline anisotropy in conductivity

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# The crystalline anisotropy



The conductivity tensor is NOT isotropic.

$$\vec{\sigma} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix}$$
$$\vec{j} = \sigma_{xx} \cdot \vec{E}$$

$$j_\alpha = \sum_\beta \sigma_{\alpha\beta} E_\beta$$

For example:

$$j_x = \sigma_{xx} E_x + \sigma_{xy} E_y + \sigma_{xz} E_z$$

Misused term (not recommended, but will encounter):

$$j_{xx} \equiv \sigma_{xx} E_x$$

# Review of semi-classical theory

- Semiclassical view of current:

$$\vec{j} = \mathbf{n} \vec{v} q \rightarrow \vec{j} = -\frac{1}{4\pi^3} \int e \vec{v}_k f d\vec{k} \text{ due to } \mathbf{n} \rightarrow \frac{1}{4\pi^3} \int f d\vec{k}$$

- Distribution function

$$f = f_0 + f_1$$

$f_0$ : equilibrium part,  $f_1$ : non-equilibrium part due to the electric field

$$\vec{j} = -\frac{1}{4\pi^3} \int e \vec{v} \mathbf{f}_1 d\vec{k}$$

- Relaxation time

$$f_1 = \frac{\partial f}{\partial t} \tau$$

$$\frac{\partial f}{\partial t} = \nabla_{\vec{k}} f \frac{d\vec{k}}{dt} = \frac{\partial f}{\partial \epsilon} \nabla_{\vec{k}} \epsilon \frac{d\vec{k}}{dt}$$

$$\nabla_{\vec{k}} \epsilon = \hbar \vec{v}, \frac{d\vec{k}}{dt} = -\frac{e \vec{E}}{\hbar} \rightarrow \vec{\sigma} = -\frac{e^2}{4\pi^3} \int \tau \frac{\partial f_0}{\partial \epsilon} \vec{v} \vec{v} d\vec{k}$$

- Fermi surface

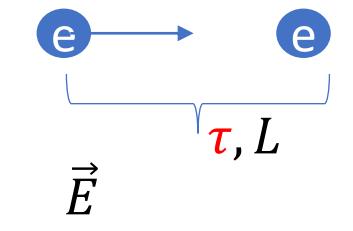
$$-\frac{\partial f_0}{\partial \epsilon} = \delta(E_F) \rightarrow \vec{\sigma} = \frac{e^2}{4\pi^3} \int \tau \vec{v} \vec{v} \frac{1}{\hbar v} dS_{E_F}$$

$S_{E_F}$ : Fermi surface area, conduction only occurs on Fermi surface

*Semiclassical*

$$\vec{a} = -\frac{eE}{m}$$

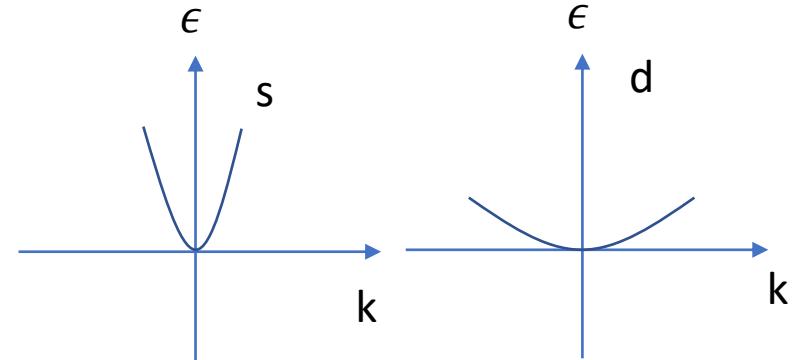
$$\frac{d\vec{p}}{dt} = m\vec{a} \rightarrow \frac{\hbar d\vec{k}}{dt} = -\frac{eE}{\hbar}$$



$$\vec{\sigma} = \frac{e^2}{4\pi^3} \int \tau \vec{v} \vec{v} \frac{1}{\hbar v_F} dS_{E_F}$$

# More about the Fermi surface for 3d transition metal like Fe, Co, Ni

- The conductivity also depends on the density of states
- s electrons dominate the transport because of the small effective mass



	s electron	d electron
Atomic overlap	large	Small
Energy range	large	Small
Effective mass $\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \epsilon}{\partial k^2}$	small	large
Density of states	small	large
Speed	faster	slower

# Nature of relaxation time $\tau$

- The relaxation time depends on the scattering rate

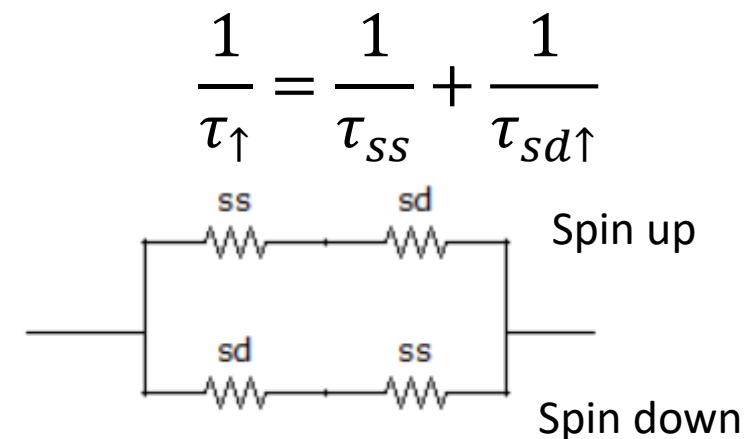
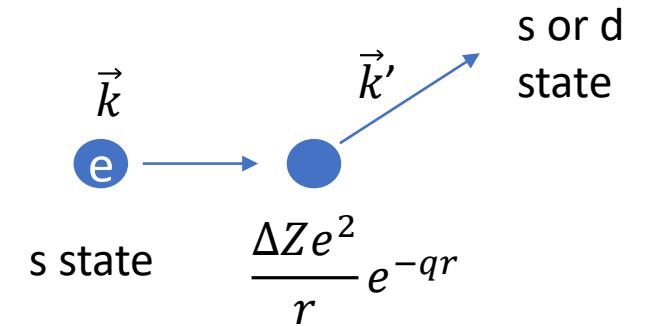
$$\frac{1}{\tau_{ss}} = \frac{2\pi}{\hbar} N_s(E_F) \int_0^\pi |\langle \psi_s | V_{scatt} | \psi_{s'} \rangle|^2 d\theta$$

$$\frac{1}{\tau_{sd}} = \frac{2\pi}{\hbar} N_d(E_F) |\langle \psi_s | V_{scatt} | \psi_d \rangle|^2$$

$\langle \psi_s | V_{scatt} | \psi_s \rangle$  and  $|\langle \psi_s | V_{scatt} | \psi_d \rangle|$  are the transition matrix elements

- Scattering potential (screened coulomb)

$$V_{scatt} = \frac{\Delta Z e^2}{r} e^{-qr}$$



$$\vec{\sigma} = \frac{e^2}{4\pi^3} \int \textcolor{red}{\tau} \vec{v} \vec{v} \frac{1}{\hbar v_F} dS_{E_F}$$

# Calculating the scattering matrix

- ss scattering

$$\langle \psi_s | V_{scatt} | \psi_s' \rangle = \int e^{i\vec{k} \cdot \vec{r}} \frac{\Delta Z e^2}{r} e^{-qr} e^{i\vec{k}' \cdot \vec{r}} dr^3 = \frac{4\pi \Delta Z e^2}{(\vec{k} - \vec{k}')^2 + q^2}$$

$$\frac{1}{\tau_{ss}} = \frac{2\pi}{\hbar} N_s(E_F) \int_0^\pi |\langle \psi_s | V_{scatt} | \psi_s' \rangle|^2 d\theta = \frac{4(\pi \Delta Z e^2)^2}{q^2(2k_F^2 - q^2)}$$

$\theta$ : angle between  $\vec{k}$  and  $\vec{k}'$ . This is isotropic.

- sd scattering  $\phi_m(\vec{r}) = xy$  as an example.

$$\langle \psi_s | V_{scatt} | \phi_{xy} \rangle \propto \int \psi_s^* V_{scatt}(r) \textcolor{red}{xy} dr^3 = -32\pi \Delta Z e^2 \frac{\textcolor{red}{k_x k_y}}{(k^2 + q^2)^3} = \alpha \textcolor{red}{k_x k_y}$$

Similarly

$$\begin{aligned} \langle \psi_s | V_{scatt} | \phi_{x^2-y^2} \rangle &\propto \int \psi_s^* V_{scatt}(r) (\textcolor{red}{x^2 - y^2}) dr^3 = -32\pi \Delta Z e^2 \frac{\textcolor{red}{k_x^2 - k_y^2}}{(k^2 + q^2)^3} \\ &= \alpha (\textcolor{red}{k_x^2 - k_y^2}) \end{aligned}$$

This is anisotropic

$$V_{scatt} = \frac{\Delta Z e^2}{r} e^{-qr}$$

$$\psi_s = e^{i\vec{k} \cdot \vec{r}}$$

$$\psi_{dm} = \phi_m(\vec{r}) f(r)$$

$$f(r) \propto e^{-r \frac{z}{3a_0}}$$

# Simplified case

$$\overleftrightarrow{\sigma} = \frac{e^2}{4\pi^3} \int \color{red}\tau\color{black} \vec{v} \vec{v} \frac{1}{\hbar v_F} dS_{E_F}$$

- *The incident is always s electron, which has parabolic (free electron gas) dispersion.*

$$\vec{v} = \frac{\hbar \vec{k}_F}{m}$$

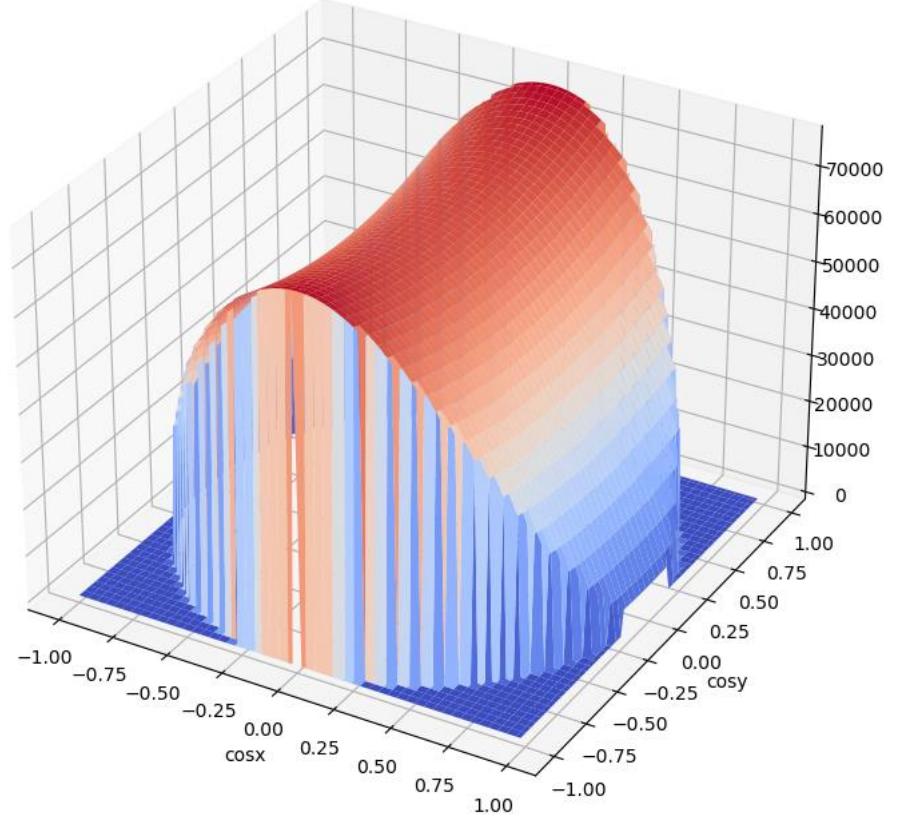
- *For an extreme case, consider only the  $d_{xy}$  state is on the Fermi surface*

$$\begin{aligned} \sigma_{ij} &= \frac{e^2 \hbar}{4\pi^3 m^2 v_F} \int \frac{1}{\frac{1}{\tau_{ss}} + \frac{1}{\tau_{sd}}} k_i k_j dS_{E_F} \\ &= \frac{e^2 \hbar}{4\pi^3 m^2 v_F} \int \frac{1}{\frac{1}{\tau_{ss}} + \frac{2\pi}{\hbar} N_d(E_F) |\alpha k_x k_y|^2} k_i k_j dS_{E_F} \end{aligned}$$

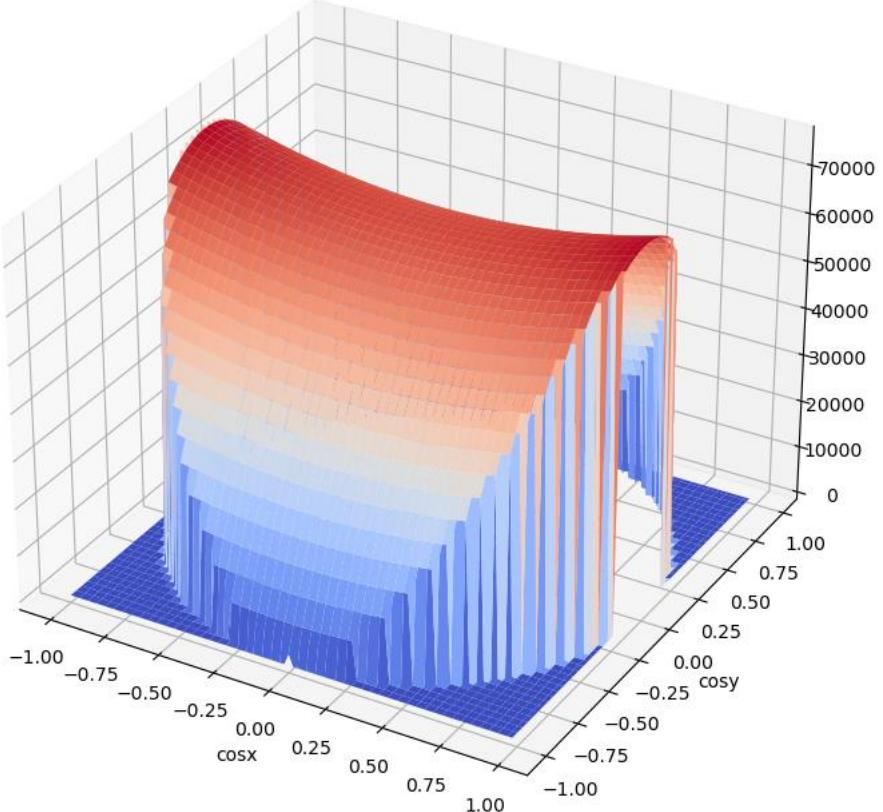
To visualize  $\sigma_{ij}$ , we plot the longitudinal conductivity

$$(\overleftrightarrow{\sigma} \cdot \hat{E}) \cdot \hat{E}$$

# Examples



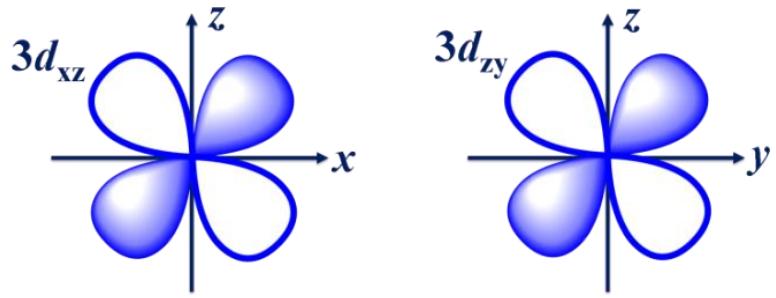
$$\vec{v} = \frac{\hbar \vec{k}}{m}$$



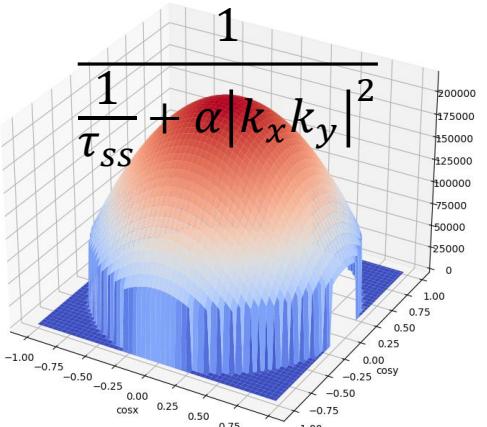
$$xz \quad \frac{1}{\tau_{ss} + \alpha |k_x k_z|^2}$$

$$\frac{1}{\tau_{ss}} \ll \alpha |k_x k_z|^2$$

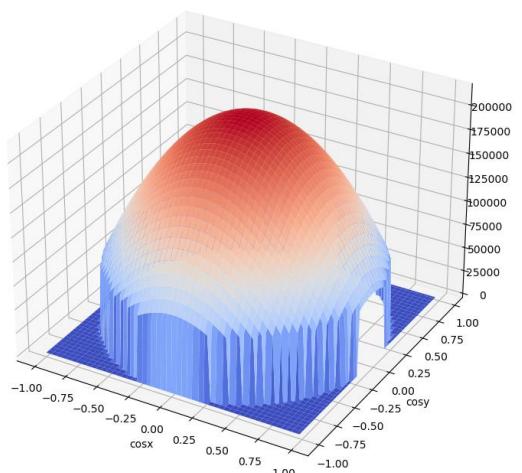
$$yz \quad \frac{1}{\tau_{ss} + \alpha |k_z k_y|^2}$$



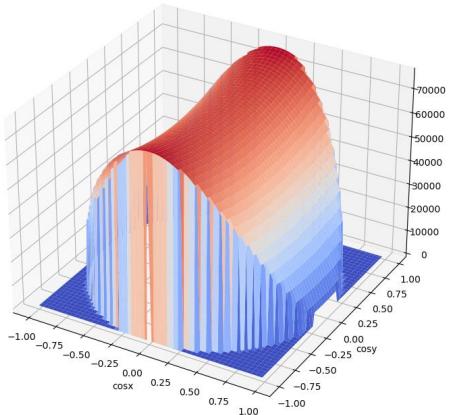
# Examples



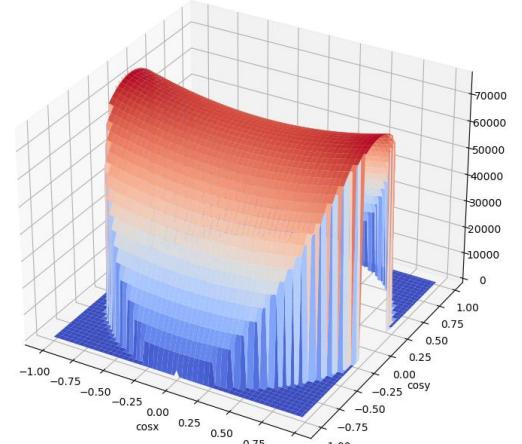
xy



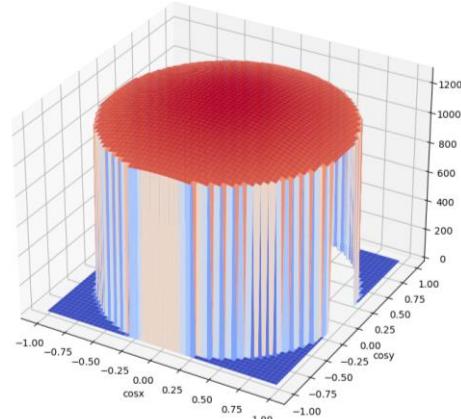
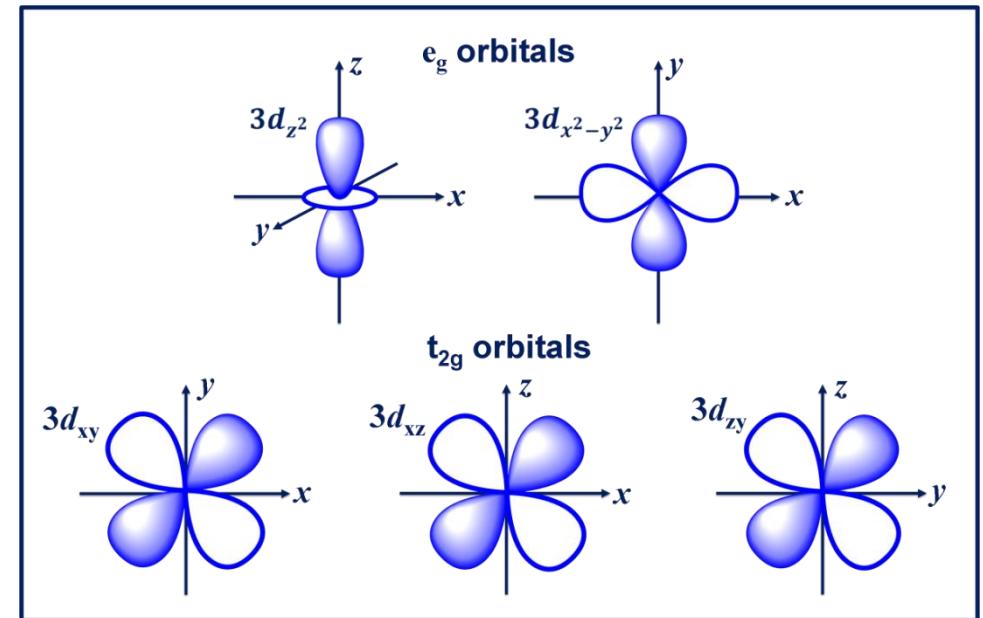
xx-yy



xz

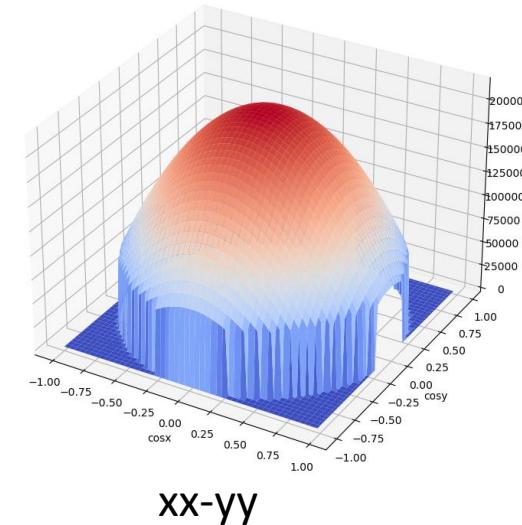
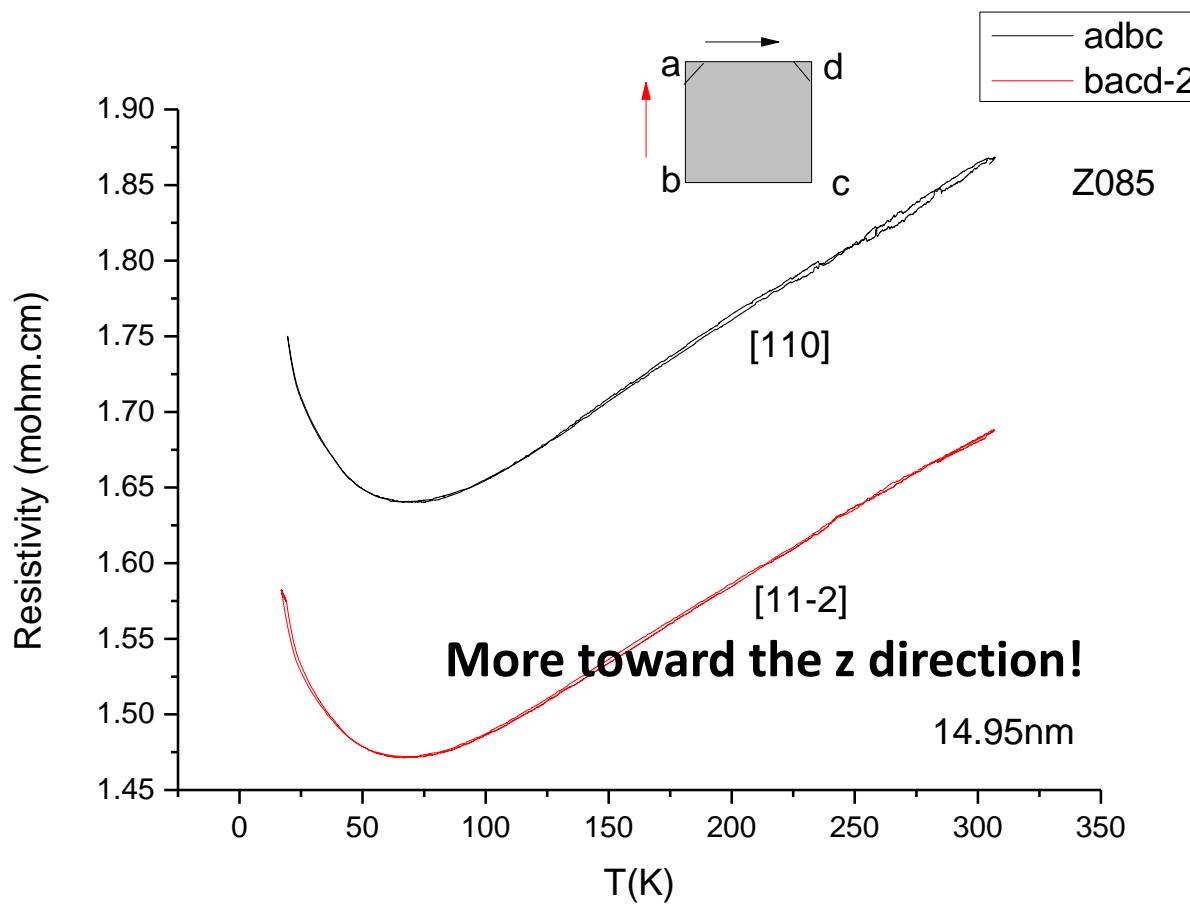


yz

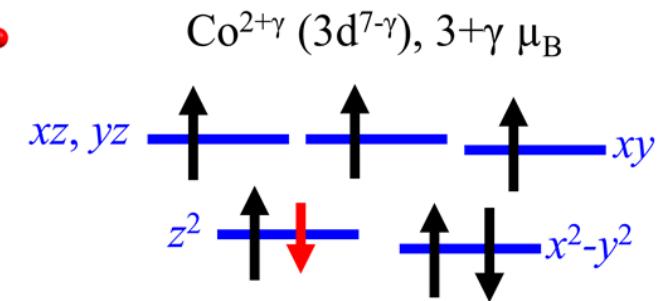
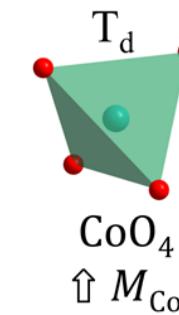
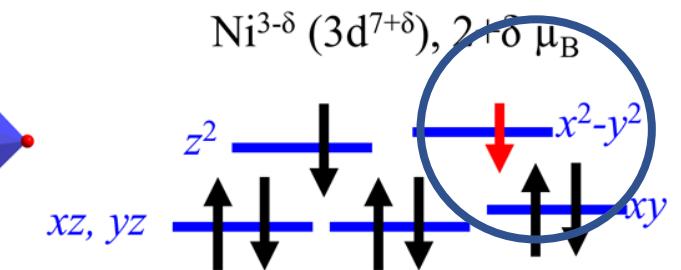
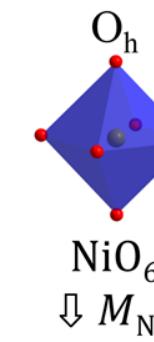


3zz-rr

# Experimental evidence



xx-yy



# Conclusion

- The semiclassical theory relies on relaxation time approximation
- Relaxation time depends on the s-d scattering.
- The s-d scattering causes the conductivity anisotropy.