• PHYS 570 days at 10-ID

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Homework Assignment #06: Chapter 6: 1,6,7,8,9 due Tuesday, April 14, 2015

1 April 10, 2015, 09:00 - 16:00

2 April 24, 2015, 09:00 - 16:00

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- 8 Activities
 - Absolute flux measurement
 - Reflectivity measurement
 - EXAFS measurement
 - Rocking curve measurement (possibly)

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- 6 Let me know when you plan to come!

	$\zeta_{\rm d}^{\rm fwhm} imes 10^6$								
	(111)			(220)			(400)		
Diamond	61.0			20.9			8.5		
<i>a</i> = 3.5670 Å	3.03	0.018	-0.01	1.96	0.018	-0.01	1.59	0.018	-0.01
Silicon	139.8			61.1			26.3		
<i>a</i> = 5.4309 Å	10.54	0.25	-0.33	8.72	0.25	-0.33	7.51	0.25	-0.33
Germanium	347.2			160.0			68.8		
<i>a</i> = 5.6578 Å	27.36	-1.1	-0.89	23.79	-1.1	-0.89	20.46	-1.1	-0.89

the quantities below the widths are $f^0(Q)$, f', and f'' (for $\lambda = 1.5405$ Å). For an angular width, multiply times $\tan \theta$ and for π polarization, multiply by $\cos(2\theta)$.

C. Segre (IIT)

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Parameterized by the asymmetry angle 0 $< \alpha < \theta_{Bragg}$



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This leads to a beam compression

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$$\delta heta_e = \sqrt{b}(\zeta_D \tan heta)$$

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 $\delta \theta_i H_i$



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$$\delta\theta_i H_i = \frac{1}{\sqrt{b}} (\zeta_D \tan \theta) b H_e = \sqrt{b} (\zeta_D \tan \theta) = \frac{\delta\theta_e H_e}{\delta\theta_e H_e}$$

C. Segre (IIT)

The measured "rocking" curve from a two crystal system is a convolution of the Darwin curves of both crystals.

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output divergence on left, input divergence on right

C. Segre (IIT)

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output divergence on left, input divergence on right

C. Segre (IIT)

The measured "rocking" curve from a two crystal system is a convolution of the Darwin curves of both crystals. When the two crystals have a matched asymmetry, we get a triangle. When one asymmetry is much higher, then we can measure the Darwin curve of a single crystal.



output divergence on left, input divergence on right

C. Segre (IIT)

Dumond diagram: no Darwin width

Transfer function of an optical element parameterized by angle and wavelength.



Dumond diagram: no Darwin width

Transfer function of an optical element parameterized by angle and wavelength. Here Darwin width is ignored.



Dumond diagram: symmetric Bragg

Including the Darwin width, we have a bandpass in wavelength.



Dumond diagram: symmetric Bragg

Including the Darwin width, we have a bandpass in wavelength. If input beam is perfectly collimated, so is output (vertical black line).


Dumond diagram: asymmetric Bragg



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Total Cross Section



The total cross-section for photon "absorption" includes elastic (or coherent) scattering, Compton (inelastic) scattering, and photoelectric absorption.

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Characteristic absorption jumps depend on the element

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Characteristic absorption jumps depend on the element

These quantities vary significantly over many decades but can easily put on an equal footing.

$$T = \frac{I}{I_o} = e^{-\mu z}$$

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$$\mu = \frac{\rho_m N_A}{M} \sigma_a$$

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scale σ_a for different elements by E^3/Z^4 and plot together



remarkably, all values lie on a common curve above the K edge and between the L and K edges and below the L edge

C. Segre (IIT)

PHYS 570 - Spring 2015



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From first-order perturbation theory, the absorption cross section is given by $% \label{eq:perturbation}$

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$$\sigma_{a} = \frac{2\pi}{\hbar c} \frac{V^{2}}{4\pi^{3}} \int |M_{if}|^{2} \delta(\mathcal{E}_{f} - \mathcal{E}_{i}) q^{2} \sin\theta dq d\theta d\varphi$$

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The interaction Hamiltonian is expressed in terms of the electromagnetic vector potential

$$M_{if} = \langle i | \mathcal{H}_I | f \rangle$$

$$\mathcal{H}_I = \frac{e\vec{p}\cdot\vec{A}}{m} + \frac{e^2A^2}{2m}$$

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$$ec{A} = \hat{arepsilon} \sqrt{rac{\hbar}{2\epsilon_0 V \omega}} \left[a_k e^{i ec{k} \cdot ec{r}} + a_k^\dagger e^{-i ec{k} \cdot ec{r}}
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The interaction Hamiltonian is expressed in terms of the electromagnetic vector potential

The first term gives absorption

$$M_{if} = \langle i | \mathcal{H}_I | f \rangle$$

$$\mathcal{H}_{I} = \frac{e\vec{p}\cdot\vec{A}}{m} + \frac{e^{2}A^{2}}{2m}$$

$$\vec{A} = \hat{\varepsilon} \sqrt{\frac{\hbar}{2\epsilon_0 V \omega}} \left[a_k e^{i\vec{k}\cdot\vec{r}} + a_k^{\dagger} e^{-i\vec{k}\cdot\vec{r}} \right]$$

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The first term gives absorption while the second produces Thomson scattering so we take only the first into consideration now.

C. Segre (IIT)

PHYS 570 - Spring 2015

In order to evaluate the M_{if} matrix element we define the initial and final states

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the initial state has a photon and a K electron (no free electron)

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$$|i
angle = |1
angle_{\gamma}|0
angle_{e}$$

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similarly, the final state has no photon and an ejected free electron (ignoring the core hole and charged ion)

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Thus

$$\mathcal{M}_{if} = rac{e}{m} \sqrt{rac{\hbar}{2\epsilon_0 V \omega}} \left[{}_{e} \langle 1 |_{\gamma} \langle 0 | (ec{p} \cdot \hat{arepsilon}) a e^{iec{k} \cdot ec{r}} + (ec{p} \cdot \hat{arepsilon}) a^{\dagger} e^{-iec{k} \cdot ec{r}} | 1
angle_{\gamma} | 0
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angle_{\gamma} | 0
angle_{e}
ight]$$

The calculation is simplified if the interaction Hamiltonian is applied to the left since the final state has only a free electron and no photon

C. Segre (IIT)

PHYS 570 - Spring 2015

The free electron state is an eigenfunction of the electron momentum operator

$$_{e}\langle 1|ec{p}=(\hbarec{q})_{e}\langle 1|$$

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The annihilation operator applied to the left creates a photon

$$e\langle 1|\vec{p} = (\hbar \vec{q})_e \langle 1|$$

 $\gamma \langle n|a = (\sqrt{n+1})_\gamma \langle n+1|a\rangle$

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 $(1 \rightarrow (7 \rightarrow))$

The free electron state is an eigenfunction of the electron momentum operator

The annihilation operator applied to the left creates a photon while the creation operator annihilates a photon when applied to the left.

$$e\langle 1|ec{p}=(\hbarec{q})_e\langle 1|$$

 $_{\gamma}\langle n|a=(\sqrt{n+1})_{\gamma}\langle n+1|a\rangle$

$$_{\gamma}\langle n|a^{\dagger}=(\sqrt{n})_{\gamma}\langle n-1|a\rangle$$

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$${}_{e}\langle 1|_{\gamma}\langle 0|(ec{p}\cdot\hat{arepsilon})\mathsf{a}=\hbar(ec{q}\cdot\hat{arepsilon})_{e}\langle 1|_{\gamma}\langle 1|$$
$$_{e}\langle 1|ec{p}=(\hbarec{q})_{e}\langle 1|$$

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 ${}_{e}\langle 1|_{\gamma}\langle 0|(ec{p}\cdot\hat{arepsilon})a^{\dagger}=0$

$$e\langle 1|p = (hq)e\langle 1|$$

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 ${}_{e}\langle 1|_{\gamma}\langle 0|(ec{p}\cdot\hat{arepsilon})a^{\dagger}=0$

$$M_{if} = \frac{e}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V \omega}} \left[\hbar (\vec{q} \cdot \hat{\varepsilon})_e \langle 1|_\gamma \langle 1| e^{i\vec{k} \cdot \vec{r}} |1\rangle_\gamma |0\rangle_e + 0 \right]$$

$$e\langle 1|p = (hq)e\langle 1|$$

 $\gamma\langle n|a = (\sqrt{n+1})\gamma\langle n+1|a$

 $(\rightarrow) \rightarrow (\rightarrow) (\rightarrow) (\rightarrow)$

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 ${}_{e}\langle 1|_{\gamma}\langle 0|(ec{p}\cdot\hat{arepsilon})a^{\dagger}=0$

$$egin{aligned} \mathcal{M}_{if} &= rac{e}{m} \sqrt{rac{\hbar}{2\epsilon_0 V \omega}} \left[\hbar (ec{q} \cdot \hat{arepsilon})_e \langle 1 |_\gamma \langle 1 | e^{iec{k} \cdot ec{r}} | 1
angle_\gamma | 0
angle_e + 0
ight] \ &= rac{e \hbar}{m} \sqrt{rac{\hbar}{2\epsilon_0 V \omega}} (ec{q} \cdot \hat{arepsilon})_e \langle 1 | e^{iec{k} \cdot ec{r}} | 0
angle_e \end{aligned}$$

C. Segre (IIT)

$$e\langle 1|p = (hq)_e\langle 1|$$

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 $(1 \rightarrow) (1 \rightarrow)$

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$$\begin{split} M_{if} &= \frac{e}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V \omega}} \left[\hbar (\vec{q} \cdot \hat{\varepsilon})_e \langle 1|_\gamma \langle 1| e^{i\vec{k} \cdot \vec{r}} |1 \rangle_\gamma |0 \rangle_e + 0 \right] \\ &= \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V \omega}} (\vec{q} \cdot \hat{\varepsilon})_e \langle 1| e^{i\vec{k} \cdot \vec{r}} |0 \rangle_e = \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V \omega}} (\vec{q} \cdot \hat{\varepsilon}) \int \psi_f^* e^{i\vec{k} \cdot \vec{r}} \psi_i d\vec{r} \end{split}$$

$$M_{if} = \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V\omega}} (\vec{q} \cdot \hat{\varepsilon}) \int \psi_f^* e^{i\vec{k}\cdot\vec{r}} \psi_i d\vec{r}$$

$$M_{if} = \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V\omega}} (\vec{q} \cdot \hat{\varepsilon}) \int \psi_f^* e^{i\vec{k}\cdot\vec{r}} \psi_i d\vec{r} = \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V\omega}} (\vec{q} \cdot \hat{\varepsilon}) \phi(\vec{Q})$$

$$M_{if} = \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V\omega}} (\vec{q} \cdot \hat{\varepsilon}) \int \psi_f^* e^{i\vec{k}\cdot\vec{r}} \psi_i d\vec{r} = \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V\omega}} (\vec{q} \cdot \hat{\varepsilon}) \phi(\vec{Q})$$

The initial electron wavefunction is simply that of a 1s atomic state

$$M_{if} = \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V\omega}} (\vec{q} \cdot \hat{\varepsilon}) \int \psi_f^* e^{i\vec{k}\cdot\vec{r}} \psi_i d\vec{r} = \frac{e\hbar}{m} \sqrt{\frac{\hbar}{2\epsilon_0 V\omega}} (\vec{q} \cdot \hat{\varepsilon}) \phi(\vec{Q})$$

 $\psi_i = \psi_{1s}(\vec{r})$

The initial electron wavefunction is simply that of a 1s atomic state

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The integral thus becomes

which is the Fourier transform of the initial state 1s electron wave function

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$$I_3 = \int \phi^2(\vec{Q}) q^2 \sin^2 \theta \cos^2 \varphi \delta(\mathcal{E}_f - \mathcal{E}_i) q^2 \sin \theta dq d\theta d\phi$$

Calculated cross section



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C. Segre (IIT)