## Today's Outline - April 02, 2015

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- PHYS 570 days at 10-ID


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- Cross-Section of an Isolated Atom

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

## PHYS 570 days at 10-ID

(1) April 10, 2015, 09:00-16:00
(2) April 24, 2015, 09:00-16:00

## PHYS 570 days at $10-$ ID

(1) April 10, 2015, 09:00-16:00
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- Absolute flux measurement
- Reflectivity measurement
- EXAFS measurement
- Rocking curve measurement (possibly)


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- Absolute flux measurement
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(4) Make sure your badge is ready
(5) Leave plenty of time to get the badge
(6) Let me know when you plan to come!


## Darwin widths

|  | $\zeta_{\mathrm{D}}^{\text {FWHM }} \times 10^{6}$ |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | (111) |  |  | (220) |  |  | (400) |  |  |
| $\begin{gathered} \text { Diamond } \\ a=3.5670 \AA \end{gathered}$ | 61.0 |  |  | 20.9 |  |  | 8.5 |  |  |
|  | 3.03 | 0.018 | -0.01 | 1.96 | 0.018 | -0.01 | 1.59 | 0.018 | -0.01 |
| $\begin{gathered} \text { Silicon } \\ a=5.4309 \AA \end{gathered}$ | 139.8 |  |  | 61.1 |  |  | 26.3 |  |  |
|  | 10.54 | 0.25 | -0.33 | 8.72 | 0.25 | -0.33 | 7.51 | 0.25 | -0.33 |
| Germanium$a=5.6578 \AA$ | 347.2 |  |  | 160.0 |  |  | 68.8 |  |  |
|  | 27.36 | -1.1 | -0.89 | 23.79 | -1.1 | -0.89 | 20.46 | -1.1 | -0.89 |

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

## Asymmetric Geometry

In general the diffracting planes are not precisely aligned with the surface of the crystal.


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b=\frac{\sin \theta_{i}}{\sin \theta_{e}}=\frac{\sin (\theta+\alpha)}{\sin (\theta-\alpha)}
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$$



$$
\delta \theta_{e}=\sqrt{b}\left(\zeta_{D} \tan \theta\right)
$$

$$
\delta \theta_{i}=\frac{1}{\sqrt{b}}\left(\zeta_{D} \tan \theta\right)
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## Rocking Curve Measurements

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

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$\mathrm{Si}(111) \mathrm{b}=4.3-\mathrm{Si}(111) \mathrm{b}=0.23$

output divergence on left, input divergence on right

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$\mathrm{Si}(111) \mathrm{b}=4.3-\mathrm{Si}(111) \mathrm{b}=0.23$

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## Rocking Curve Measurements

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

## 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



## Double Crystal Monochromators



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## Total Cross Section



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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.

## Scaled Absorption

$$
T=\frac{l}{l_{0}}=e^{-\mu z}
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scale $\sigma_{a}$ for different elements by $E^{3} / Z^{4}$ and plot together

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## Calculation of $\sigma_{a}$

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\sigma_{a}=\frac{2 \pi}{\hbar c} \frac{V^{2}}{4 \pi^{3}} \int\left|M_{i f}\right|^{2} \delta\left(\mathcal{E}_{f}-\mathcal{E}_{i}\right) q^{2} \sin \theta d q d \theta d \varphi
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where the matrix element $M_{\text {if }}$ between the initial, $\langle i|$, and final, $|f\rangle$, states is given by

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The interaction Hamiltonian is ex-

$$
\mathcal{H}_{l}=\frac{e \vec{p} \cdot \vec{A}}{m}+\frac{e^{2} A^{2}}{2 m}
$$ pressed in terms of the electromagnetic vector potential

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

$$
\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

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$$

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

## Free electron approximation

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\end{aligned}
$$

Thus

$$
M_{i f}=\frac{e}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}\left[e\left\langle\left. 1\right|_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a e^{i \vec{k} \cdot \vec{r}}+(\vec{p} \cdot \hat{\varepsilon}) a^{\dagger} e^{-i \vec{k} \cdot \vec{r}} \mid 1\right\rangle_{\gamma}|0\rangle_{e}\right]
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$$

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

## Free electron approximation

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

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$$
e^{\langle } 11\left|\vec{p}=(\hbar \vec{q})_{e}<1\right|
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The free electron state is an eigenfunction of the electron momentum operator
The annihilation operator applied to the left creates a photon

## Free electron approximation

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& e^{\langle }\langle 1| \vec{p}=(\hbar \vec{q})_{e}\langle 1| \\
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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.

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$$
\begin{aligned}
e^{\langle }\left\langle\left. 1\right|_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a\right. & =\hbar(\vec{q} \cdot \hat{\varepsilon})_{e}\left\langle\left. 1\right|_{\gamma}\langle 1|\right. \\
e^{\langle }\left\langle\left. 1\right|_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a^{\dagger}\right. & =0
\end{aligned}
$$

## Free electron approximation

$$
\begin{aligned}
& e^{\langle }\langle 1| \vec{p}=(\hbar \vec{q}){ }_{e}\langle 1| \\
& { }_{\gamma}\langle n| a=(\sqrt{n+1}){ }_{\gamma}\langle n+1| a \\
& { }_{\gamma}\langle n| a^{\dagger}=(\sqrt{n})_{\gamma}\langle n-1| a \\
& \text { operator } \\
& e^{\langle }\left\langle 1{ }_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a=\hbar(\vec{q} \cdot \hat{\varepsilon}){ }_{e}\left\langle\left. 1\right|_{\gamma}\langle 1|\right.\right. \\
& e^{\langle 1} \mid{ }_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a^{\dagger}=0 \\
& M_{i f}=\frac{e}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}\left[\hbar(\vec{q} \cdot \hat{\varepsilon})_{e}\left\langle\left. 1\right|_{\gamma}\langle 1| e^{i \vec{k} \cdot \vec{r}} \mid 1\right\rangle_{\gamma}|0\rangle_{e}+0\right]
\end{aligned}
$$

The free electron state is an eigenfunction of the electron momentum

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

## Free electron approximation

$$
\begin{aligned}
& { }_{e}\langle 1| \vec{p}=(\hbar \vec{q}) e\langle 1| \\
& { }_{\gamma}\langle n| a=(\sqrt{n+1}){ }_{\gamma}\langle n+1| a \\
& { }_{\gamma}\langle n| a^{\dagger}=(\sqrt{n})_{\gamma}\langle n-1| a \\
& e^{\left\langle\left. 1\right|_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a=\hbar(\vec{q} \cdot \hat{\varepsilon}){ }_{e}\left\langle\left. 1\right|_{\gamma}\langle 1|\right.\right.} \\
& e^{\langle }\left\langle 1{ }_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a^{\dagger}=0\right. \\
& M_{i f}=\frac{e}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}\left[\hbar(\vec{q} \cdot \hat{\varepsilon})_{e}\left\langle\left. 1\right|_{\gamma}\langle 1| e^{i \vec{k} \cdot \vec{r}} \mid 1\right\rangle_{\gamma}|0\rangle_{e}+0\right] \\
& =\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon})_{e}\langle 1| e^{i \vec{k} \cdot \vec{r}}|0\rangle_{e}
\end{aligned}
$$

## Free electron approximation

$$
\begin{aligned}
& e^{\langle }\langle 1| \vec{p}=(\hbar \vec{q}){ }_{e}\langle 1| \\
& { }_{\gamma}\langle n| a=(\sqrt{n+1}){ }_{\gamma}\langle n+1| a \\
& { }_{\gamma}\langle n| a^{\dagger}=(\sqrt{n})_{\gamma}\langle n-1| a \\
& \text { function of the electron momentum } \\
& \text { operator } \\
& \text { The annihilation operator applied } \\
& \text { to the left creates a photon while } \\
& \text { the creation operator annihilates a } \\
& \text { photon when applied to the left. } \\
& { }_{e}\left\langle\left. 1\right|_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a=\hbar(\vec{q} \cdot \hat{\varepsilon})_{e}\left\langle\left. 1\right|_{\gamma}\langle 1|\right.\right. \\
& e^{\langle }\left\langle 1{ }_{\gamma}\langle 0|(\vec{p} \cdot \hat{\varepsilon}) a^{\dagger}=0\right. \\
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& =\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon})_{e}\langle 1| e^{i \vec{k} \cdot \vec{r}}|0\rangle_{e}=\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon}) \int \psi_{f}^{*} e^{i \vec{k} \cdot \vec{r}} \psi_{i} d \vec{r}
\end{aligned}
$$

The free electron state is an eigen-

## Photoelectron integral

$$
M_{i f}=\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon}) \int \psi_{f}^{*} e^{i \vec{k} \cdot \vec{r}} \psi_{i} d \vec{r}
$$

## Photoelectron integral

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$$

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M_{i f}=\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 $1 s$ atomic state

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$$

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

$$
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The initial electron wavefunction is simply that of a 1 s atomic state while the final state is approximated as a plane wave

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$$

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$$

$$
\psi_{i}=\psi_{1 s}(\vec{r}) \quad \psi_{f}=\sqrt{\frac{1}{V}} e^{i \vec{q} \cdot \vec{r}}
$$

$$
\phi(\vec{Q})=\sqrt{\frac{1}{V}} \int e^{-i \vec{q} \cdot \vec{r}} e^{i \vec{k} \cdot \vec{r}} \psi_{1 s}(\vec{r}) d \vec{r}
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M_{i f}=\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon}) \int \psi_{f}^{*} e^{i \vec{k} \cdot \vec{r}} \psi_{i} d \vec{r}=\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon}) \phi(\vec{Q})
$$

$$
\psi_{i}=\psi_{1 s}(\vec{r}) \quad \psi_{f}=\sqrt{\frac{1}{V}}^{i \vec{q} \cdot \vec{r}}
$$

The initial electron wavefunction is

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\phi(\vec{Q})=\sqrt{\frac{1}{V}} \int e^{-i \vec{q} \cdot \vec{r}} e^{i \vec{k} \cdot \vec{F}} \psi_{1 s}(\vec{r}) d \vec{r}
$$ simply that of a $1 s$ atomic state while the final state is approximated as a plane wave

$$
=\sqrt{\frac{1}{V}} \int \psi_{1 s}(\vec{r}) e^{i(\vec{k}-\vec{q}) \cdot \vec{r}} d \vec{r}
$$

The integral thus becomes

## Photoelectron integral

$$
\begin{aligned}
M_{i f} & =\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon}) \int \psi_{f}^{*} e^{i \vec{k} \cdot \vec{r}} \psi_{i} d \vec{r}=\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon}) \phi(\vec{Q}) \\
\psi_{i} & =\psi_{1 s}(\vec{r}) \quad \psi_{f}=\sqrt{\frac{1}{V}} e^{i \vec{q} \cdot \vec{r}} \quad \begin{array}{ll}
\text { The initial electron wavefunction is } \\
\text { simply that of a 1s atomic state } \\
\text { while the final state is approxi- } \\
\text { mated as a plane wave }
\end{array} \\
\phi(\vec{Q}) & =\sqrt{\frac{1}{V} \int e^{-i \vec{q} \cdot \vec{r}} e^{i \vec{k} \cdot \vec{r}} \psi_{1 s}(\vec{r}) d \vec{r}} \quad \begin{array}{ll}
\text { The integral thus becomes }
\end{array} \\
& =\sqrt{\frac{1}{V} \int \psi_{1 s}(\vec{r}) e^{i(\vec{k}-\vec{q}) \cdot \vec{r}} d \vec{r}} \quad \begin{array}{ll}
\text { Ther }
\end{array} \\
& =\sqrt{\frac{1}{V} \int \psi_{1 s}(\vec{r}) e^{i \vec{Q} \cdot \vec{r}} d \vec{r}} \quad
\end{aligned}
$$

## Photoelectron integral

$$
\begin{aligned}
& M_{i f}=\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon}) \int \psi_{f}^{*} e^{i \vec{k} \cdot \vec{r}} \psi_{i} d \vec{r}=\frac{e \hbar}{m} \sqrt{\frac{\hbar}{2 \epsilon_{0} V \omega}}(\vec{q} \cdot \hat{\varepsilon}) \phi(\vec{Q}) \\
& \psi_{i}=\psi_{1 s}(\vec{r}) \quad \psi_{f}=\sqrt{\frac{1}{V}}^{i \vec{q} \cdot \vec{r}} \\
& \phi(\vec{Q})=\sqrt{\frac{1}{V}} \int e^{-i \vec{q} \cdot \vec{r}} e^{i \vec{k} \cdot \vec{F}} \psi_{1 s}(\vec{r}) d \vec{r} \\
& =\sqrt{\frac{1}{V}} \int \psi_{1 s}(\vec{r}) e^{i(\vec{k}-\vec{a}) \cdot \vec{r}} d \vec{r} \\
& =\sqrt{\frac{1}{V}} \int \psi_{1 s}(\vec{r}) e^{\vec{Q} \cdot \vec{r}} d \vec{r} \\
& \text { The initial electron wavefunction is } \\
& \text { simply that of a } 1 \mathrm{~s} \text { atomic state } \\
& \text { while the final state is approxi- } \\
& \text { mated as a plane wave } \\
& \text { The integral thus becomes } \\
& \text { which is the Fourier transform of } \\
& \text { the initial state } 1 s \text { electron wave } \\
& \text { function }
\end{aligned}
$$

## Photoelectron cross-section

the overall matrix element squared for a particular photoelectron final direction $(\varphi, \theta)$ is

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\left|M_{i f}\right|^{2}=\left(\frac{e \hbar}{m}\right)^{2} \frac{\hbar}{2 \epsilon_{0} V^{2} \omega}\left(q^{2} \sin ^{2} \theta \cos ^{2} \varphi\right) \phi^{2}(\vec{Q})
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and the final cross-section per $K$ electron can now be computed as

$$
\sigma_{a}=\frac{2 \pi}{\hbar c} \frac{V^{2}}{4 \pi^{3}}\left(\frac{e \hbar}{m}\right)^{2} \frac{\hbar}{2 \epsilon_{0} V^{2} \omega} I_{3}
$$

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$$

where the integral $I_{3}$ is given by

## Photoelectron cross-section

the overall matrix element squared for a particular photoelectron final direction $(\varphi, \theta)$ is

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and the final cross-section per $K$ electron can now be computed as

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\sigma_{a}=\frac{2 \pi}{\hbar c} \frac{V^{2}}{4 \pi^{3}}\left(\frac{e \hbar}{m}\right)^{2} \frac{\hbar}{2 \epsilon_{0} V^{2} \omega} I_{3}=\left(\frac{e \hbar}{m}\right)^{2} \frac{1}{4 \pi^{2} \epsilon_{0} c \omega} I_{3}
$$

where the integral $I_{3}$ is given by

$$
I_{3}=\int \phi^{2}(\vec{Q}) q^{2} \sin ^{2} \theta \cos ^{2} \varphi \delta\left(\mathcal{E}_{f}-\mathcal{E}_{i}\right) q^{2} \sin \theta d q d \theta d \phi
$$

## Calculated cross section



## Calculated cross section



## Calculated cross section



