Today’s Outline - October 24, 2016

- Modulated structures
- Lattice vibrations
- Powder diffraction
- Bragg & Laue geometries
- Reflection for a Single Layer
- Kinematical Approach for Many Layers
- Darwin Curve
- Dynamical Diffraction Theory

Homework Assignment #05:
Chapter 5: 1, 3, 7, 9, 10
due Wednesday, November 02, 2016

No class on Wednesday, November 9, 2016
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Modulated structures

By definition crystals have always been considered to have long range order.

\[ x = an + u \cos(qan), \]

where:
- \( a \) is the lattice parameter,
- \( u \) is the amplitude of the displacement, and
- \( q = \frac{2\pi}{\lambda_m} \) is the wave vector of the modulation.

If \( \lambda_m \) is a multiple or a rational fraction of \( a \), it is called a commensurate modulation but if \( \lambda_m = ca \), where \( c \) is an irrational number, then it is an incommensurate modulation.
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However, it is common to see structures where the positions of the atoms is modulated (e.g. charge density waves, magnetic lattices, etc.) according to $x_n = an + u \cos(qan)$, where: $a$ is the lattice parameter, $u$ is the amplitude of the displacement, and $q = \frac{2\pi}{\lambda_m}$ is the wave vector of the modulation.
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Diffraction from a modulation

For simple a 1D modulated structure, we can compute the scattering

\[ A(Q) = N - 1 \sum_{n=0}^{N-1} e^{iQx_n} \approx N - 1 \sum_{n=0}^{N-1} e^{iQan}[1 + iQu \cos(qan)] \]

\[ I(Q) = N(2\pi a)\sum_h \delta(Q-Gh) + \left(Qu^2\right)\left[\delta(Q+q-Gh) + \delta(Q-q-Gh)\right] \]

the diffraction pattern has main Bragg peaks plus satellite peaks
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If the modulation of the structure is a multiple of the lattice parameter, the modulation is simply a superlattice and the actual lattice parameter will be changed.

![Graph showing intensity vs. Q for quasiperiodic scattering](image)
Quasicrystals

The only rotational symmetries which permit a space-filling lattice are 2-, 3-, 4-, and 6-fold.
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![Diagrams of quasicrystals](image-url)
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In 2011 Shechtman was awarded the Nobel Prize in Chemistry.
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This metastable phase was also found with Fe and Cr in the place of Mn. Other groups have discovered stable icosahedral phases with three and two elements.

Quasicrystal diffraction patterns

The $\text{Al}_{65}\text{Cu}_{20}\text{Fe}_{15}$ system was one of the first stable quasicrystals to be discovered. Later discovery of stable quasicrystals in the Ta-Te, Cd-Ca, and Cd-Yb systems enabled large crystals to be grown.

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Lattice Vibrations

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For a 1D lattice, we replace the position of the atom with its *instantaneous* position, $\vec{R}_n + \vec{u}_n$ where $\vec{u}_n$ is the displacement from the equilibrium position, $\vec{R}_n$. 

Computing the intensity:

$$I = \langle \sum_m f(\vec{Q}) e^{i \vec{Q} \cdot (\vec{R}_m + \vec{u}_m)} \sum_n f^*(\vec{Q}) e^{-i \vec{Q} \cdot (\vec{R}_n + \vec{u}_n)} \rangle$$

The last term is a time average which can be simplified using the Baker-Hausdorff theorem,

$$\langle e^{ix} \rangle = e^{ -\langle x^2 \rangle / 2} \langle e^{i \vec{Q} \cdot (\vec{u}_m - \vec{u}_n)} \rangle = e^{ -\langle Q^2 (\vec{u}_m - \vec{u}_n)^2 \rangle / 2}$$
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\[ = e^{-2M} \left[ 1 + e^{Q^2\langle u_{Qm}u_{Qn} \rangle} - 1 \right] \]

The first term is just the elastic scattering from the lattice with the addition of the term \( e^{-Q^2\langle u_{Q}^2 \rangle} = e^{-Q^2\langle u_{Qm}^2 \rangle / 2} e^{-Q^2\langle u_{Qn}^2 \rangle / 2} \), called the Debye-Waller factor.

The second term is the Thermal Diffuse Scattering and actually increases with mean squared displacement.
\[ \langle e^{iQ(u_{Qm} - u_{Qn})} \rangle = e^{-Q^2 \langle u_{Qm}^2 \rangle / 2} e^{-Q^2 \langle u_{Qn}^2 \rangle / 2} e^{Q^2 \langle u_{Qm} u_{Qn} \rangle} \]

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Substituting into the expression for intensity
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\[ + \sum_{m} \sum_{n} f(Q)e^{-M} e^{i\vec{Q} \cdot \vec{R}_m} f^*(\vec{Q})e^{-M} e^{-i\vec{Q} \cdot \vec{R}_n} \left[ e^{Q^2\langle u_{Qm}u_{Qn} \rangle} - 1 \right] \]
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\[ + \sum_m \sum_n f(Q)e^{-M} e^{i\overrightarrow{Q} \cdot \overrightarrow{R}_m} f^*(Q)e^{-M} e^{-i\overrightarrow{Q} \cdot \overrightarrow{R}_n} \left[ e^{Q^2\langle u_{Qm}u_{Qn} \rangle} - 1 \right] \]

The first term is just the elastic scattering from the lattice with the addition of the term \( e^{-M} = e^{-Q^2\langle u_{Q}^2 \rangle / 2} \), called the Debye-Waller factor.
Lattice Vibrations

\[ \langle e^{iQ(u_{Qm} - u_{Qn})} \rangle = e^{-Q^2\langle u_{Qm}^2 \rangle/2} e^{-Q^2\langle u_{Qn}^2 \rangle/2} e^{Q^2\langle u_{Qm}u_{Qn} \rangle} \]

\[ = e^{-Q^2\langle u_{Q}^2 \rangle} e^{Q^2\langle u_{Qm}u_{Qn} \rangle} = e^{-2M} e^{Q^2\langle u_{Qm}u_{Qn} \rangle} \]

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The second term is the Thermal Diffuse Scattering and actually increases with mean squared displacement.
Thermal Diffuse Scattering

\[ I^{\text{TDS}} = \sum_m \sum_n f(\vec{Q}) e^{-M} e^{i\vec{Q} \cdot \vec{R}_m} f^*(\vec{Q}) e^{-M} e^{-i\vec{Q} \cdot \vec{R}_n} \left[ e^{Q^2\langle u_{Qm} u_{Qn} \rangle} - 1 \right] \]

The TDS has a width determined by the correlated displacement of atoms which is much broader than a Bragg peak. These correlated motions are just phonons.

A 0.5mm Si wafer illuminated by 28keV x-rays from an APS undulator were used to measure the phonon dispersion curves of silicon incident beam along (100).
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Incident beam along (100)

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Properties of the Debye-Waller Factor

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for isotropic atomic vibrations

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In general, Debye-Waller factors can be anisotropic
The Debye Model

The Debye model can be used to compute $B_T$ by integrating a linear phonon dispersion relation up to a cutoff frequency, $\omega_D$, called the Debye frequency.

$$B_T = \frac{6\hbar^2 m}{A k_B \Theta} \left[ \phi\left(\frac{\Theta}{T}\right) + \frac{\Theta}{T} + 1 \right]$$

$$\phi(x) = \int_{\Theta/T_0}^{\Theta/T} \xi e^{-\xi} d\xi$$

$$B_T [\text{\AA}^2] = 11492T[K]A\Theta^2[K^2] \left[ \phi\left(\frac{\Theta}{T}\right) + 2873A\Theta[K] \right]$$
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\[
B_T \approx 6 \frac{\hbar^2}{m A} k_B \Theta \left[ \phi \left( \frac{\Theta}{T} \right) + 1 \right] \]

\[
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C. Segre (IIT)
PHYS 570 - Fall 2016
October 24, 2016 12 / 20
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Debye Temperatures

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<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>( \Theta ) (K)</th>
<th>( B_{4.2} )</th>
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*diamond
\[ B_T = \frac{11492 T}{A \Theta^2} \phi(\Theta / T) + \frac{2873}{A \Theta} \]

diamond is very stiff and \( \Theta \) does not vary much with temperature.

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Copper has a much lower Debye temperature and a wider variation of thermal factor with temperature.

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PHYS 570 - Fall 2016

October 24, 2016

13 / 20
Powder diffraction

(a) Ambient pressure

(b) 4.9 GPa (49 kbar)
CaO-CaO\textsubscript{2} reaction kinetics

CaO is a possible material to be used for carbon sequestration.
CaO-CaO₂ reaction kinetics

CaO is a possible material to be used for carbon sequestration.

CaO will absorb CO₂ at temperatures as low as 450°C forming CaCO₃ and can be regenerated by calcination at temperatures above 700°C.
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CaO-CaO$_2$ reaction kinetics
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Final conversion fraction depends on temperature but also some other parameter (what?)
CaO-CaO$_2$ reaction kinetics

Reaction kinetics much faster than previously observed (0.28/s)
CaO-CaO\textsubscript{2} reaction kinetics

A - 450°C (fit up to 50% of the final CaO conversion)
CaO-CaO$_2$ reaction kinetics

Initial crystallite size is one of the determining factors in initial rate of conversion and fraction converted.

CaO crystallite size can be related to porosity which is key to the conversion process.