AtomicControl: A Crystallography Simulator

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Outline

• Motivations and objectives
• Capabilities
• Software model
• Building crystals
• Generating an x-ray diffraction pattern
• Classroom demos
Motivation

• Visualizing crystal structures is difficult without models
• Instant feedback and interactivity useful for learning
• Classroom use in 3.012 and 3.014

Objectives of AtomicControl

• Interactively build arbitrary crystal structures
• Visualize crystal structures
• Simulate X-ray diffraction patterns
AtomicControl Capabilities

- Model arbitrary crystal structures
- Save and load previously created structures
- Models allow free rotation of crystal
- Instant visual feedback on modifications
- Relative atom sizes can be represented
- X-ray diffraction patterns generated
- Reciprocal lattice visualization
Software Model

• Programming Language: Java

• Cross-Platform: Windows, Mac OS X, Linux, Athena

• Modularity
  – Crystal Builder, diffractometer, and graphical interface independant
  – Standardized interfaces for interacting between objects
  – Main module Interface: Crystal
Software Model
Building Crystals: Space Groups

A space group can be mathematically defined as a set of equipoint transformations of the form:

\[
\begin{bmatrix}
u' \\
v' \\
w'
\end{bmatrix} = \begin{bmatrix}
R_{11} & R_{12} & R_{13} \\
R_{21} & R_{22} & R_{23} \\
R_{31} & R_{32} & R_{33}
\end{bmatrix}
\begin{bmatrix}
u \\
v \\
w
\end{bmatrix} + \begin{bmatrix}
T_1 \\
T_2 \\
T_3
\end{bmatrix}
\]

<table>
<thead>
<tr>
<th>Positions</th>
<th>Multiplicity, Wyckoff letter, Site symmetry</th>
<th>Coordinates</th>
<th>Reflection conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 i 1</td>
<td></td>
<td>(0, 0, 0) + \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) +</td>
<td>General:</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Akh : h + (k + l = 2n)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Ak0 : h, (k = 2n)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>O0l : k + (l = 2n)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>hkl : 2(a + l = 4n)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>GOl : (l = 4n)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H00 : h = 2n</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>H(\overline{0}0) : h = 2n</td>
</tr>
</tbody>
</table>
Build Algorithm

Apply translation vectors to basis atom list
do(
  for each atom(
    for each transformation(
      Apply transform to atom
      Normalize the transformed location
      Create a copy of the atom at the transformed location
    )
  )
  remove duplicates from atom list
) while atom list is bigger than before, repeat
do
  remove atoms outside the unit cell
XRD: Bragg Condition

\[ \lambda = 2d \sin \theta \iff \Delta k = G \]
Powder Diffraction

\[ I(2\theta) = |F|^2 \cdot p \cdot \left( \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right) \]

Handling Multiplicies:

\[ I(2\theta) = \sum |F|^2 \cdot \left( \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right) \]
X-ray Diffraction Algorithm

for each $h$ from $-h_{\text{max}}$ to $h_{\text{max}}$:
for each $k$ from $-k_{\text{max}}$ to $k_{\text{max}}$:
for each $l$ from $-l_{\text{max}}$ to $l_{\text{max}}$:
  $G_{\text{mag}} = |hb_1 + kb_2 + lb_3|^2$
  if $G_{\text{mag}} \cdot \lambda/4\pi < 1$ :
    add $[h \ k \ l]$ to list of allowed $G$

for each allowed $G_i$ :
  for each basis atom $j$:
    $R_j = \text{Atom}_j$’s Centroid
    $s = |G_i|/4\pi$
    $F_i = F_i + f_j(s) \ e^{R_j \cdot G_i}$
  save $F_i$
Convert to $I(2\theta)$

for each $G_i$:
\[
\theta_i = \sin^{-1}\left( \frac{\lambda |G_i|}{4\pi} \right)
\]
\[
I(2\theta_i) = I(2\theta_i) + |F_i|^2
\]

for each $\theta_n$:
\[
I(2\theta_n) = I(2\theta_n) \ast LP(\theta_n)
\]
X-Ray diffraction comparison

FCC Gold

Experimental data from Swanson and Tage 1953
Classroom Demos

- Redefining the Unit Cell:
  Conventional BCC vs. Primitive BCC

- Cu₃Au Order-Disorder Transformation:
  Simple Cubic to Face-Centered Cubic

- Martensitic Transformation:
  Cubic to Tetragonal
Conclusions

- Build and Visualize Crystal Structure
- Simulate Powder Pattern
- All in an easy to use package

Future Directions

- Classroom Use
- Availability online, Open Source
- Expanded diffraction capability, customizability
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http://pruffle.mit.edu/atomiccontrol