AtomicControl:
A Crystallography Simulator

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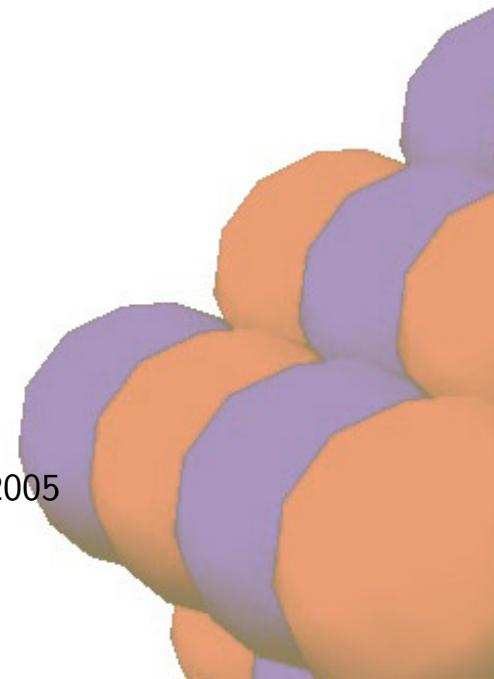
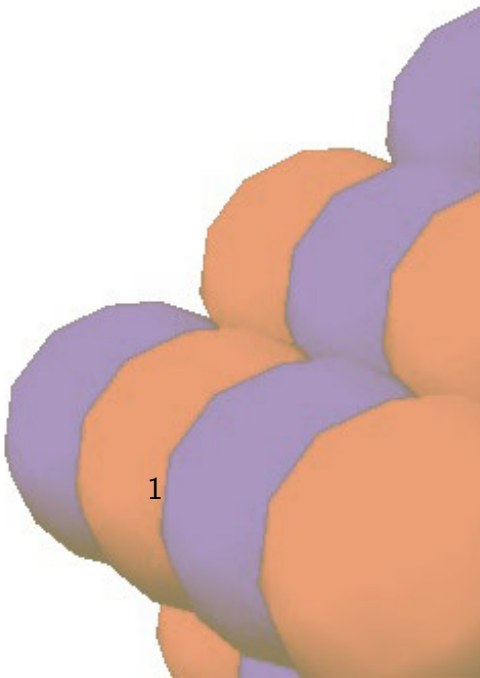


Outline

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

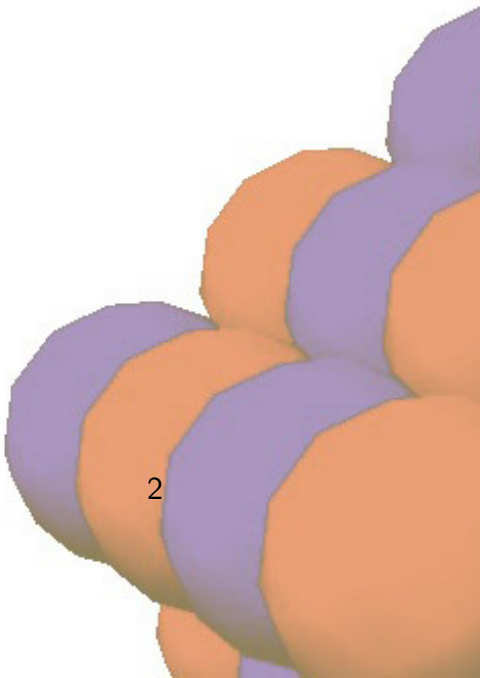


Motivation

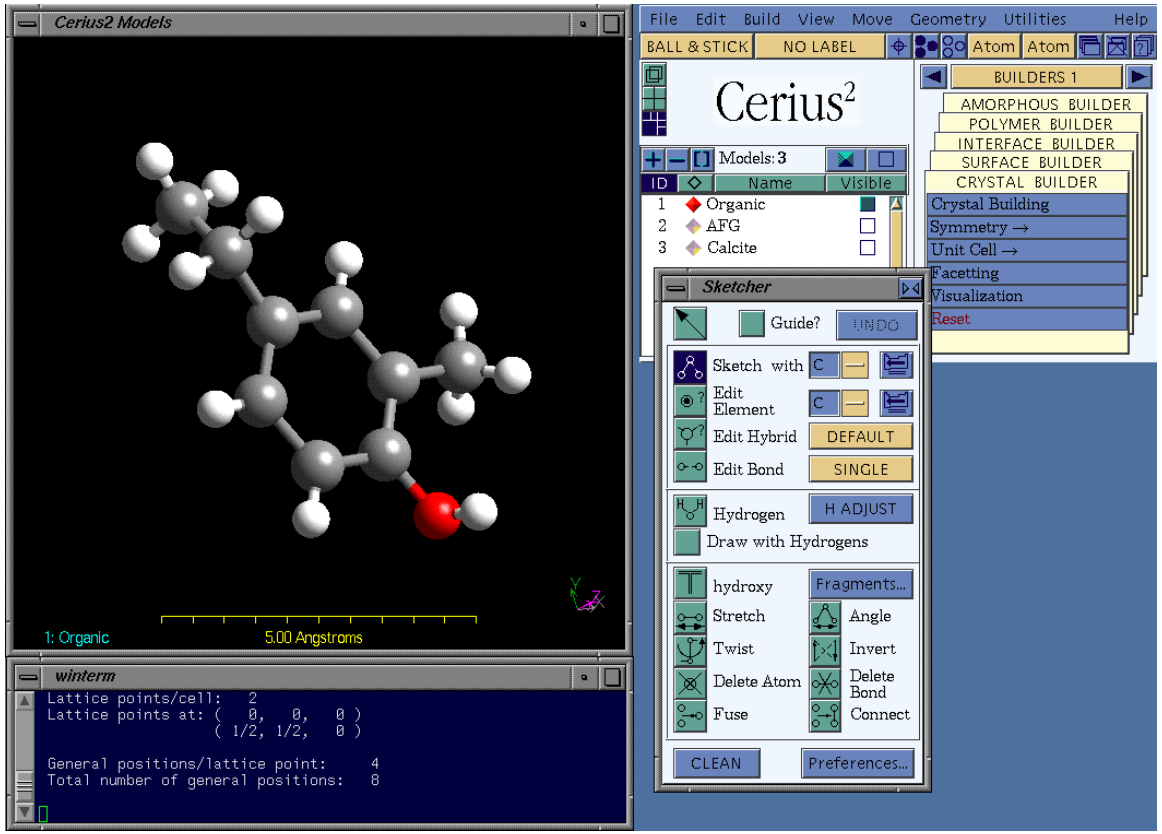
- Visualizing crystal structures is difficult without models
- Instant feedback and interactivity useful for learning
- Classroom use in 3.012 and 3.014

Objectives of AtomicControl

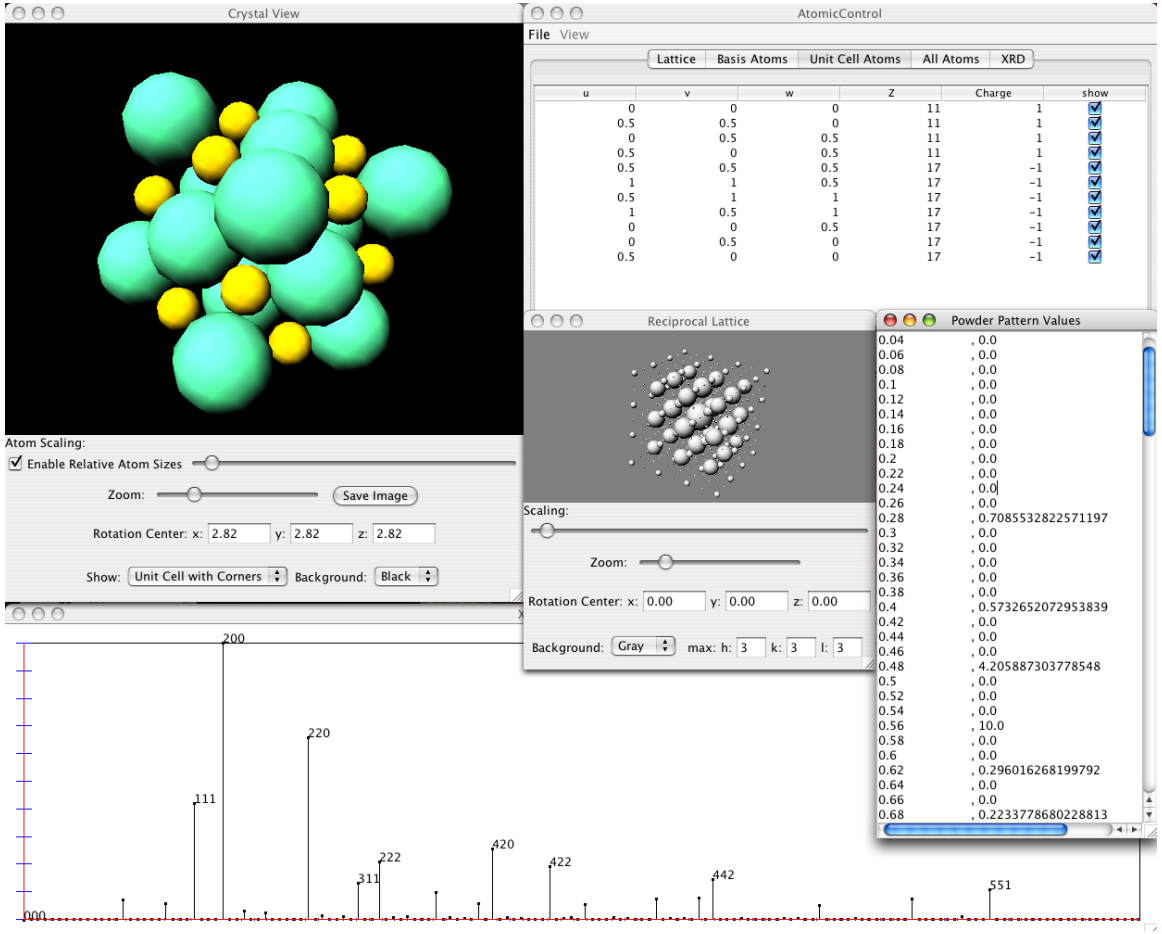
- Interactively build arbitrary crystal structures
- Visualize crystal structures
- Simulate X-ray diffraction patterns



Cerius^2

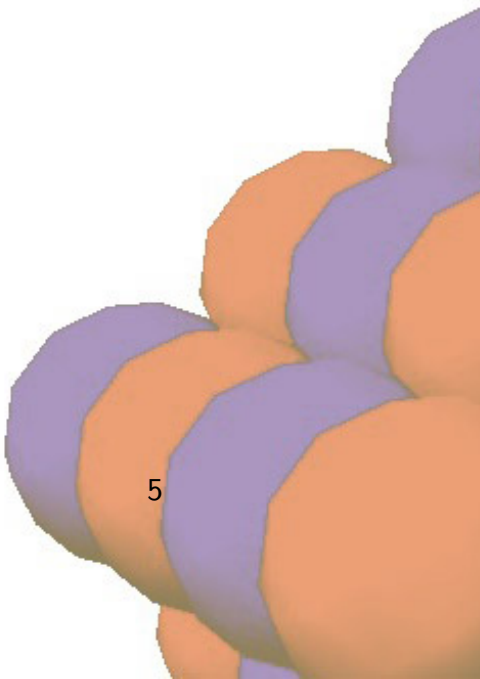

Cerius2 Models
1: Organic
5.00 Angstroms
winterm
Lattice points/cell: 2
Lattice points at: (0, 0, 0)
(1/2, 1/2, 0)
General positions/lattice point: 4
Total number of general positions: 8
File Edit Build View Move Geometry Utilities Help
BALL & STICK
NO LABEL
Atom
Atom
Cerius2
Models: 3
ID
Name
Visible
1 Organic
2 AFG
3 Calcite
BUILDERS 1
AMORPHOUS BUILDER
POLYMER BUILDER
INTERFACE BUILDER
SURFACE BUILDER
CRYSTAL BUILDER
Crystal Building
Symmetry →
Unit Cell →
Facetting
Visualization
Reset
Sketcher
Guide?
UNDO
Sketch with
C
Edit Element
C
Edit Hybrid
DEFAULT
Edit Bond
SINGLE
Hydrogen
H ADJUST
Draw with Hydrogens
hydroxy
Fragments...
Stretch
Angle
Twist
Invert
Delete Atom
Delete Bond
Fuse
Connect
CLEAN
Preferences...

AtomicControl



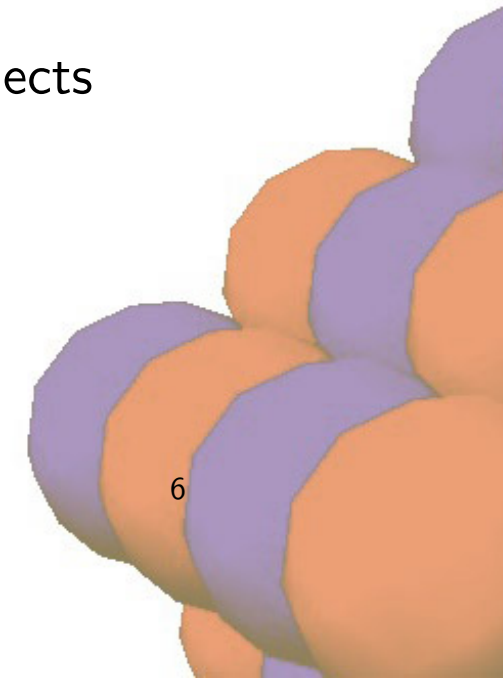
AtomicControl Capabilities

- 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

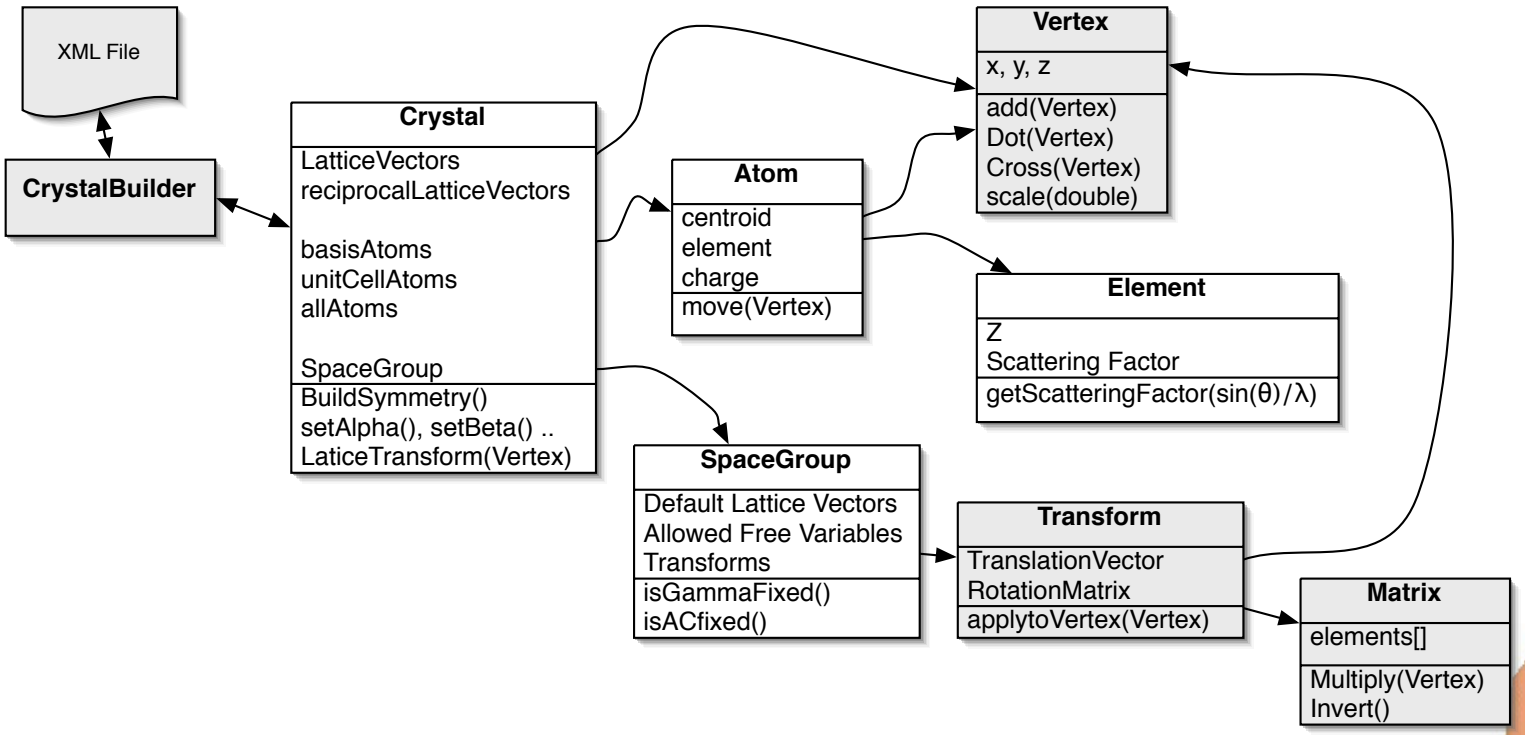


Software Model

- 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



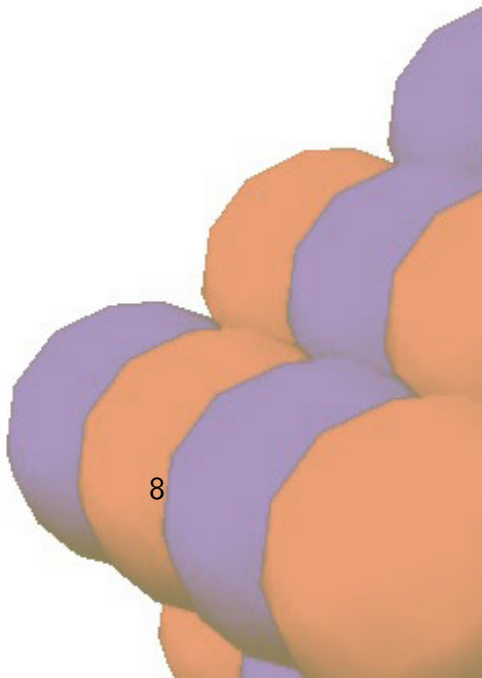
Building Crystals: Space Groups

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
		(0, 0, 0) +	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ +	
32 *i* 1	(1) x, y, z		(2) $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$	General:
	(3) $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$		(4) $y + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$	$hkl : h + k + l = 2n$
	(5) $\bar{x} + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$		(6) $x, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$	$hk0 : h, k = 2n$
	(7) $y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$		(8) $\bar{y}, \bar{x}, \bar{z}$	$0kl : k + l = 2n$
	(9) $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$		(10) $x + \frac{1}{2}, y, \bar{z} + \frac{3}{4}$	$hhl : 2h + l = 4n$
	(11) $y, \bar{x}, \bar{z}$		(12) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$	$00l : l = 4n$
	(13) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$		(14) $\bar{x}, y, z$	$h00 : h = 2n$
	(15) $\bar{y} + \frac{1}{2}, \bar{x}, z + \frac{3}{4}$		(16) $y, x + \frac{1}{2}, z + \frac{1}{4}$	$h\bar{h}0 : h = 2n$



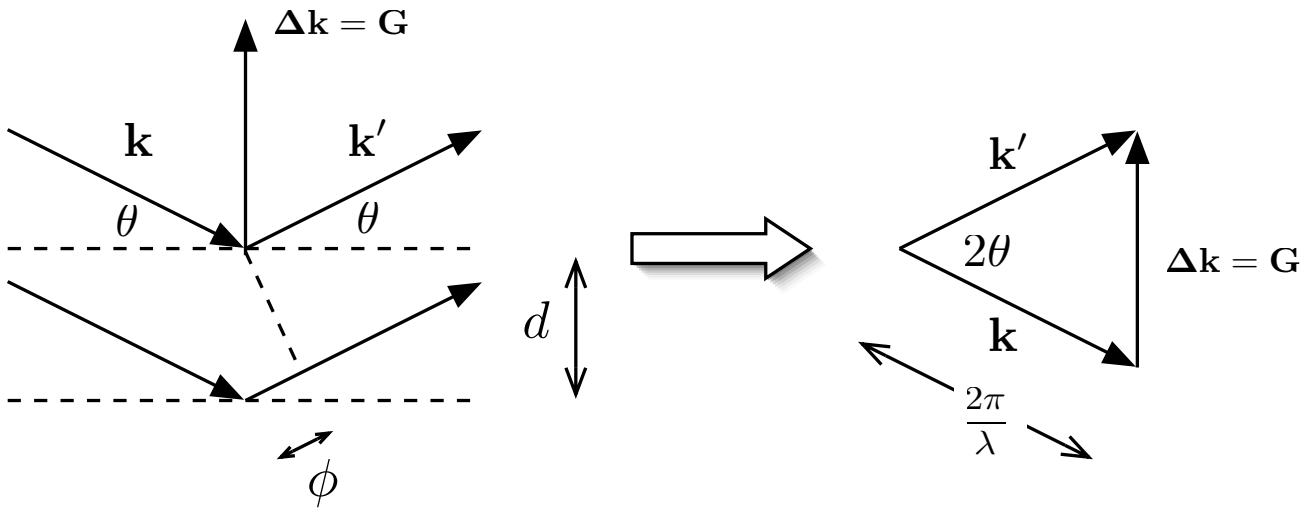
Build Algorithm

```
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

$$\lambda = 2d \sin\theta \iff \boldsymbol{\Delta k} = \boldsymbol{G}$$

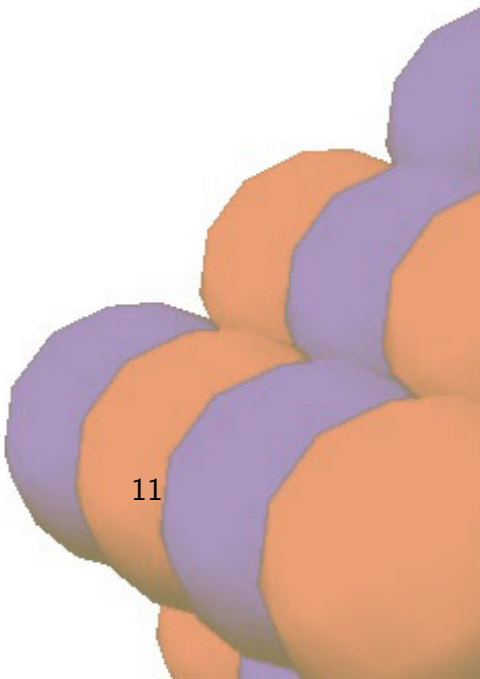


Powder Diffraction

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

Handling Multiplicies:

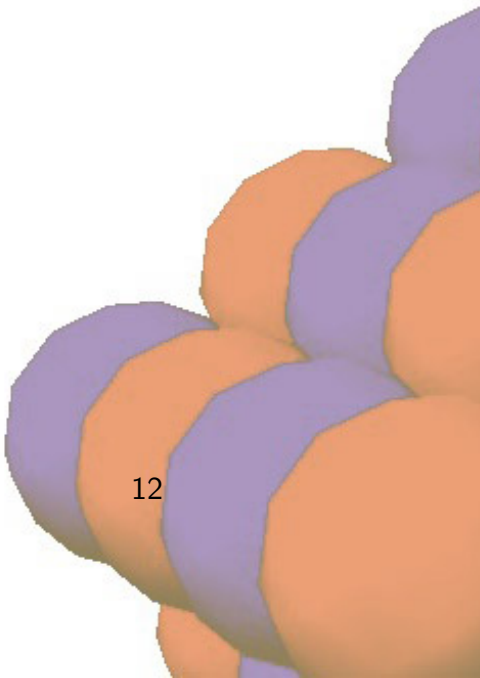
$$I(2\theta) \;=\; \sum |F|^2 \cdot \left(\frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}\right)$$



X-ray Diffraction Algorithm

```
for each h from -h_max to h_max:
    for each k from -k_max to k_max:
        for each l from -l_max to l_max:
            Gmag = |h b_1 + k b_2 + l b_3|^2
            if Gmag·λ/4π < 1 :
                add [h k l] to list of allowed G

for each allowed G_i :
    for each basis atom_j:
        R_j = Atom_j's Centroid
        s = |G_i|/4π
        F_i = F_i + f_j(s) e^(R_j · G_i)
    save F_i
```



Convert to $I(2\theta)$

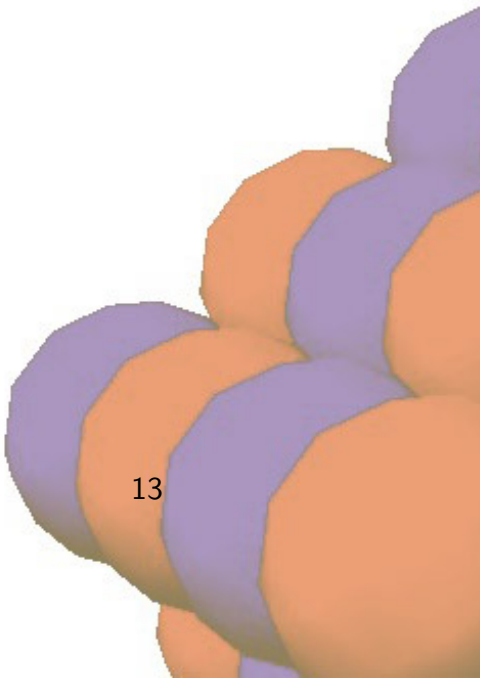
for each $\boldsymbol{G_i}$:

$$\theta_i = \sin^{-1}\left(\frac{\lambda \ |\boldsymbol{G_i}|}{4\pi}\right)$$

$$\mathtt{I}(2\theta_i) = \mathtt{I}(2\theta_i) + |F_i|^2$$

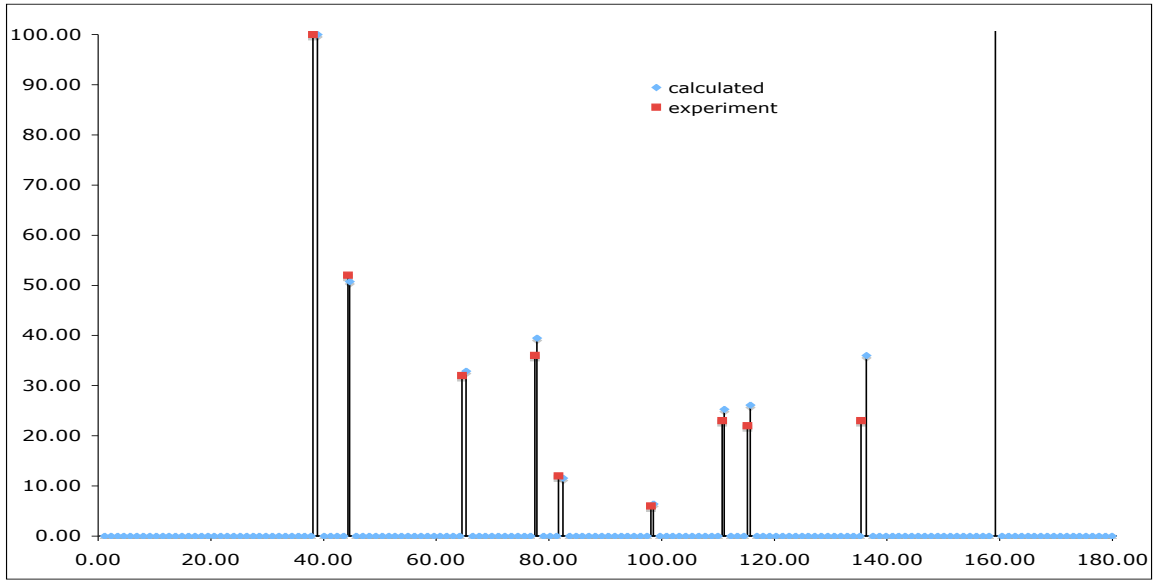
for each θ_n :

$$\mathtt{I}(2\theta_n) = \mathtt{I}(2\theta_n) * \mathtt{LP}(\theta_n)$$

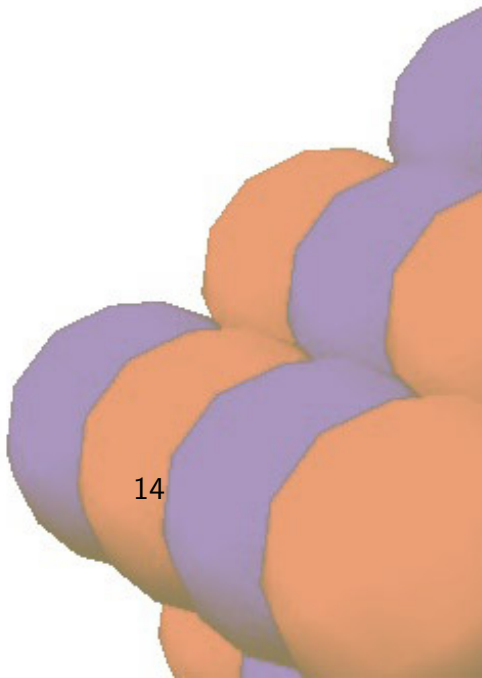


X-Ray diffraction comparison

FCC Gold

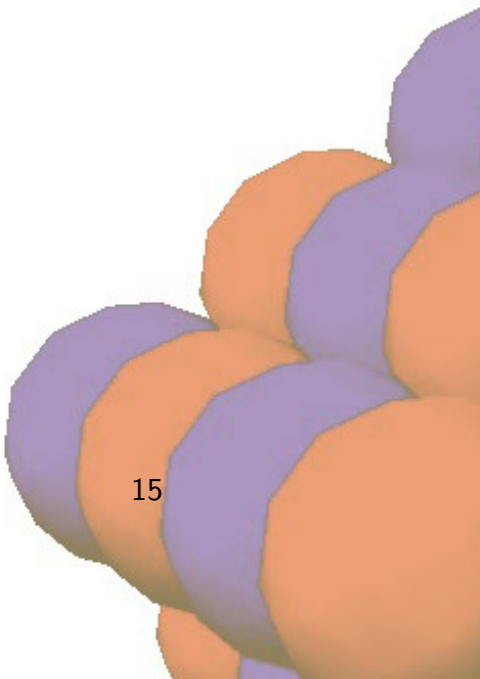


Experimental data from Swanson and Tage 1953



Classroom Demos

- Redefining the Unit Cell:
  Conventional BCC vs. Primitive BCC
- Cu_3Au Order-Disorder Transformation:
  Simple Cubic to Face-Centered Cubic
- Martensitic Transformation:
  Cubic to Tetragonal

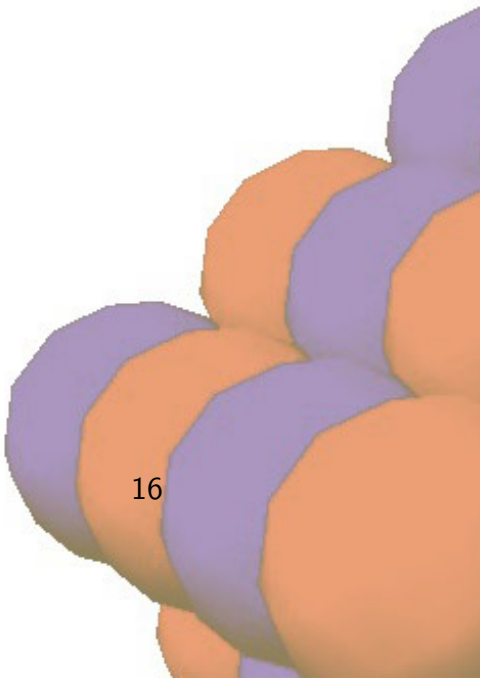


Conclusions

- 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