JEMS tutorial

Part 1: Simulating diffraction patterns for Al FCC with JEMS

Open the structure file for an FCC material with single atom motif (here Al).

(a) Simulate the diffraction pattern on different zone axes ([0 0 1], [1 1 0], [1 1 1], …).

(b) How does the pattern change when you change: camera length; convergence angle ("Beam half conv."); acceptance angle ("Accept."); "Deviation".

Camera length → magnification of pattern | Deviation → length of relrod
Acceptance angle → objective aperture

(c) Polls: How can you change convergence angle and acceptance angle on a microscope? What does "Deviation" relate to?

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(d) Change acceleration voltage using the “Voltage” setting. What happens? Why?

Voltage ↑ ⇒ $\lambda \downarrow$. Scattering angles ↓ ⇒ pattern "demagnifies"

- $2\theta_B \simeq \frac{\lambda}{d}$ - And Ewald sphere flatter ⇒ see more diffraction spots

(e) Methods demonstration: adding higher order Laue zones. Is there a first order Laue zone for the [1 0 1] zone axis? Why?

(FOLZ: $hU+kV+lW=1$)

$hU+kV+lW = h+l = 1$

Not possible for h, k, l all odd or all even

(f) Methods demonstration: setting up a “2-beam” condition. Select “All beams” Dynamical calculation (Crystal / matrix tab) for the full effect.

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Part 2: Pattern simulation using other structures

2.1 $AuCu_3$

(a) Restart JEMS. Select $AuCu_3$ in cubic. Simulate the SADP on various zone axes.

No systematic absences

(b) Compare its pattern on [0 0 1] zone axis to that from Al on [0 0 1]. What difference do you notice in the diffracting planes? Why is there this difference for the two structures?

Au : 0,0,0 Cu : face centered sites

$$F_g = f_{Au} + f_{Cu}\left[e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(h+l)}\right]$$

If h, k, l all even / all odd : $F_g = f_{Au} + 3f_{Cu}$

— mixed : $F_g = f_{Au} - f_{Cu}$

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FCC with 2 atoms per lattice point:

0, 0, 0

$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

2.2 Si

(a) Now select Si in cubic. Si has the diamond structure. How does this structure compare to that of Al? Simulate the SADP on various zone axes.

{002} planes are also systematically absent

(b) Compare its pattern on [0 0 1] zone axis to that from Al on [0 0 1]. What difference do you notice in the diffracting planes? Why is there this difference for the two structures?

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$a = b \neq c$

$\alpha = \beta = 90^\circ \quad \gamma = 120^\circ$

2.3 Graphite

(a) Now select Graphite in hexagonal. What is the defining symmetry of graphite? How can you see this in its diffraction pattern(s)?