

Lecture 5

Screw Motion

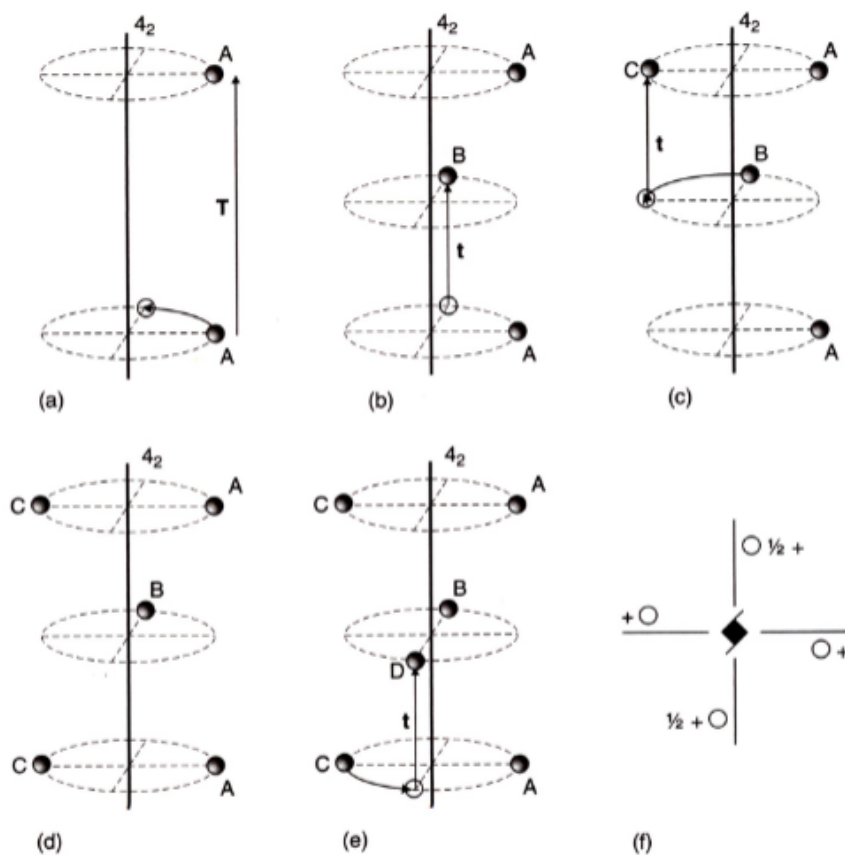


Figure 1: 42 axis

- Compound Operation: rotation then translation
- Notation n_p , where the atom is rotated by $\frac{2\pi}{n}$ anticlockwise and shifted upwards by $\frac{p}{n}T$, where T is the lattice repeat
- Note that if n and p have common factors, the final angle of the same particle at $z = 0$ and $z = T$ are different, so each “layer” has more than 1 atom, as lattices have to repeat

Space Group Lattice Symbols

- A: A-face centred
- B: B-face centred
- C: C-face centred

Space Group Symbols

- a: glide vector along a
- b: glide vector along b
- c: glide vector along c
- n: diagonal glide plane
- d: diamond glide plane

Space Group P4

- p4 plane group stretched vertically

Multiplicity	Wyckoff letter	Site symmetry	Coordinates of equivalent positions
4	d	1	$(x, y, z), (\bar{x}, \bar{y}, z), (\bar{y}, x, z), (y, \bar{x}, z)$
2	c	2	$(0, \frac{1}{2}, z), (\frac{1}{2}, 0, z)$
1	b	4	$(\frac{1}{2}, \frac{1}{2}, z)$
1	a	4	$(0, 0, z)$

Space Group P41

Multiplicity	Wyckoff letter	Site symmetry	Coordinates of equivalent positions
4	a	1	$(x, y, z), (\bar{x}, \bar{y}, z), (\bar{y}, x, z), (y, \bar{x}, z)$

Complete Specification of Any 2-D or 3-D Crystal Structure

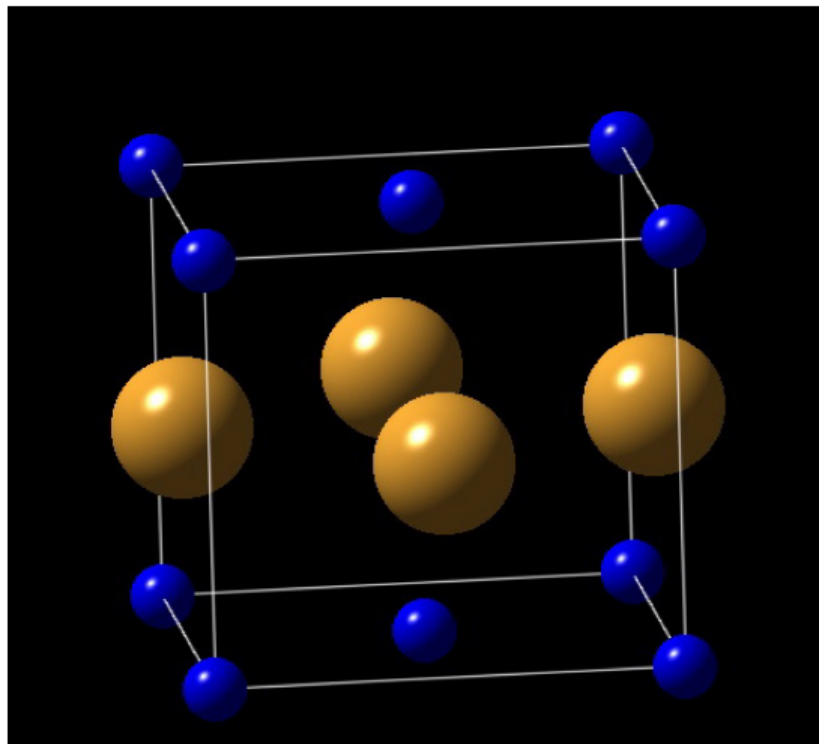
- Lattice Parameters
 - p, c, etc
- Space Group Symbol
 - 2, 4, 6, etc
- List of atom types and coordinates (Wyckoff letter)

AuCu

Structure 4 *Prototype:* AuCu

SBS/PS: L1₀/tP4 (or tP4 with centered cell) *SG # 123:* **P4/mmm** (D_{4h}^1)

Lattice complex: Au @ $2e(0, \frac{1}{2}, \frac{1}{2})$; Cu @ $1a(0,0,0)$ and $1c(\frac{1}{2}, \frac{1}{2}, 0)$



- tP4
- $P \frac{4}{m} \frac{2}{m} \frac{2}{m}$
- Wyckoff letters
 - e at $(0, \frac{1}{2}, \frac{1}{2})$
 - a at $(0, 0, 0)$
 - c at $(\frac{1}{2}, \frac{1}{2}, 0)$