# Analytical Methods for Materials

Lesson 13
Crystallography and Crystal Structures – continued

## Suggested Reading

- Chapter 6 in Waseda
- Excerpt from ASM Metals Handbook.

# Notation for crystal structures

1. Hermann-Mauguin (HM)…
   aka the ‘International’ system
2. Pearson
3. Strukturbericht
4. Schoenflies

The International (i.e., **Hermann-Maugin**) system is preferred for describing crystal structures in metals and ceramics.

The other systems have their uses too.

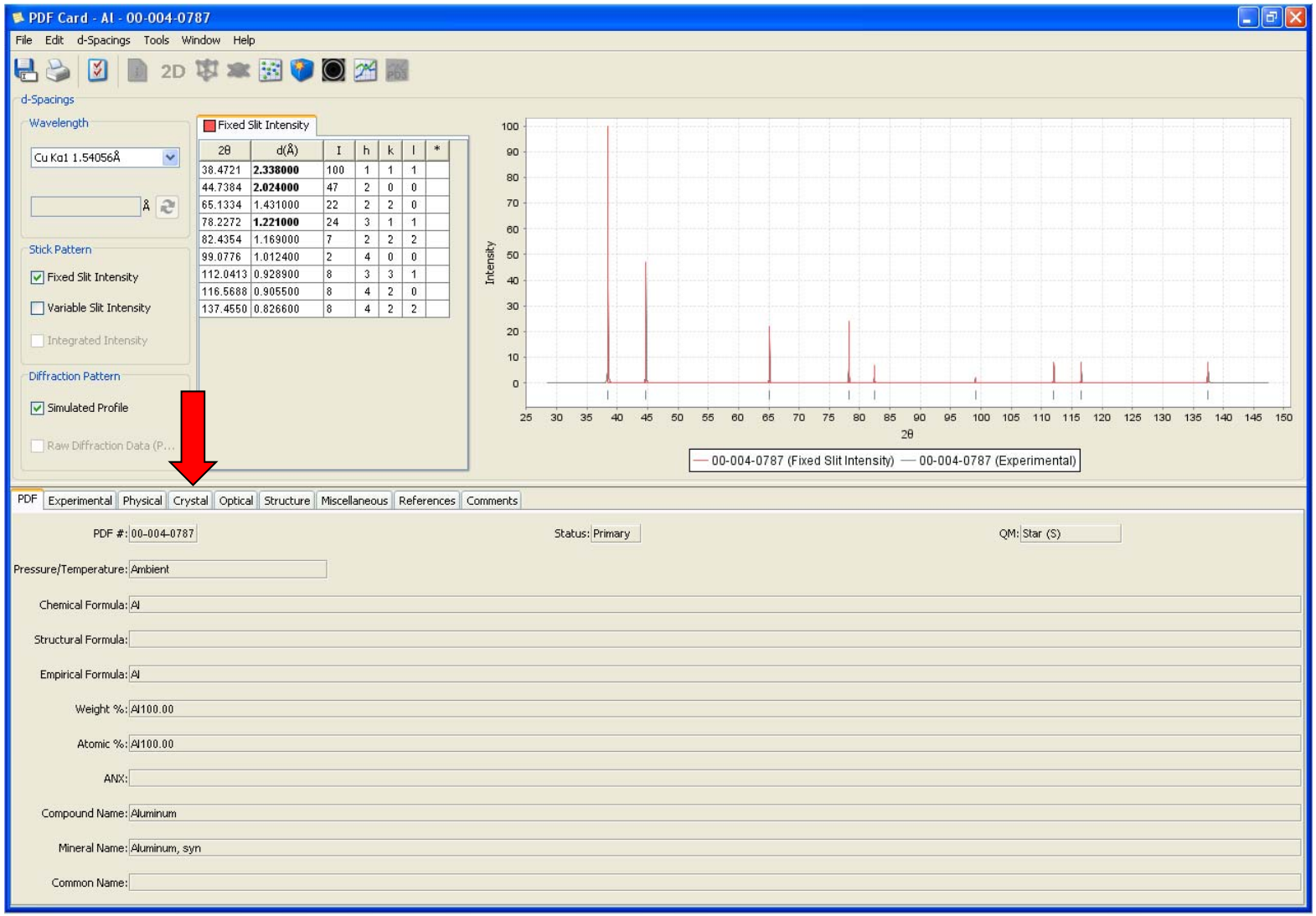
***We use all of them to describe space groups!***

Space group data allows us to define allowed and missing reflections in a diffraction pattern.

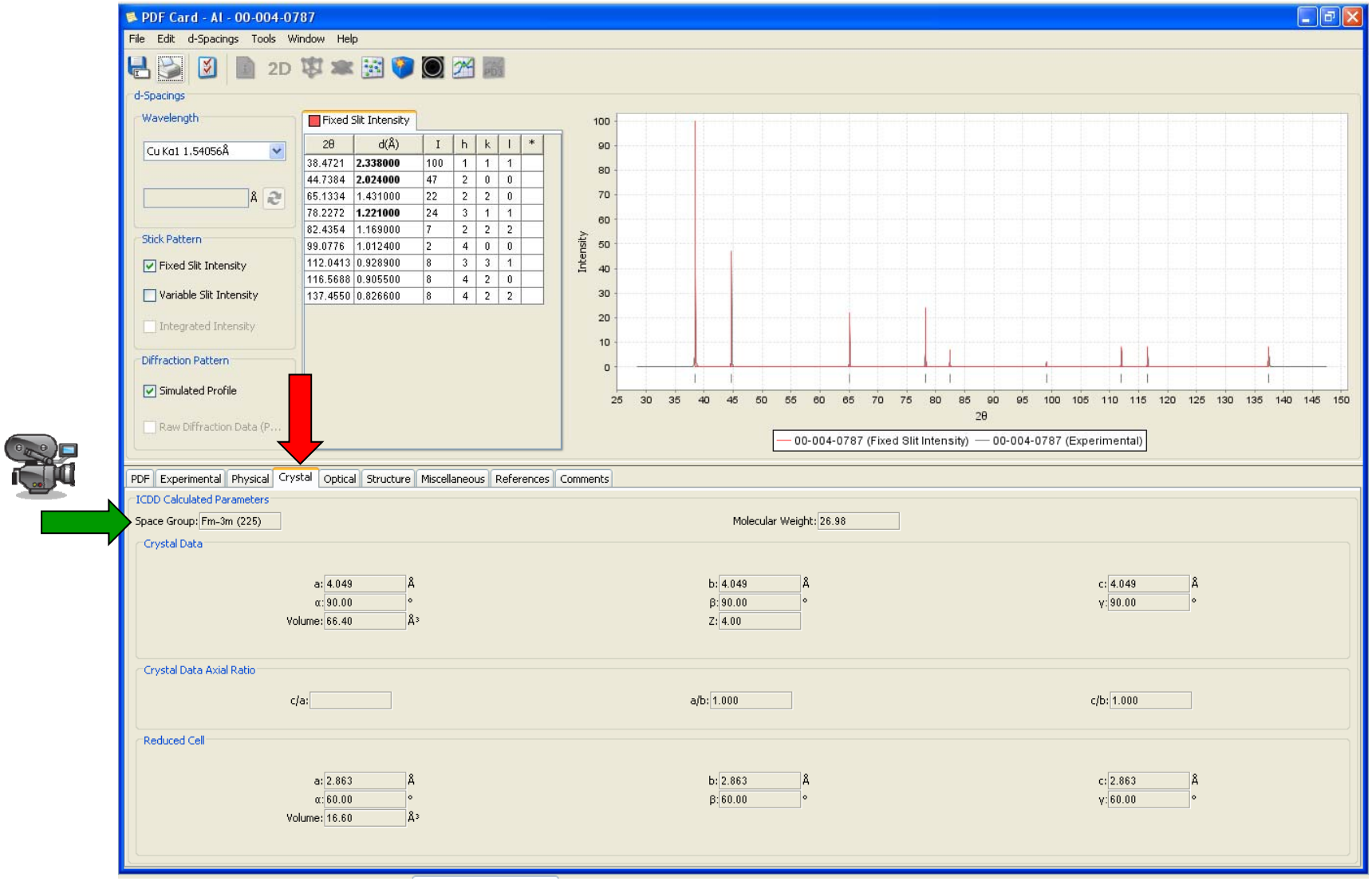
*Tells us everything we need to know about symmetry and motif placement!*

In this class, the first place you'll see this is on X-ray (i.e., ICDD, JCPDS, or PDF) cards.

# ICDD (i.e., JCPDF)card



# ICDD (i.e., JCPDF)card



# ICDD (i.e., JCPDF)card for Al

**00-004-0787** Oct 18, 2011 10:36 AM (CAF User)

**Status** Primary **QM:** Star (S) **Pressure/Temperature:** Ambient **Chemical Formula:** Al **Empirical Formula:** Al
**Weight %:** Al100.00 **Atomic %:** Al100.00 **Compound Name:** Aluminum **Mineral Name:** Aluminum, syn

**Radiation:** CuKα1 **λ:** 1.5406Å **Intensity:** Diffractometer **I/Ic:** 3.62

**SYS:** Cubic **SPGR:** Fm-3m (225)
**Author's Cell [ AuthCell a:** 4.0494Å **AuthCell Vol:** 66.40Å³ **AuthCell Z:** 4.00 **AuthCell MolVol:** 16.60 ]
**Dcalc:** 2.699g/cm³ **SS/FOM:** F(9) = 91.8(0.0109, 9)

**Space Group:** Fm-3m (225) **Molecular Weight:** 26.98
**Crystal Data [ XtlCell a:** 4.049Å **XtlCell b:** 4.049Å **XtlCell c:** 4.049Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 66.40Å³ **XtlCell Z:** 4.00 ] **Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 ]
**Reduced Cell [ RedCell a:** 2.863Å **RedCell b:** 2.863Å **RedCell c:** 2.863Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 16.60Å³ ]

**Crystal (Symmetry Allowed):** Centrosymmetric

**CAS:** 7429-90-5 **Pearson:** cF4.00 **Prototype Structure:** Cu **Prototype Structure (Alpha Order):** Cu
**LPF Prototype Structure:** Cu,cF4,225 **LPF Prototype Structure (Alpha Order):** Cu
**Mineral Classification:** Gold (Supergroup), 1C-disordered (Group)

**Subfile(s):** Primary Pattern, Inorganic, Forensic, Mineral Related (Mineral , Synthetic), Pigment/Dye, Common Phase, Metals & Alloys, Educational Pattern, Explosive, NBS Pattern

**Last Modification Date:** 01/15/2010

**Cross-Ref PDF #'s:**

| | | | |
|---|---|---|---|
| 01-085-1327 (Alternate), | 04-001-0564 (Alternate), | 04-001-1007 (Alternate), | 04-001-7364 (Alternate), |
| 04-002-3717 (Alternate), | 04-002-6895 (Alternate), | 04-002-8919 (Alternate), | 04-003-1376 (Alternate), |
| 04-003-4137 (Alternate), | 04-003-4850 (Alternate), | 04-003-6600 (Alternate), | 04-003-7059 (Alternate), |
| 04-004-2353 (Alternate), | 04-004-8465 (Alternate), | 04-004-8742 (Alternate), | 04-004-8743 (Alternate), |
| 04-005-9305 (Alternate), | 04-006-2586 (Alternate), | 04-006-6522 (Alternate), | 04-007-0410 (Alternate), |
| 04-007-5139 (Alternate), | 04-007-9709 (Alternate), | 04-007-9967 (Alternate), | 04-010-6160 (Alternate), |
| 04-012-3402 (Alternate), | 04-012-3461 (Alternate), | 04-012-7848 (Primary) | |

**Experimental Data Reference:** Swanson, Tatge. Natl. Bur. Stand. (U.S.), Circ. 539 I, 11 (1953).
**Physical Data Reference(s):** Ibid.

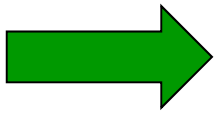
**Database Comments:** Additional Patterns: See PDF 01-085-1327. Analysis: The chemical analysis (%): Si 0.011, Cu 0.006, Fe 0.007, Ti 0.0001, Zr 0.003, Ga 0.004, Mo 0.00002, S 0.0001, Al 99.9+ (by difference). Color: Light gray metallic. General Comments: Mineral species of doubtful validity, Am. Mineral., 65 205 (1980). Sample Preparation: The material used for the NBS sample was a melting point standard sample of aluminum prepared at NBS, Gaithersburg, Maryland, USA. Temperature of Data Collection: Pattern taken at 298 K. Unit Cell Data Source: Powder Diffraction.

**00-004-0787 (Fixed Slit Intensity) - Cu Kα1 1.54056Å**

| 2θ | d(Å) | I | h | k | l | * | 2θ | d(Å) | I | h | k | l | * | 2θ | d(Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 38.4721 | **2.338000** | 100 | 1 | 1 | 1 | | 78.2272 | **1.221000** | 24 | 3 | 1 | 1 | | 112.0413 | 0.928900 | 8 | 3 | 3 | 1 | |
| 44.7384 | **2.024000** | 47 | 2 | 0 | 0 | | 82.4354 | 1.169000 | 7 | 2 | 2 | 2 | | 116.5688 | 0.905500 | 8 | 4 | 2 | 0 | |
| 65.1334 | 1.431000 | 22 | 2 | 2 | 0 | | 99.0776 | 1.012400 | 2 | 4 | 0 | 0 | | 137.4550 | 0.826600 | 8 | 4 | 2 | 2 | |

Space group data allows us to define allowed and missing reflections in a diffraction pattern.

*Tells us everything we need to know about symmetry and motif placement!*

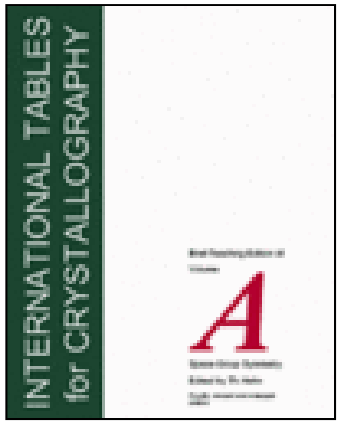


Another place you'll see this is in the International Tables for Crystallography.

# International Tables for Crystallography

From the data tabulated in the International Tables, we can get the following:

- Herman-Mauguin (HM) Symbol (Long, Short)
- Point Group (HM, Schoenflies)
- Location and identification of symmetry elements
- Wyckoff site multiplicity and symmetry
- Location of general and special positions
- Extinction conditions for X-rays
- Possible subgroups and supergroups




You don’t need to worry about some of these things… “yet.”

# RECALL
# Herman – Mauguin (International) Symbol

The HM symbol is derived from the type of Bravais lattice and the symmetry elements present in the crystal.

(Letter) · (primary) · (secondary) · (tertiary)

Each letter describes centering present in the lattice:

| | |
|---|---|
| P – Primitive | I – Body centered |
| C – C-centered | F – Face centered |
| B – B-centered | R – Rhombohedral |
| A – A-centered | H – Hexagonal |

*See the next viewgraph.*

## Space Group Letter Symbols

| Letter symbol | Lattice type | Number of lattice points per unit cell | "Centering" Coordinates of lattice points |
|---|---|---|---|
| *P* | P | 1 | 0,0,0 |
| *A* | *A*-face centered | 2 | 0, 0, 0 ; 0, ½, ½ |
| *B* | *B*-face centered | 2 | 0, 0, 0 ; ½, 0, ½ |
| *C* | *C*-face centered | 2 | 0, 0, 0 ; ½, ½, 0 |
| *I* | Body centered | 2 | 0, 0, 0 ; ½, ½, ½ |
| *F* | Face centered (all) | 4 | 0, 0, 0 ; ½, ½, 0 ; ½, 0, ½ ; 0, ½, ½ |
| *R* | Primitive (Rhombohedral axes) | 1 | 0, 0, 0 |
| | Centered (Hexagonal axes) | 3 | 0, 0, 0 ; ⅔, ⅓, ⅓ ; ⅓, ⅔, ⅔ (obverse setting)<br>0, 0, 0 ; ⅓, ⅔, ⅓ ; ⅔, ⅓, ⅔ (reverse setting) |
| *H* | Centered Hexagonal | 3 | 0, 0, 0 ; ⅔, ⅓, 0 ; ⅓, ⅔, 0 |

We use specific symbols to denote crystal systems ….

# The next three symbols denote symmetry elements present in certain directions:

| Crystal System | Symmetry Direction | | |
|---|---|---|---|
| | **Primary** | **Secondary** | **Tertiary** |
| Triclinic | None | | |
| Monoclinic* | [010] | | |
| Orthorhombic | [100] | [010] | [001] |
| Tetragonal | [001] | [100]/[010] | [110] |
| Hexagonal/ Trigonal | [001] | [100]/[010] | [120]/[1(-1)0] |
| Cubic | [100]/[010]/ [001] | [111] | [110] |

* For this structure list primary in secondary slot.
Place “1” in primary and tertiary slots for Long notation.

The bracketed numbers
on the previous page represent
directions originating from the crystal origin:

[100] – Axis parallel or plane perpendicular to the *a*-axis.

[010] – Axis parallel or plane perpendicular to the *b*-axis.

[001] – Axis parallel or plane perpendicular to the *c*-axis.

[110] – Axis parallel or plane perpendicular to the line running at 45° to the *a*-axis and *b*-axis.

$[1\bar{1}0]$ – Axis parallel or plane perpendicular to the long face diagonal of the *ab* face of a hexagonal cell.

[111] – Axis parallel or plane perpendicular to the body diagonal.

# Symmetry elements in space group symbols

| Symbol | Lattice type | Comments |
|---|---|---|
| $m$ | Mirror plane | reflection |
| $a$ | Axial glide plane $\perp$ [010],[001] | Glide vector $a/2$ |
| $b$ | Axial glide plane $\perp$ [001],[100] | Glide vector $b/2$ |
| $c$ | Axial glide plane $\perp$ [100],[010] | Glide vector $c/2$ |
| | $\perp$ $[1\bar{1}0]$,[110] | Glide vector $c/2$ |
| | $\perp$ [100],[010],$[\bar{1}\bar{1}0]$ | Glide vector $c/2$, hexagonal axes |
| | $\perp$ $[1\bar{1}0]$,[120],$[\bar{2}\bar{1}0]$,$[\bar{1}\bar{1}0]$ | Glide vector $c/2$, hexagonal axes |
| $n$ | Diagonal glide plane $\perp$ [001]; [100]; [010] | Glide vector $\frac{1}{2}(a+b)$; $\frac{1}{2}(b+c)$; $\frac{1}{2}(a+c)$ |
| | Diagonal glide plane $\perp$ $[1\bar{1}0]$; $[01\bar{1}]$; $[\bar{1}01]$ | Glide vector $\frac{1}{2}(a+b+c)$; $\frac{1}{2}(a+c)$ |
| | Diagonal glide plane $\perp$ [110]; [011]; [101] | Glide vector $\frac{1}{2}(-a+b+c)$; $\frac{1}{2}(a-b+c)$; $\frac{1}{2}(a+b-c)$ |
| $d$ | Diamond glide plane $\perp$ [001]; [100]; [010] | Glide vector $\frac{1}{4}(a\pm b)$; $\frac{1}{4}(b\pm c)$; $\frac{1}{4}(a\pm c)$ |
| | Diamond glide plane $\perp$ $[1\bar{1}0]$; $[01\bar{1}]$; $[\bar{1}01]$ | Glide vector $\frac{1}{4}(a+b\pm c)$; $\frac{1}{4}(\pm a+b+c)$; $\frac{1}{4}(a\pm b+c)$ |
| | Diamond glide plane $\perp$ [110]; [011]; [101] | Glide vector $\frac{1}{4}(-a+b\pm c)$; $\frac{1}{4}(\pm a-b+c)$; $\frac{1}{4}(a\pm b-c)$ |
| 1 | None | – – – |
| 2, 3, 4, 6 | $n$ – fold rotation axis | A counter clockwise rotation of $360°/n$ |
| $\bar{1}$ | Center of symmetry | – – – |
| $\bar{2}=m$, $\bar{3}$, $\bar{4}$, $\bar{6}$ | $\bar{n}$ – fold rotoinversion axis | A counter clockwise rotation of $360°/n$ followed by inverstion |
| $2_1$, $3_1$, $3_2$, $4_1$, $4_2$, $4_3$, $6_1$, $6_2$, $6_3$, $6_4$, $6_5$ | $n$ – fold screw axis, $n_p$ | A counter clockwise right-handed screw rotation of $360°/n$ followed by translation by $(p/n)T$ |

**We use specific symbols to denote internal symmetry.**

# The full Herman-Mauguin symbol shows:

- Both rotation/screw axes running parallel to the specified direction.
- Any mirror/glide plane perpendicular to the same direction.

or

- The two symbols separated by a forward slash (/)

Some examples:

| | | | |
|---|---|---|---|
| C | 1 | 2/m | 1 |
| P | $2_1$ | $2_1$ | 2 |
| P | 2/m | 2/n | $2_1$/a |
| I | $4_1$/a | 2/m | 2/d |
| P | $6_3$/m | 2/m | 2/c |
| F | 4/m | 3 | 2/m |

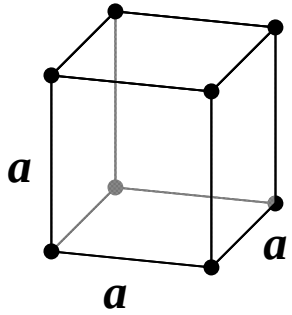
# The short Herman-Mauguin symbol

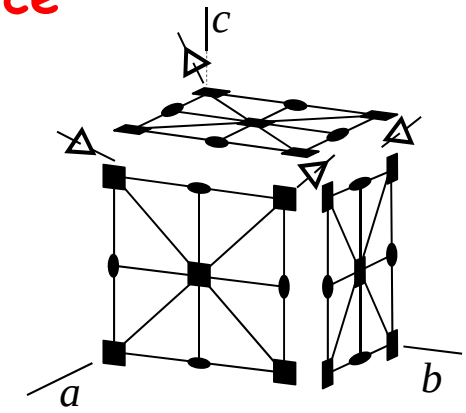
- Short HM symbols contain only the mirror/glide plane components for primary, secondary and tertiary directions.
- If no mirror/glide plane, contains the rotation/screw axis.
- In certain cases (monoclinic, tetragonal and hexagonal), both the rotation/screw axis and the mirror/glide plane are retained for the primary direction only.

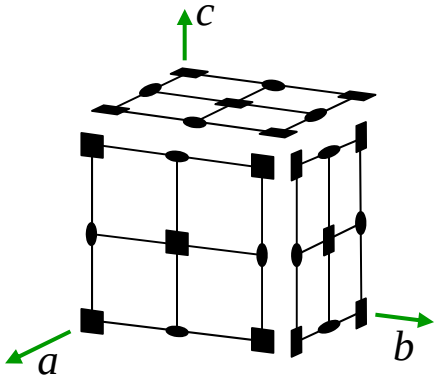
| Long | Short |
|---|---|
| C 1 2/m 1 | **C2/m** |
| P $2_1$ $2_1$ 2 | **P$2_12_12$** |
| P 2/m 2/n $2_1$/a | **Pmna** |
| I $4_1$/a 2/m 2/d | **I$4_1$/amd** |
| P $6_3$/m 2/m 2/c | **P$6_3$/mmc** |
| F 4/m 3 2/m | **Fm3m** |

# Symmetry of a Cubic *P*-Lattice

P $4/m$ $\bar{3}$ $2/m$ LONG
$\langle 100 \rangle$ $\langle 111 \rangle$ $\langle 110 \rangle$
P $m$ $\bar{3}$ $m$ SHORT

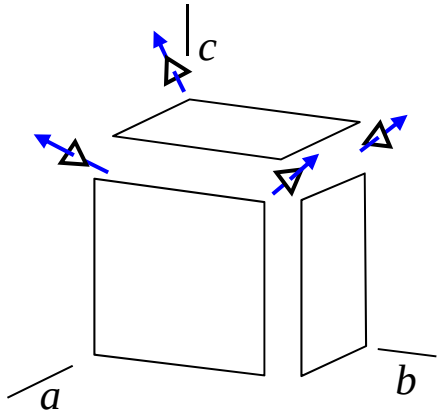


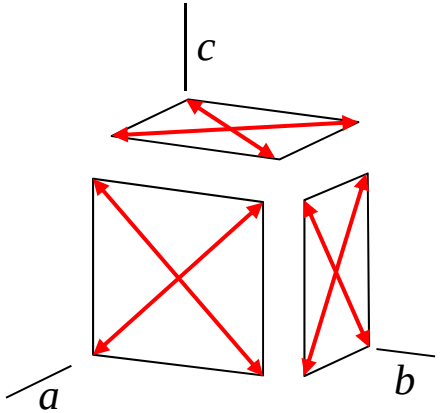

P $4/m$
$\langle 100 \rangle$

**Primary**




P ...$\bar{3}$...
$\langle 111 \rangle$

**Secondary**



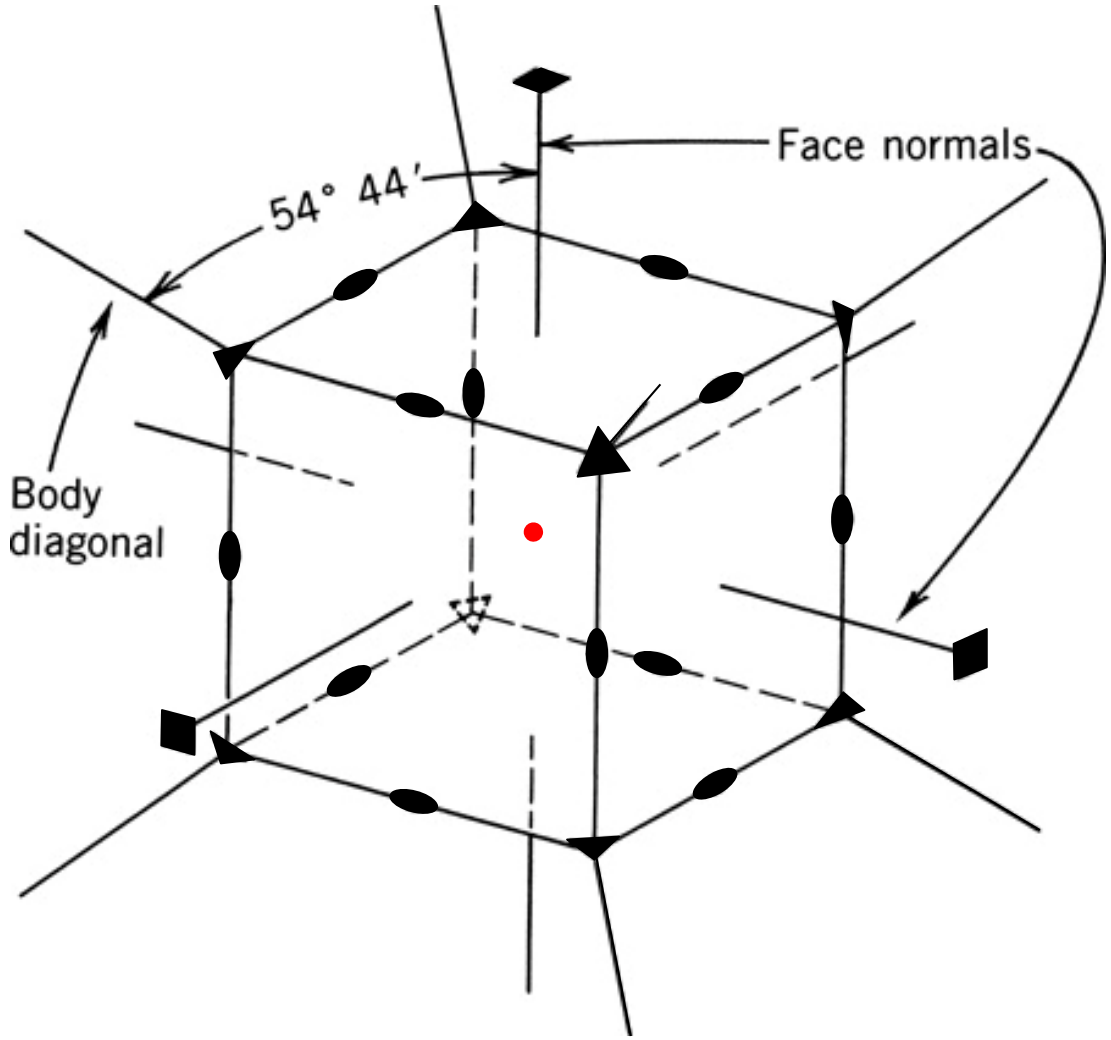

P ....$2/m$
$\langle 110 \rangle$

**Tertiary**

Fig. (a) Cubic unit cell. (b) Space group P $4/m$ $\bar{3}$ $2/m$. In diagrams (c), (d) and (e), only the symetry elements corresponding to the symmetry directions <100>, <111>, <110> are shown.

P $4/m$ $\bar{3}$ $2/m$.
$\langle 100 \rangle$ $\langle 111 \rangle$ $\langle 110 \rangle$

Adapted from W. Borchardt-Ott, *Crystallography, 2nd Edition*, Springer, Berlin, Germany, 1995, p. 99




3 tetrad axes

4 triad axes

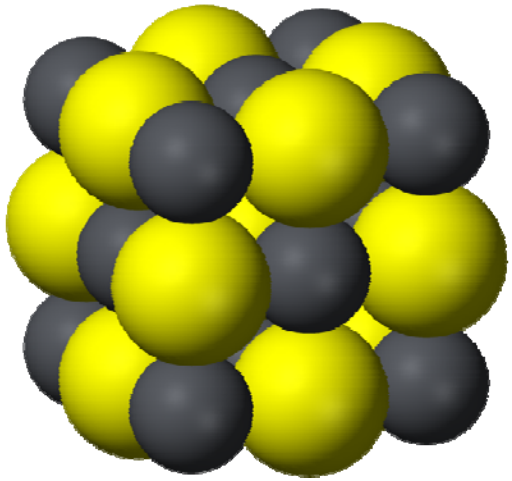
6 diad axes

9 mirror planes
(hidden)

**Fig. 6.18** The location of 4-, 3-, and 2-fold symmetry axes with respect to a cubic outline for 432. Note that the axes connect symbols on the opposite sides of the crystal and run through the center. Adapted from C. Klein and B. Dutrow, Manual of Mineral Science, 23rd Edition (John Wiley & Sons, 2007)

# Galena (PbS)

http://crystal-cure.com/pics/galena.jpg



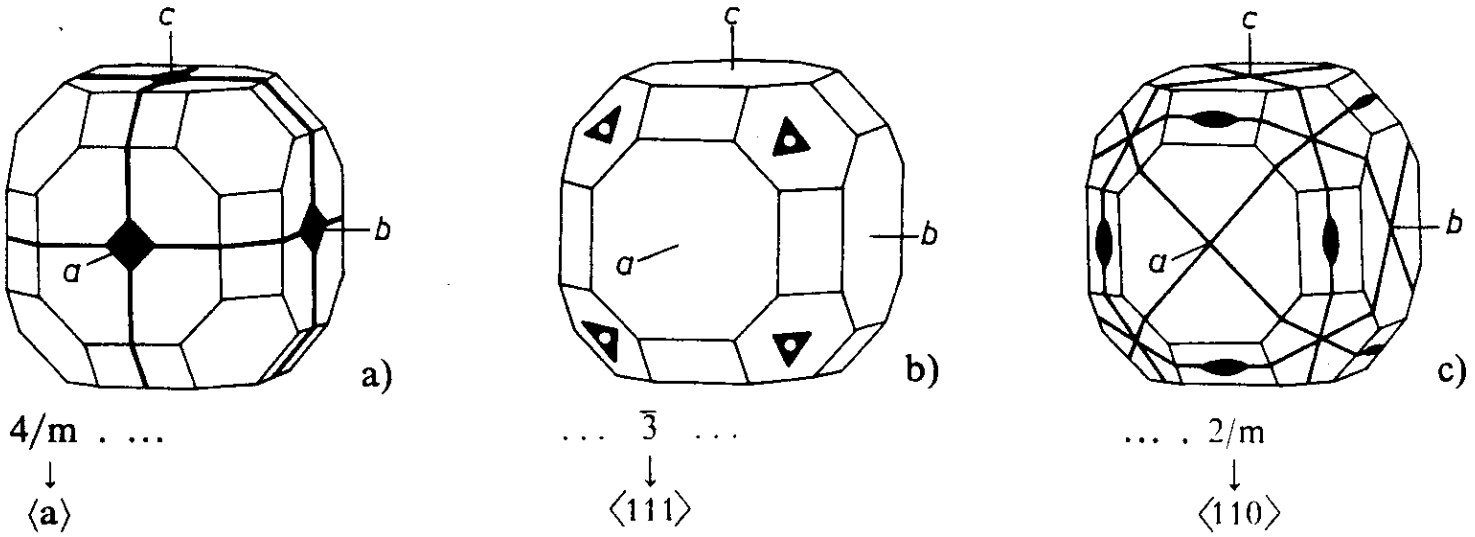
http://en.wikipedia.org/wiki/File:Galena-unit-cell-3D-ionic.png

$4/m\ \bar{3}\ 2/m$

F$m$3$m$

http://www.minservice.com/cartshop3/catalog/FERR0240_galena_p.jpg

# Crystal Forms



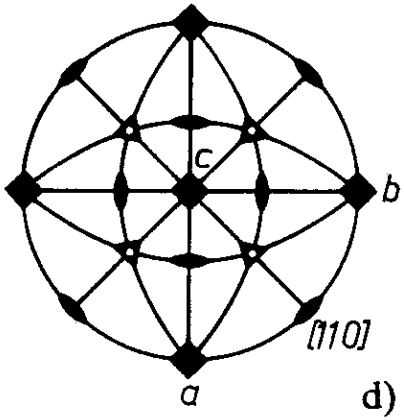
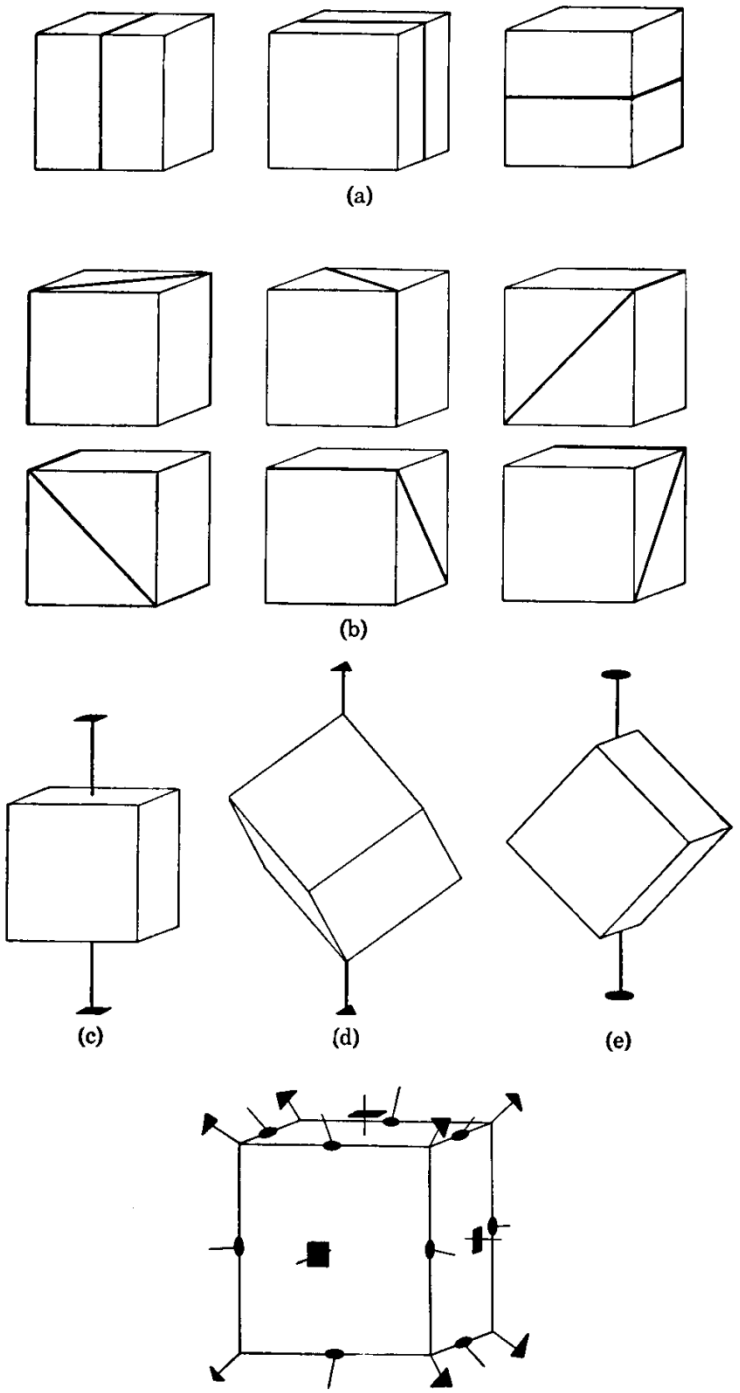




**Fig. 8.4a–d.** A galena crystal in point group 4/m $\bar{3}$ 2/m.
↓ ↓ ↓
⟨a⟩ ⟨111⟩ ⟨110⟩

In **a**, only those symmetry elements which relate to the a-axis and equivalent directions (i.e. the b- and c-axes) have been drawn in (4/m → ⟨a⟩); in **b**, only those relating to the [111] and equivalent directions ($\bar{3}$ → ⟨111⟩); in **c**, only those relating to the [110] and equivalent directions (2/m → ⟨110⟩). The stereogram of the symmetry elements is given in **d**

Adapted from W. Borchardt-Ott, *Crystallography, 2nd Edition*, Springer, Berlin, Germany, 1995, p. 124

**Fig. 1.9.** (a) the three planes of symmetry parallel to the faces of a cube. (b) The six diagonal planes of symmetry of a cube. (c) One of the tetrad axes of a cube. (d) one of the triad axes of a cube. (e) one of the diad axes of a cube. (f) The thirteen axes of symmetry shown by a cube. From C. Kittel, Introduction to Solid State Physics, 2nd Edition, (John Wiley & Sons, New York, 1959) p. 23.



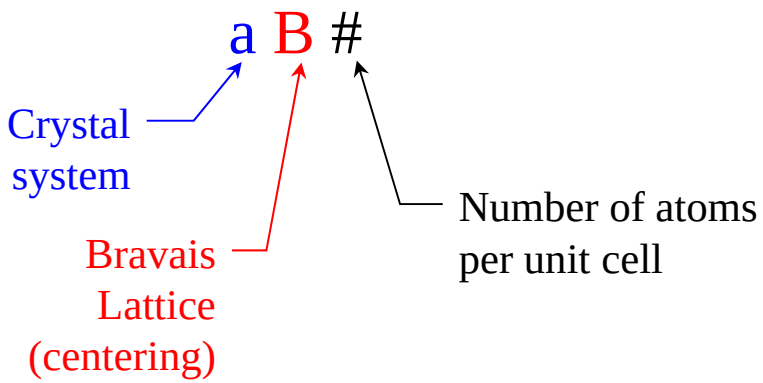
# How do we identify the crystal system from a HM symbol?

- **Cubic** - Secondary symmetry symbol 3 or $\bar{3}$ (i.e. I*a*3, P*m*3*m*, Fd3*m*)
- **Tetragonal** - Primary symmetry symbol 4, $\bar{4}$, $4_1$, $4_2$ or $4_3$ (i.e. $P4_12_12$, I4/*m*, P4/*mcc*)
- **Hexagonal** - Primary symmetry symbol 6, $\bar{6}$, $6_1$, $6_2$, $6_3$ or $6_5$ (i.e. P6*mm*, $P6_3/m3m$)
- **Trigonal** - Primary symmetry symbol 3, $\bar{3}$, $3_1$, or $3_2$ (i.e. P31*m*, R3, R3*c*, P312)
- **Orthorhombic** - All three symbols following the lattice descriptor are mirror planes, glide planes, 2-fold rotation or screw axes (i.e. P*nma*, $Cmc2_1$, P*nc*2)
- **Monoclinic** - Lattice descriptor followed by a single mirror plane, glide plane, 2-fold rotation or screw axis or an axis/plane symbol (i.e. C*c*, P2, $P2_1/n$)
- **Triclinic** - Lattice descriptor followed by either a 1 or $\bar{1}$

# Pearson Symbols

- W.B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys,* Wiley-Interscience, New York, 1972.

- Classification of structures based on:
  - Crystal system
  - Bravais lattice
  - Number of atoms per unit cell



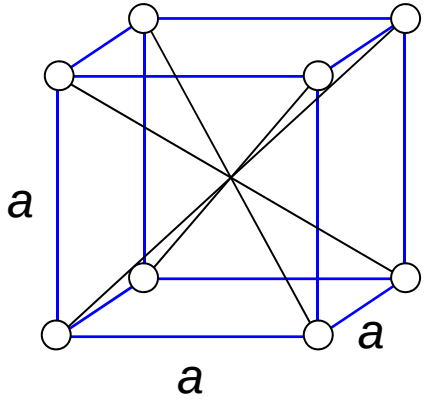
# Notation for Crystal Structures – cont'd

*Symbols for the 14 Bravais Lattices*

| Symbol | System | Lattice Symbol |
|---|---|---|
| **aP** | Triclinic | P |
| **mP** | Simple monoclinic | P |
| **mC** | Base-centered monoclinic | C |
| **oP** | Simple orthorhombic | P |
| **oC** | Base-centered orthorhombic | C |
| **oF** | Face-centered orthorhombic | F |
| **oI** | Body-centered orthorhombic | I |
| **tP** | Simple tetragonal | P |
| **tI** | Body-centered tetragonal | I |
| **hP** | Hexagonal | P |
| **hR** | Rhombohedral | R |
| **cP** | Simple cubic | P |
| **cF** | Face-centered cubic | F |
| **cI** | Body-centered cubic | I |

# Pearson Symbols for Some Typical Crystal Structures

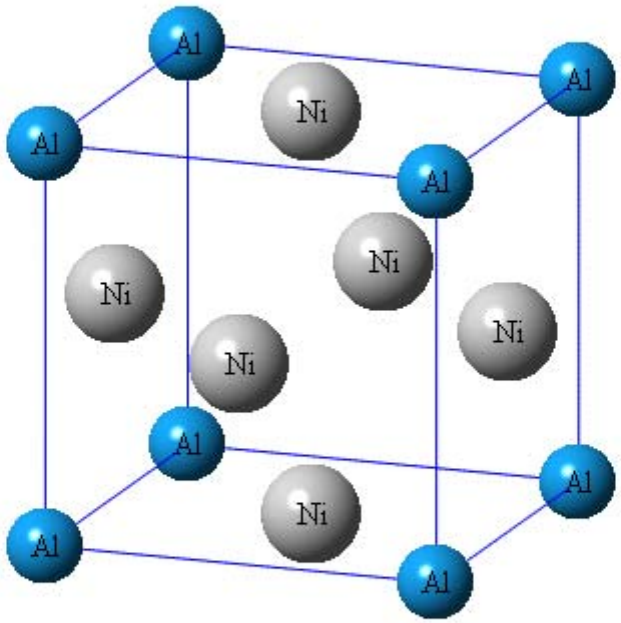
| Crystal structure | Pearson Symbol |
|---|---|
| Simple cubic | cP1 |
| Body-centered cubic | cI2 |
| Face-centered cubic | cF4 |
| Hexagonal close-paced | hP2 |
| CsCl | cP2 |
| NaCl | cF8 |
| Diamond cubic | cF8 |
| Zinc blende | cF8 |
| Fluorite | cF12 |

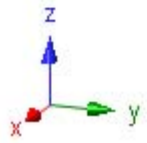



⇐ cP1

# What's the Pearson symbol for this one?

$AlNi_3$



# Strukturbericht

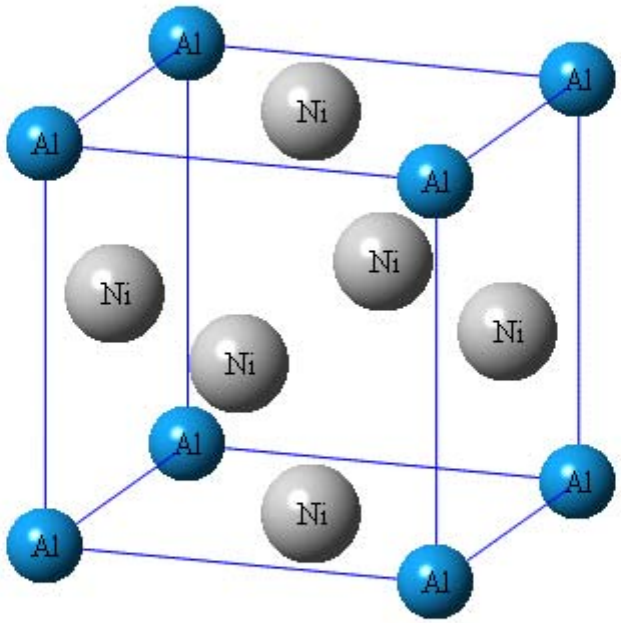
- Symbols designate the type of crystal structure.
  - A – elements;
  - B – AB type compounds (i.e., composition near 50-50 at.%);
  - C – $AB_2$ compounds;
  - D - $A_mB_n$ compounds;
  - E, F, G, H ⋯ K – More complex compounds ;
  - L – Alloys;
  - O – Organic compounds ;
  - S – Silicates.

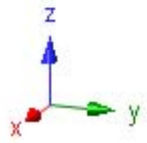
- Many visual examples can be viewed at:
  - http://cst-www.nrl.navy.mil/lattice/struk/index.html

- This system is inconsistent. For example, TiAl is denoted as $L1_0$ even though it has AB stoichiometry (see the next viewgraph).

# What's the Strukturbericht symbol for this one?
# What is the international symbol for this one?

$AlNi_3$



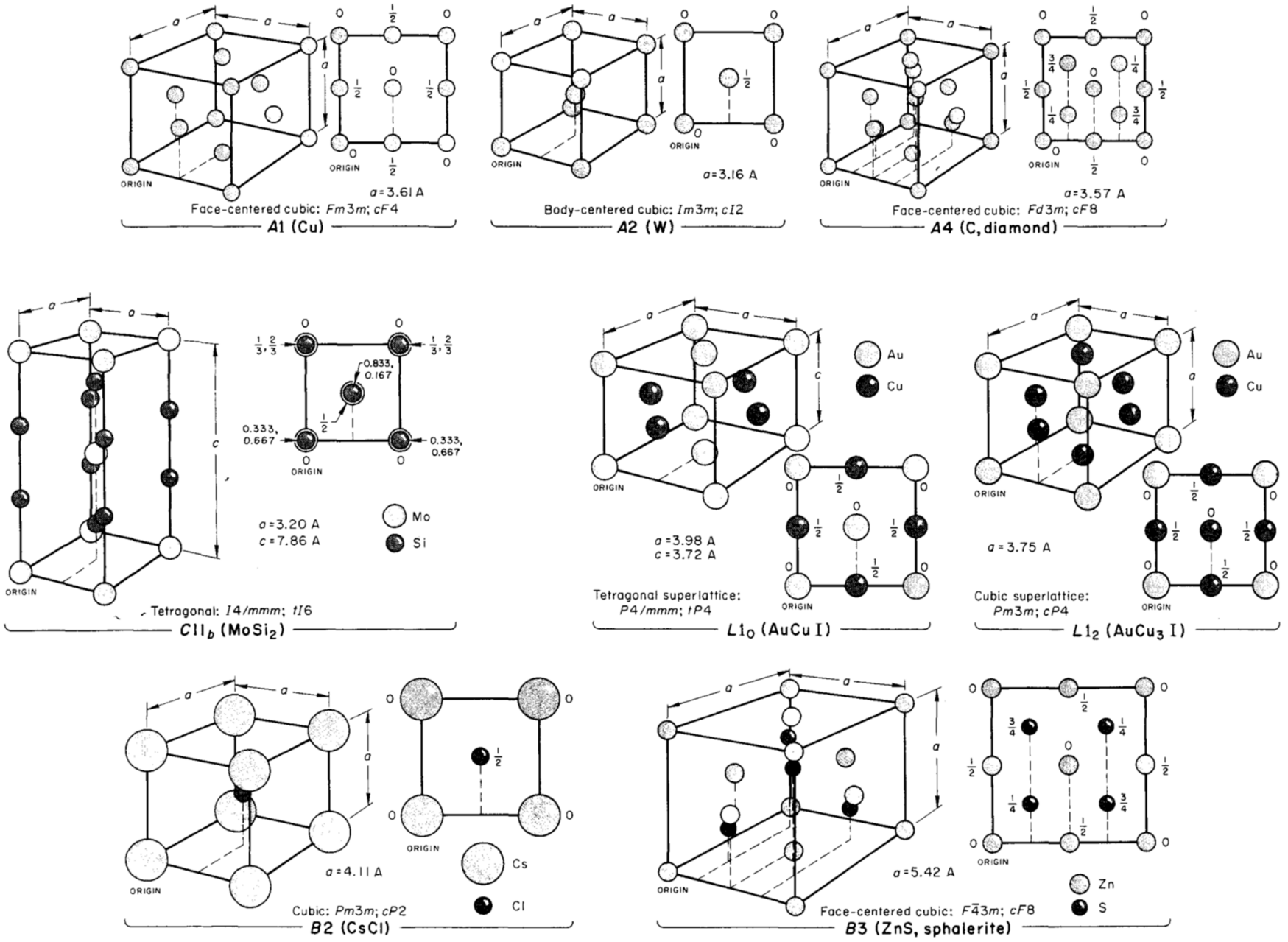



***Fig. 1. Atom positions, structure symbols, prototypes, space-group notations, Pearson symbols, and lattice parameters for some of the simple metallic crystals*** (continued on next two pages)

Excerpt from C.S. Barrett, “Crystal Structure of Metals,” in *ASM Handbook, 8th Edition*, vol. 8 (1973), ASM International, Metals Park, OH, pp. 233-250.

*A1* Copper type. Face-centered cubic: *Fm3m*; *cF*4. Four atoms per cell, at 0,0,0; ½,0,½; 0,½,½ and ½,½,0. For Cu, $a$ = 3.61 A. See Fig. 1. **Examples:** Ag, Al, Au, $\alpha$-Ca, $\alpha$-Ce, $\beta$-Co, Cu, $\gamma$-Fe, Ir, Ni, Pb, Pd, Pt, Rh, $\alpha$-Sr, $\alpha$-Th.

*A2* Tungsten type. Body-centered cubic: *Im3m*; *cI*2. Two atoms per cell, at 0,0,0 and ½,½,½. For W, $a$ = 3.16 A. See Fig. 1. **Examples:** Ba, Cb, Cr, Cs, $\beta$ Cu-Zn (HT), $\alpha$-Fe, $\delta$-Fe, K, $\beta$-Li, Mo, $\beta$-Na, Rb, Ta, V, W.

*A4* Carbon (diamond) type. Face-centered cubic: *Fd3m*; *cF*8. Eight atoms per cell, at 0,0,0; 0,½,½; ½,0,½; ½,½,0; ¼,¼,¼; ¼,¾,¾; ¾,¼,¾ and ¾,¾,¼. For C (diamond), $a$ = 3.57 A. See Fig. 1. **Examples:** C (diamond), Ge, Si, $\alpha$-Sn.

*C11$_b$* $MoSi_2$ type. Tetragonal: *I*4/*mmm*; *tI*6. Two molybdenum atoms at 0,0,0 and ½,½,½; four silicon atoms at 0,0,$z$; 0,0,$\bar{z}$; ½,½,½+$z$ and ½,½,½−$z$ (with $z$ = 0.333). For $MoSi_2$, $a$ = 3.20 A and c = 7.86 A. See Fig. 1. **Examples:** $AgZr_2$, $AlCr_2$, $Au_2Be$, $Au_2Mn$, $CuTi_2$, $Hg_2Mg$, $MoSi_2$, $Ni_2Ta$, $Si_2W$.

*L1$_0$* AuCu I type. Tetragonal superlattice: *P*4/*mmm*; *tP*4. Two gold atoms at 0,0,0 and ½,½,0; two copper atoms at 0,½,½ and ½,0,½. See Fig. 1. **Examples:** AgTi, AlTi, AuCu I, $\theta$ CdPt, FePd, $\gamma''$ FePt, $\theta$ MnNi, NiPt.

*L1$_2$* $AuCu_3$ I type. Cubic superlattice: *Pm3m*; *cP*4. One gold atom at 0,0,0; three copper atoms at 0,½,½; ½,0,½ and ½,½,0. See Fig. 1. **Examples:** $\alpha'$ $AlNi_3$, $AlZr_3$, $Au_3Cu$, $AuCu_3$ I, $CoPt_3$, $Cr_3Pt$, $Fe_3Ga$, $FePd_3$, $Ni_3Fe$, $Ni_3Mn$, $Sn_3U$.

*B2* CsCl or $\beta'$ Cu-Zn type. Cubic: *Pm3m*; *cP*2. One cesium atom at 0,0,0; and one chlorine atom at ½,½,½. For CsCl, $a$ = 4.11 A. See Fig. 1. **Examples:** AgCd, CoTi, CsCl, FeAl, FeCo, FeTi, FeV, $\beta$ NiAl, $\beta$ NiGa, $\delta$ NiIn, NiTi, $\beta'$ Cu-Zn.

*B3* ZnS (sphalerite, or zinc blende) type. Face-centered cubic: $F\bar{4}3m$; *cF*8. Four zinc atoms at 0,0,0; 0,½,½; ½,0,½ and ½,½,0; four sulfur atoms at ¼,¼,¼; ¼,¾,¾; ¾,¼,¾ and ¾,¾,¼. For ZnS (sphalerite), $a$ = 5.42 A. See Fig. 1. **Examples:** CdS, CdSe, CdTe, $CuFeS_2$ (HT), GaP, GaSb, InAs, InP, InSb, $\beta$ MnS, $\beta$ SiC, ZnO, ZnS (sphalerite), ZnSe.

Excerpt from C.S. Barrett, “Crystal Structure of Metals,” in *ASM Handbook, 8th Edition*, vol. 8 (1973), ASM International, Metals Park, OH, pp. 233-250.

A very good place to look for crystallography data is the Bilbao Crystallographic Server

http://www.cryst.ehu.es/