Approfondimento Lezione 5

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1. The periodic Table - Crystal Structure

V·T·E

Crystal structure of elements in the periodic table

https://en.wikipedia.org/wiki/Periodic_table_(crystal_structure)

1 H HEX																	2 He HCP
3 Li BCC	4 Be HCP											5 B RHO	6 C HEX	7 N HEX	8 O SC	9 F SC	10 Ne FCC
11 Na BCC	12 Mg HCP											13 Al FCC	14 Si DC	15 P ORTH	16 S ORTH	17 Cl ORTH	18 Ar FCC
19 K BCC	20 Ca FCC	21 Sc HCP	22 Ti HCP	23 V BCC	24 Cr BCC	25 Mn BCC	26 Fe BCC	27 Co HCP	28 Ni FCC	29 Cu FCC	30 Zn HCP	31 Ga ORTH	32 Ge DC	33 As RHO	34 Se HEX	35 Br ORTH	36 Kr FCC
37 Rb BCC	38 Sr FCC	39 Y HCP	40 Zr HCP	41 Nb BCC	42 Mo BCC	43 Tc HCP	44 Ru HCP	45 Rh FCC	46 Pd FCC	47 Ag FCC	48 Cd HCP	49 In TETR	50 Sn TETR	51 Sb RHO	52 Te HEX	53 I ORTH	54 Xe FCC
55 Cs BCC	56 Ba BCC	57* La DHCP	72 Hf HCP	73 Ta BCC/TETR	74 W BCC	75 Re HCP	76 Os HCP	77 Ir FCC	78 Pt FCC	79 Au FCC	80 Hg RHO	81 Tl HCP	82 Pb FCC	83 Bi RHO	84 Po SC/RHO	85 At [FCC]	86 Rn FCC
87 Fr [BCC]	88 Ra BCC	89** Ac FCC	104 Rf [HCP]	105 Db [BCC]	106 Sg [BCC]	107 Bh [HCP]	108 Hs [HCP]	109 Mt [FCC]	110 Ds [BCC]	111 Rg [BCC]	112 Cn [HCP]	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og [FCC]

*	58 Ce DHCP/FCC	59 Pr DHCP	60 Nd DHCP	61 Pm DHCP	62 Sm RHO	63 Eu BCC	64 Gd HCP	65 Tb HCP	66 Dy HCP	67 Ho HCP	68 Er HCP	69 Tm HCP	70 Yb FCC	71 Lu HCP
**	90 Th FCC	91 Pa TETR	92 U ORTH	93 Np ORTH	94 Pu MON	95 Am DHCP	96 Cm DHCP	97 Bk DHCP	98 Cf DHCP	99 Es FCC	100 Fm [FCC]	101 Md [FCC]	102 No [FCC]	103 Lr [HCP]

- BCC: body centered cubic
- FCC: face centered cubic (cubic close packed)
- HCP: hexagonal close packed
- DHCP: double hexagonal close packed
- ORTH: orthorhombic
- TETR: tetragonal
- RHO: rhombohedral
- HEX: hexagonal
- SC: simple cubic
- DC: diamond cubic
- MON: monoclinic
- unknown or uncertain

1. Piani cristallini e Indici di Miller

Distanze tra piani e indici di Miller (***hkl***)

Formule per il calcolo della distanza tra piani (d_{hkl}) per famiglie di piani con indici di Miller **hkl** in una cella unitaria con parametri **a**, **b**, **c**, **α**, **β**, **γ**. Le barre verticali (triclinico) indicano il determinante «della matrice . Nel caso trigonale **a=b=c=A**; **α=β=γ**.

Orthorhombic

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Tetragonal

$$\frac{1}{d_{hkl}^2} = \left[h^2 + k^2 + l^2\left(\frac{a}{c}\right)^2\right]\frac{1}{a^2}$$

Cubic

$$\frac{1}{d_{hkl}^2} = (h^2 + k^2 + l^2)\frac{1}{a^2}$$

Monoclinic

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2 \sin^2\gamma} + \frac{k^2}{b^2 \sin^2\gamma} - \frac{2hk\cos\gamma}{ab\sin^2\gamma} + \frac{l^2}{c^2}$$

Hexagonal

$$\frac{1}{d_{hkl}^2} = \left[\frac{4}{3}(h^2 + k^2 + hk) + l^2\left(\frac{a}{c}\right)^2\right]\frac{1}{a^2}$$

Triclinic

$$\frac{1}{d_{hkl}^2} = \begin{bmatrix} \frac{h}{a} & \cos\gamma & \cos\beta \\ \frac{k}{b} & 1 & \cos\alpha \\ \frac{l}{c} & \cos\alpha & 1 \end{bmatrix} + \frac{k}{b}\begin{vmatrix} 1 & \frac{h}{a} & \cos\alpha \\ \cos\gamma & \frac{k}{b} & \cos\alpha \\ \cos\beta & \frac{l}{c} & 1 \end{vmatrix} + \frac{l}{c}\begin{vmatrix} 1 & \cos\gamma & \frac{h}{a} \\ \cos\gamma & 1 & \frac{k}{b} \\ \cos\beta & \cos\alpha & \frac{l}{c} \end{vmatrix} \cdot \begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}^{-1}$$

Trigonal (rhombohedral)

$$\frac{1}{d_{hkl}^2} = \left[(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + lh)(\cos^2\alpha - \cos\alpha)\right]\frac{1}{A^2(1 + 2\cos^3\alpha - 3\cos^2\alpha)}$$

Visitate i link :

https://www.doitpoms.ac.uk/tlplib/miller_indices/index.php

https://www.doitpoms.ac.uk/tlplib/xray-diffraction/index.php

https://www.doitpoms.ac.uk/tlplib/reciprocal_lattice/index.php

https://www.doitpoms.ac.uk/tlplib/crystallographic_texture/index.php

Per visualizzare i concetti di indici di Miller, piani cristallini, spazio reciproco, diffrazione X, cristallografia nei materiali policristallini, ed effettuare utili esercizi online.