

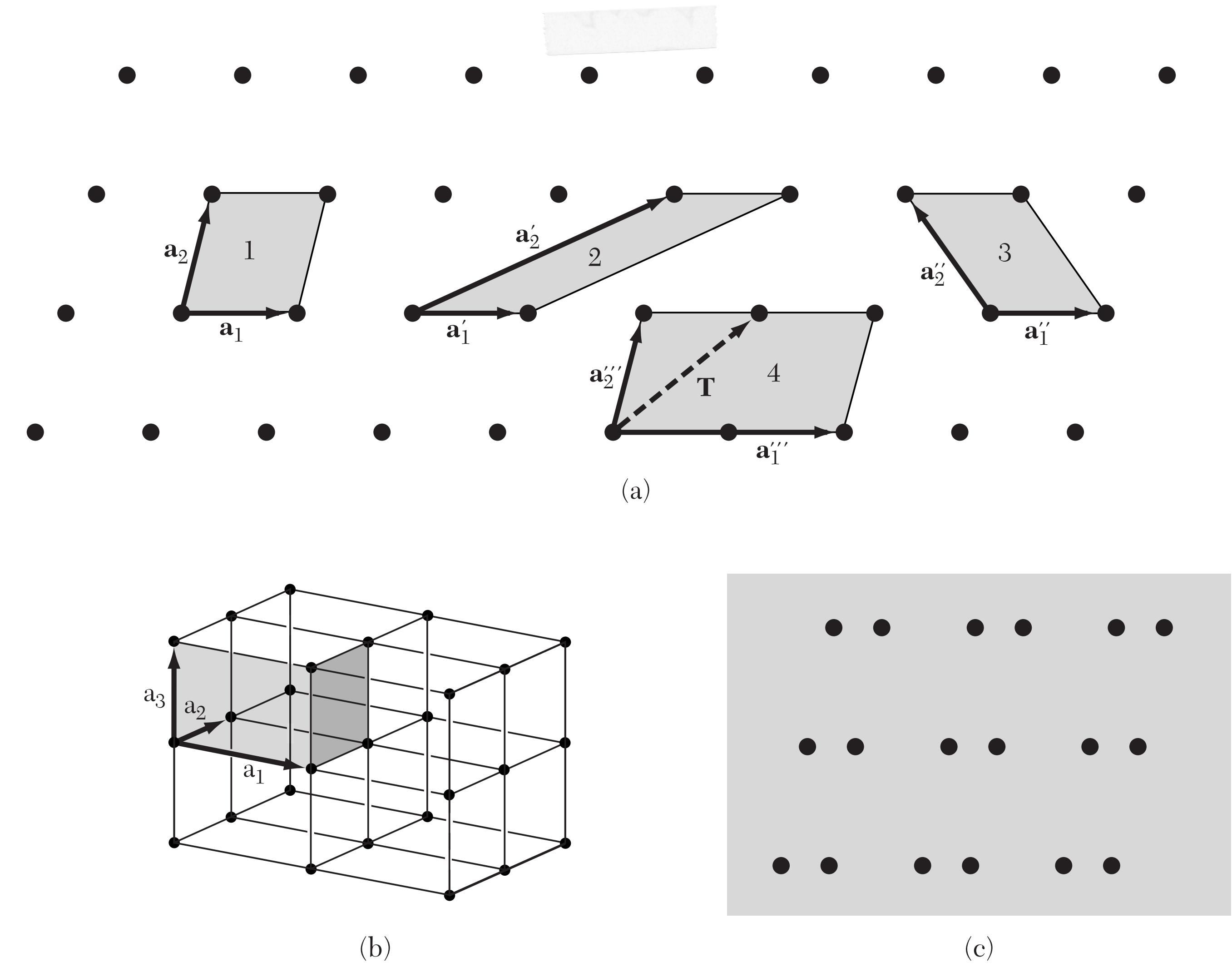
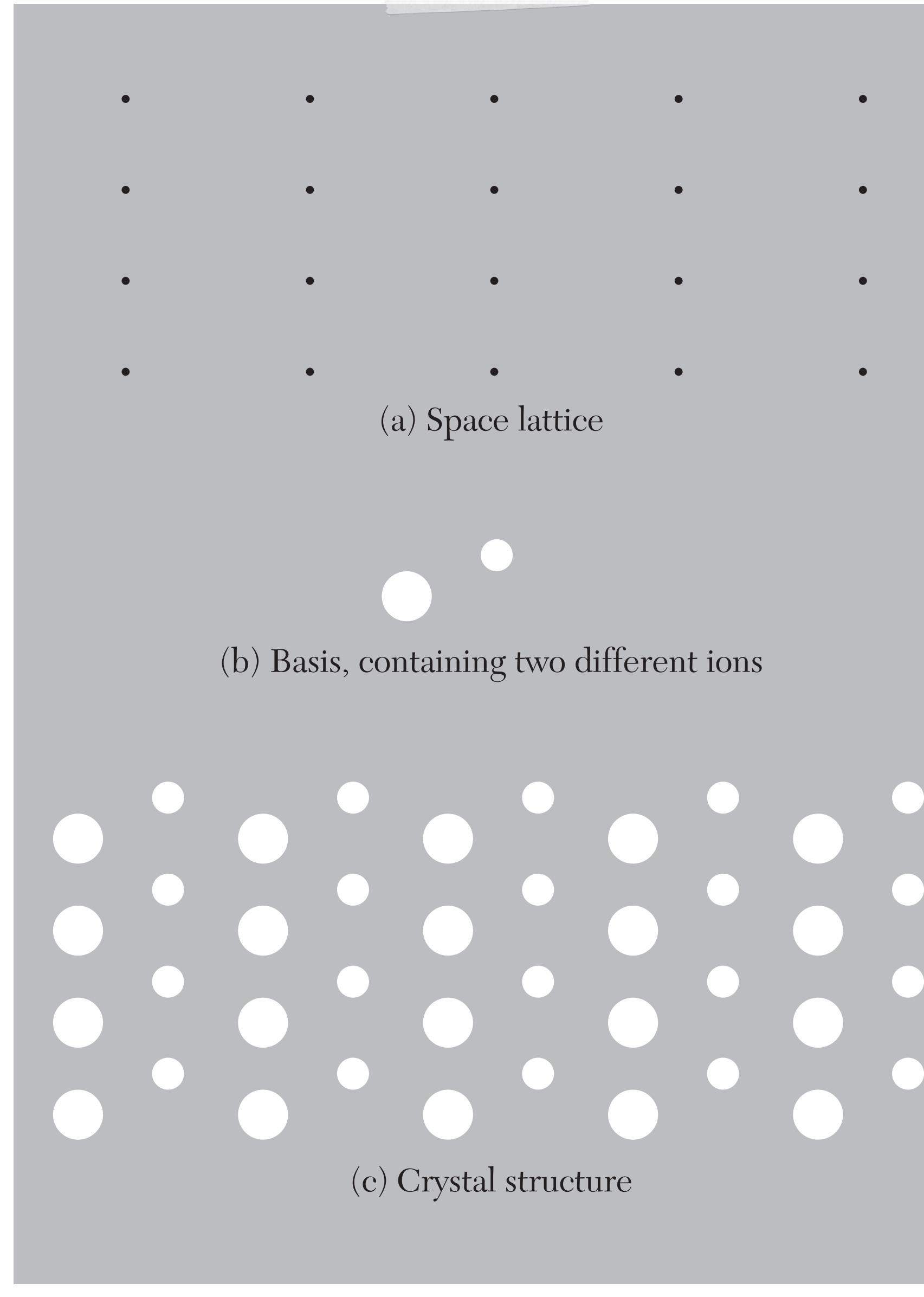


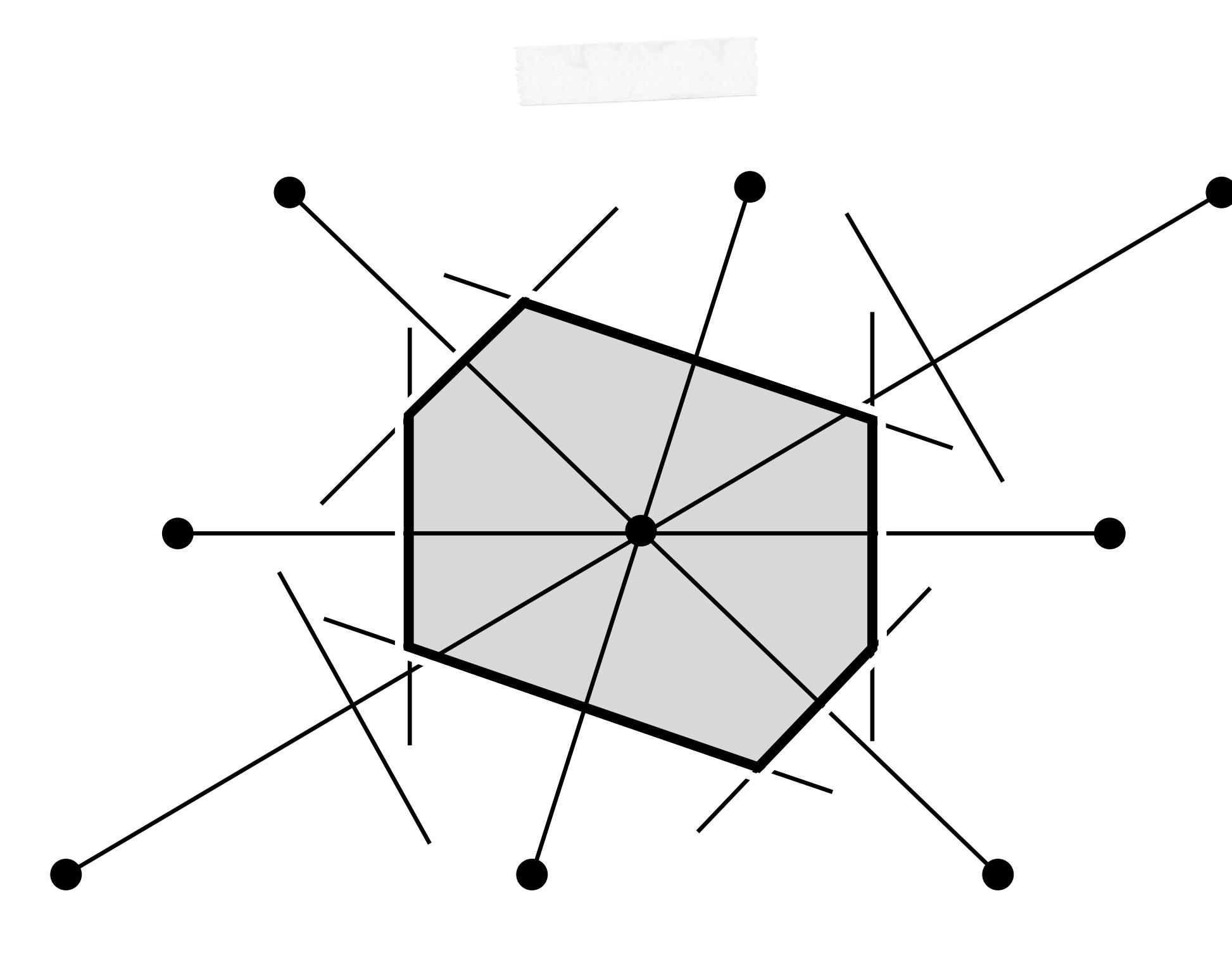
“Chapter 1” Crystalline Structure: Symmetry and Groups

¹A. C. García-Castro

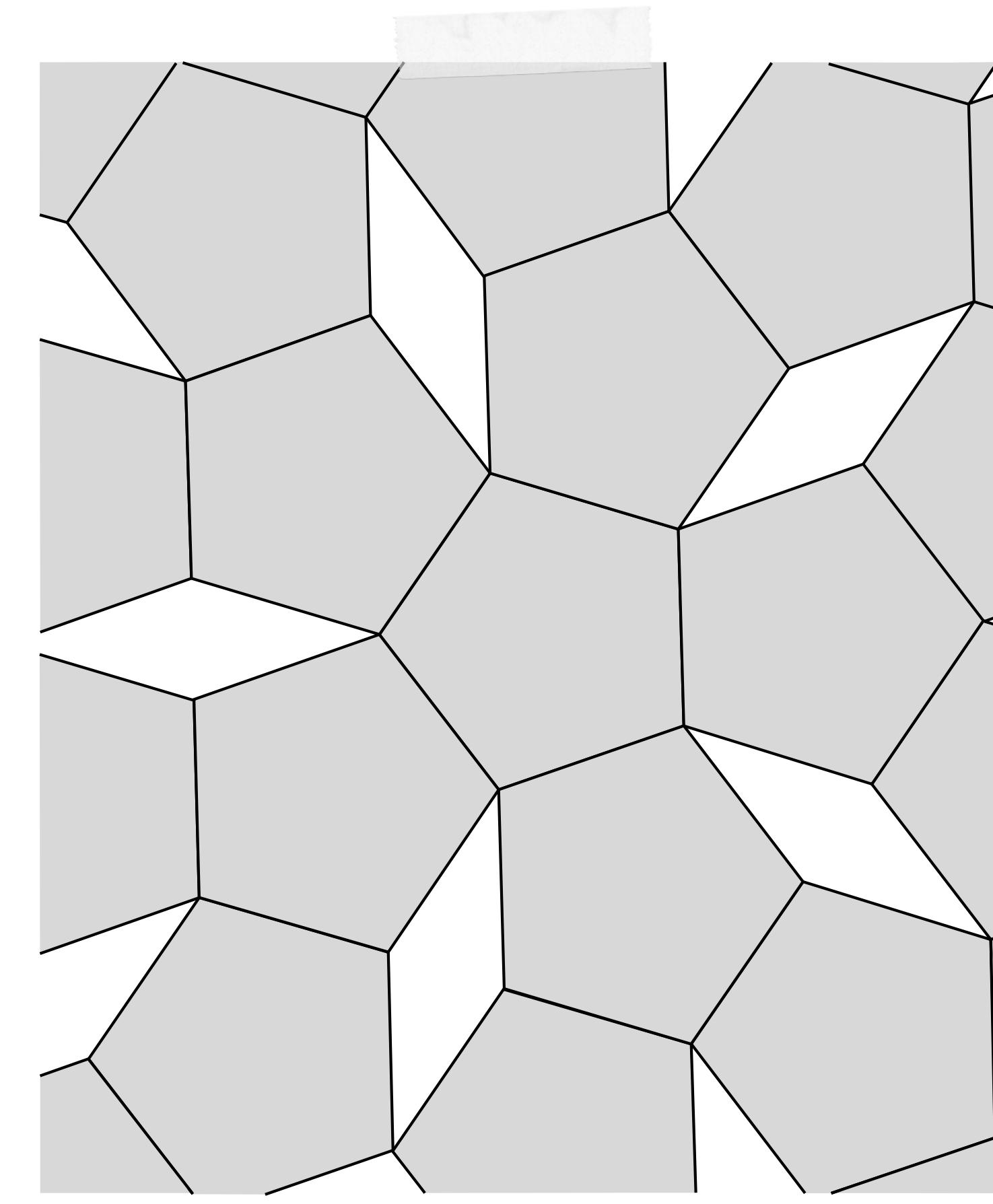
¹School of Physics, Universidad Industrial de Santander, Bucaramanga (Colombia).



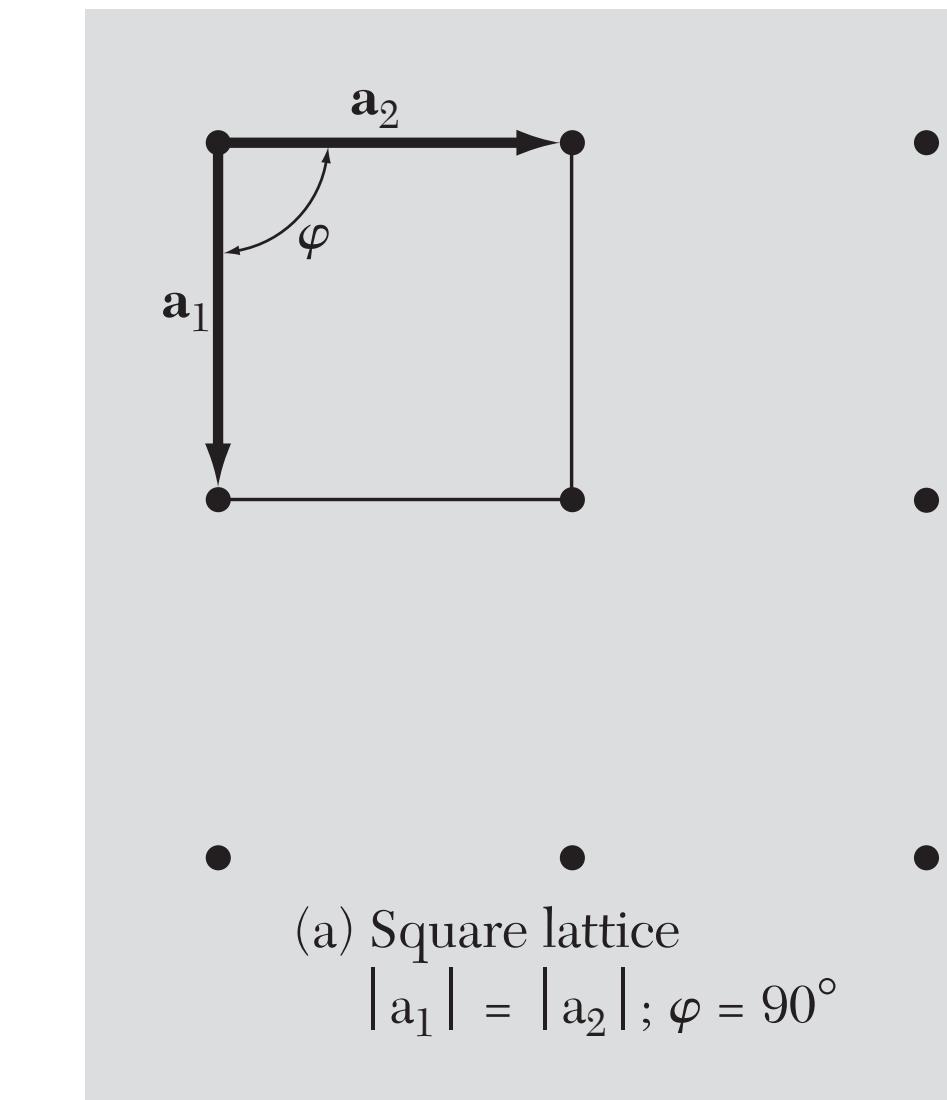




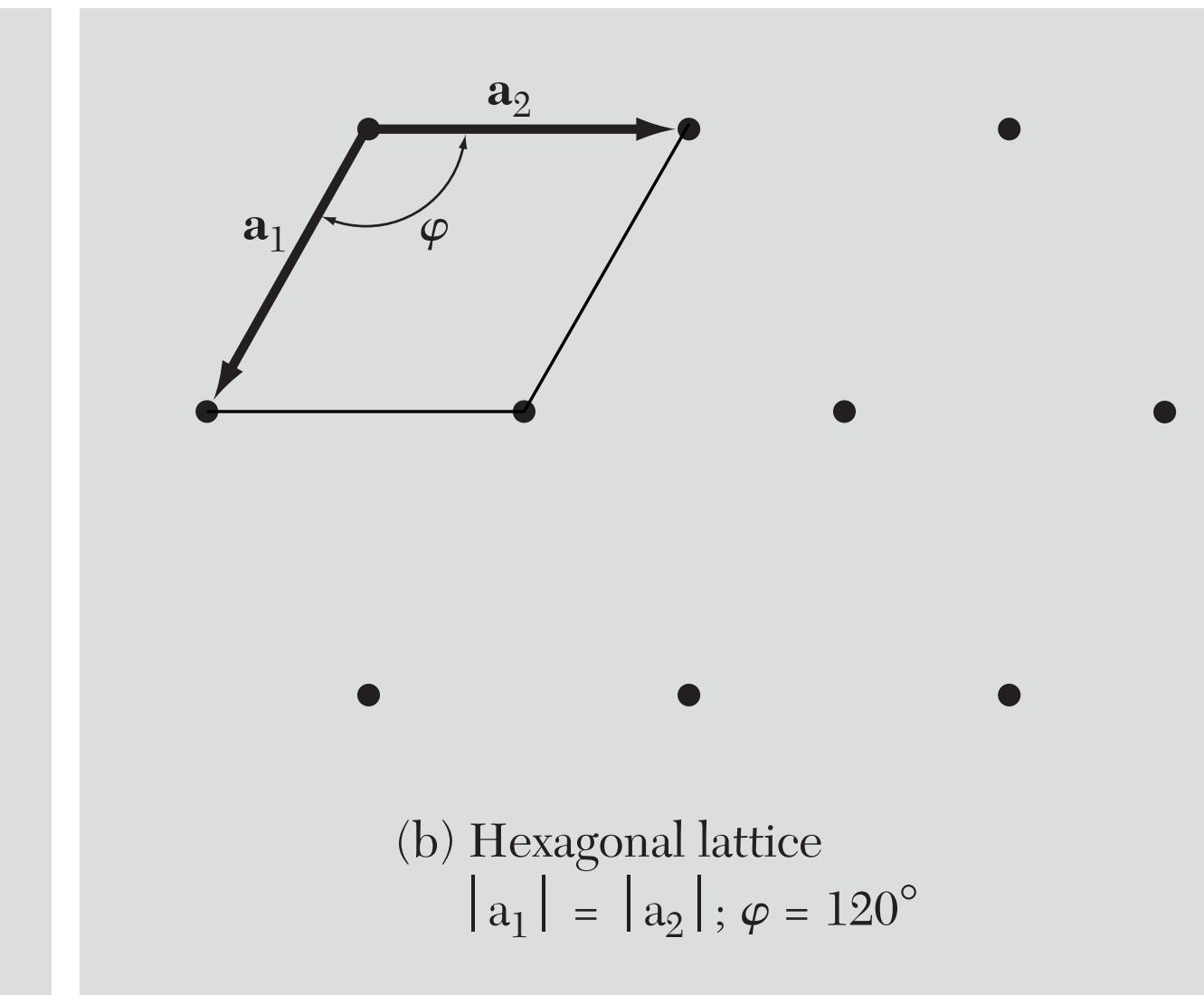
Wigner-Seitz primitive cell



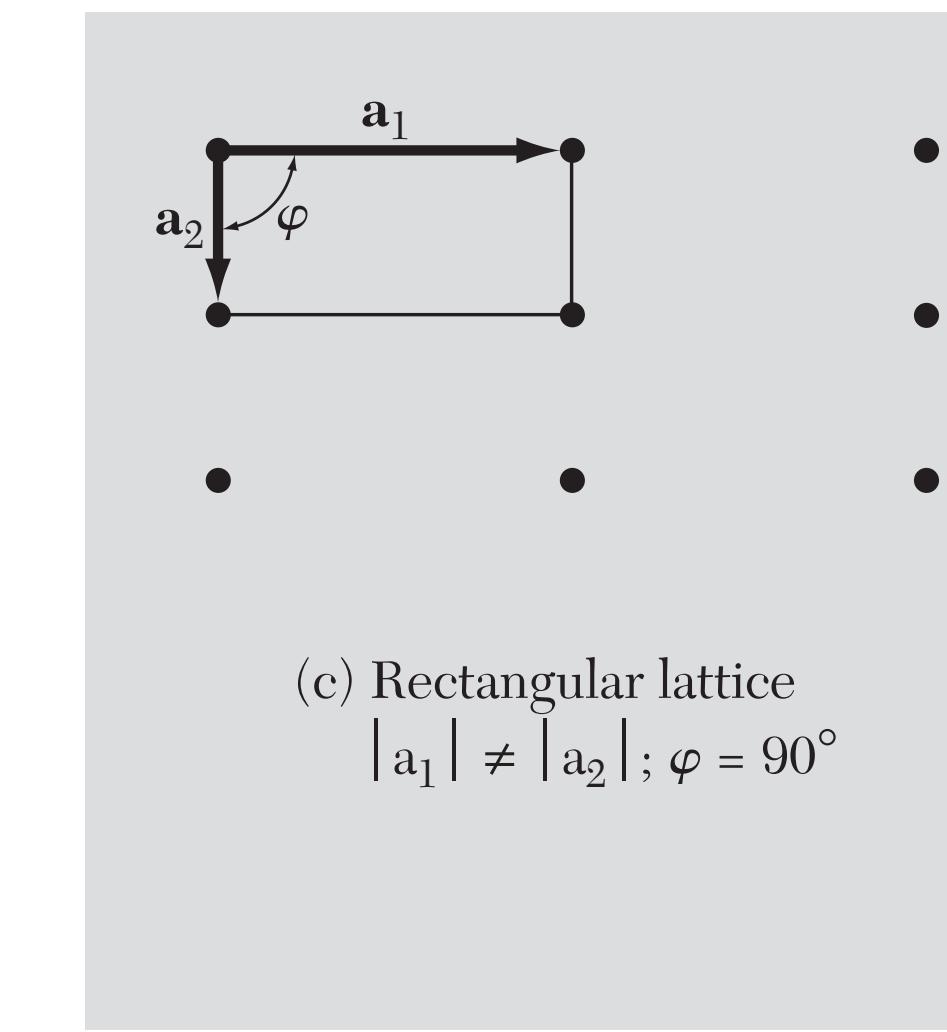
5-fold symmetry “cannot” exist.... Until that moment...
Quasicrystals!



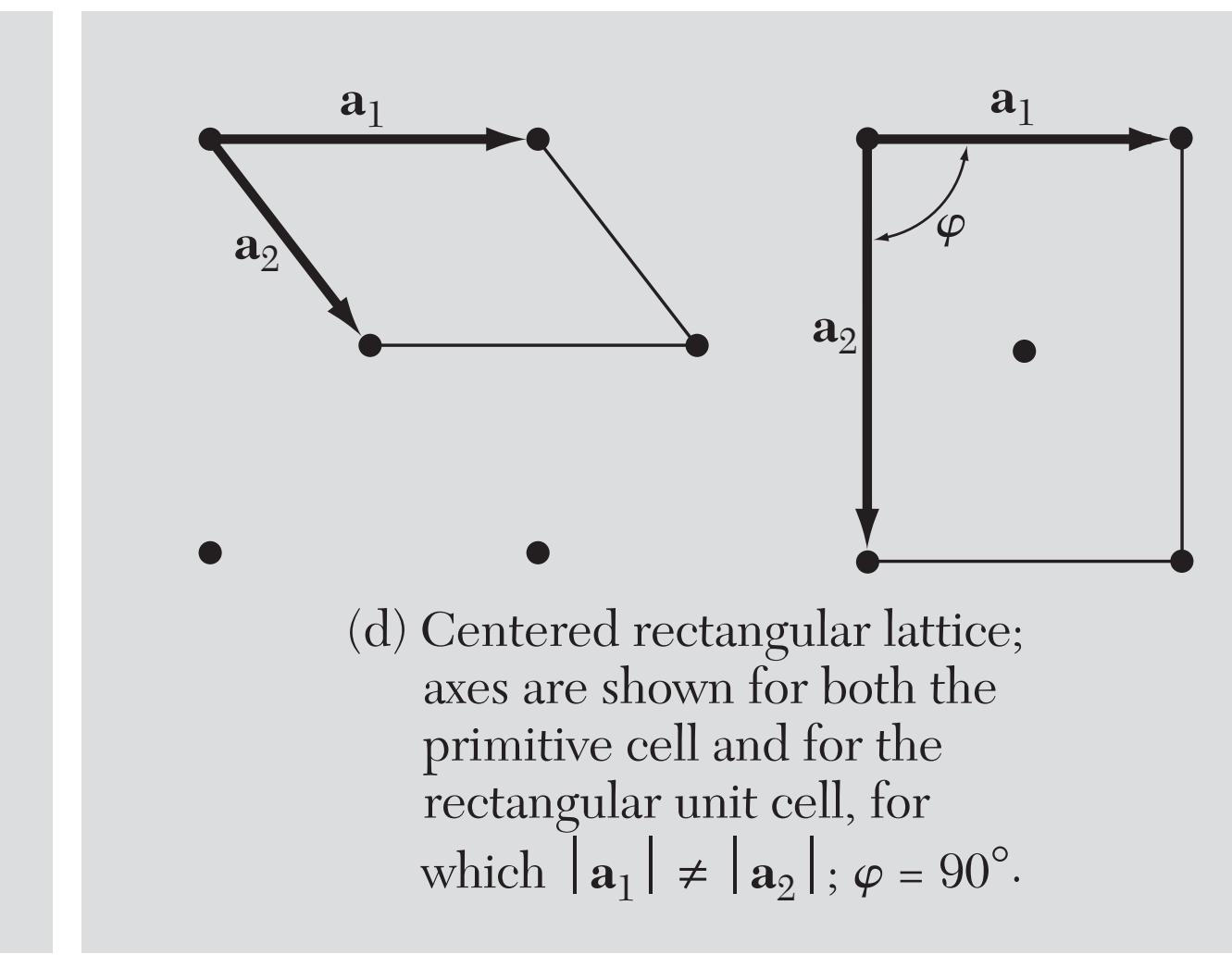
(a) Square lattice
 $|\mathbf{a}_1| = |\mathbf{a}_2|; \varphi = 90^\circ$



(b) Hexagonal lattice
 $|\mathbf{a}_1| = |\mathbf{a}_2|; \varphi = 120^\circ$



(c) Rectangular lattice
 $|\mathbf{a}_1| \neq |\mathbf{a}_2|; \varphi = 90^\circ$



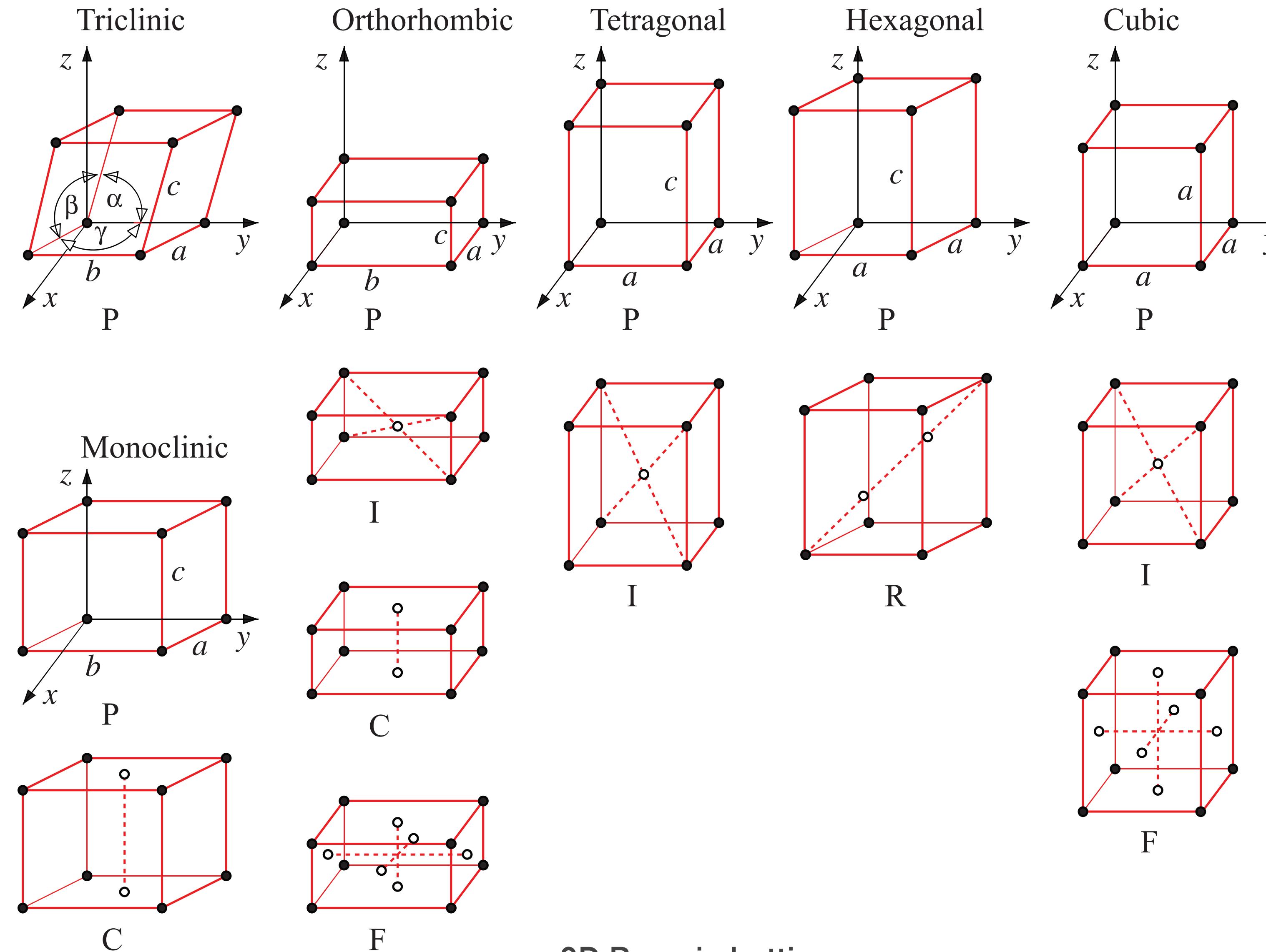
(d) Centered rectangular lattice;
axes are shown for both the
primitive cell and for the
rectangular unit cell, for
which $|\mathbf{a}_1| \neq |\mathbf{a}_2|; \varphi = 90^\circ$.

2D Bravais Lattices

Table 3.2 The seven crystal systems (first column) and the associated 32 point groups (last column) for crystals in three dimensions. The relations between the cell sides (a, b, c) and cell angles (α, β, γ) are shown and the corresponding lattices are labeled P = primitive, I = body centered, C = side centered, F = face centered, R = rhombohedral.

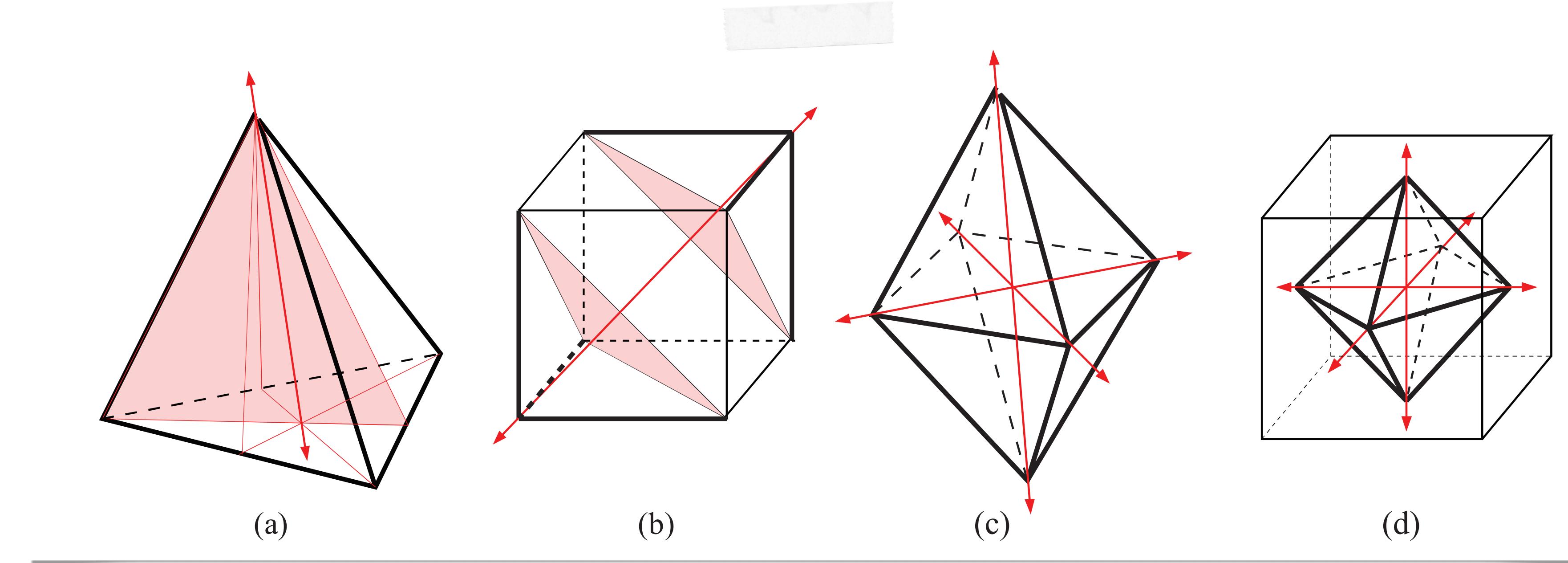
System	Cell sides	Cell angles	Lattices	Point groups
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$	P	C_1, C_i
Monoclinic	$a \neq b \neq c$	$\alpha = \beta = \frac{\pi}{2} \neq \gamma$	P, C	C_2, C_s, C_{2h}
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$	P, I, C, F	D_2, D_{2h}, C_{2v}
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$	P, I	$C_4, S_4, C_{4h}, D_4,$ C_{4v}, D_{2d}, D_{4h}
Trigonal	$a = b = c$	$\alpha = \beta = \gamma \neq \frac{\pi}{2}$	P	$C_3, C_{3i}, C_{3v}, D_3, D_{3d}$
Hexagonal	$a = b \neq c$	$\alpha = \beta = \frac{\pi}{2}, \gamma = \frac{2\pi}{3}$	P, R	$C_6, C_{3h}, C_{6h}, C_{6v},$ D_{3h}, D_6, D_{6h}
Cubic	$a = b = c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$	P, I, F	T, T_h, O, T_d, O_h

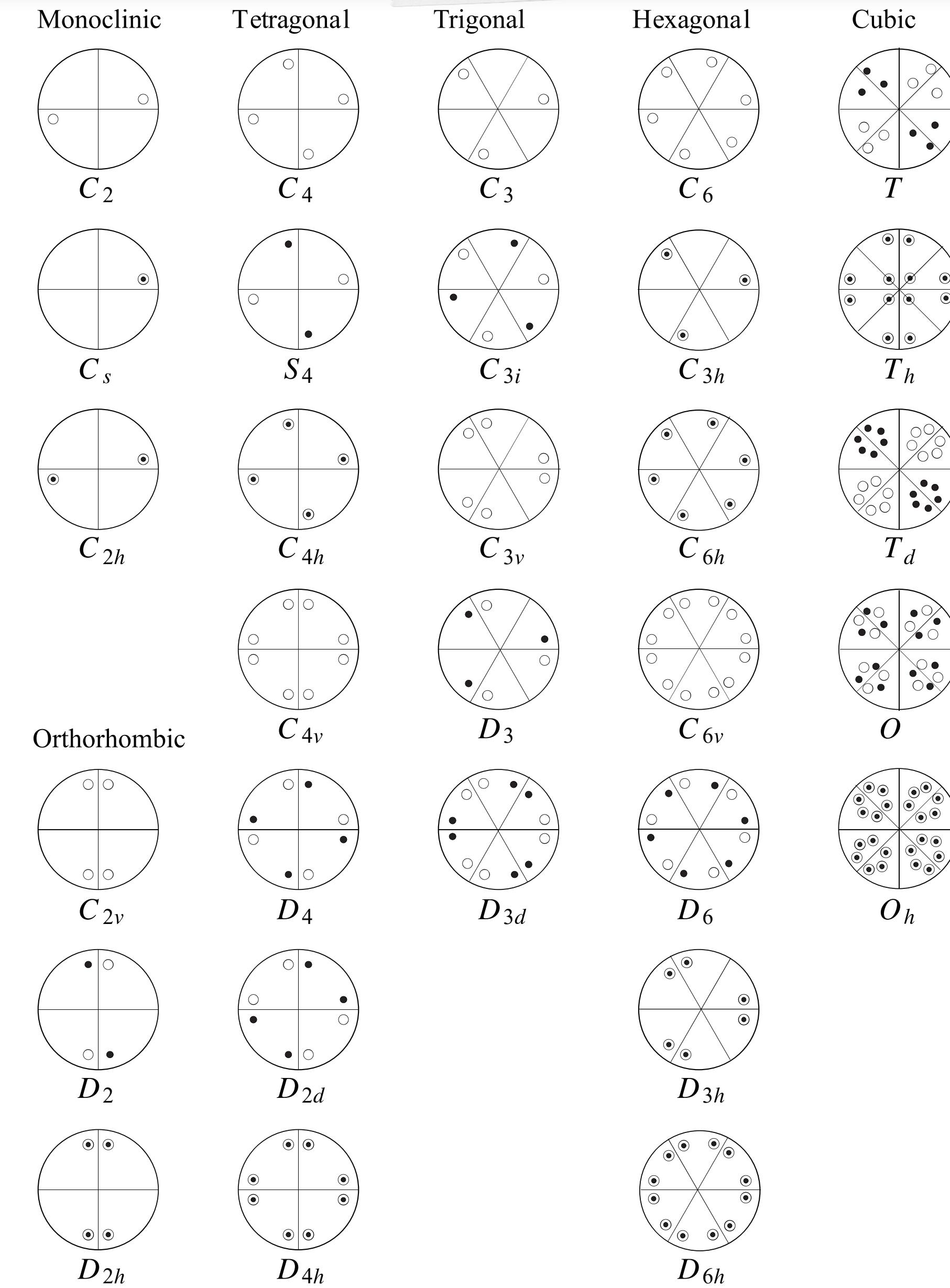
3D Bravais Lattices



Point groups and symmetries:

- C: for “cyclic,” when there is a single axis of rotation; a number subscript indicates the -fold symmetry around this axis (can be 2, 3, 4, 6).
- D: for “dihedral,” when there are twofold axes at right angles to another axis.
- T: for “tetrahedral,” when there are four sets of rotation axes of threefold symmetry, as in a tetrahedron.
- O: for “octahedral,” when there are fourfold rotation axes combined with perpendicular twofold rotation axes, as in an octahedron.





C_i and C_1 are not shown because they are trivial

Open circles refer to the north pole. Whereas the full circles refer to the south.

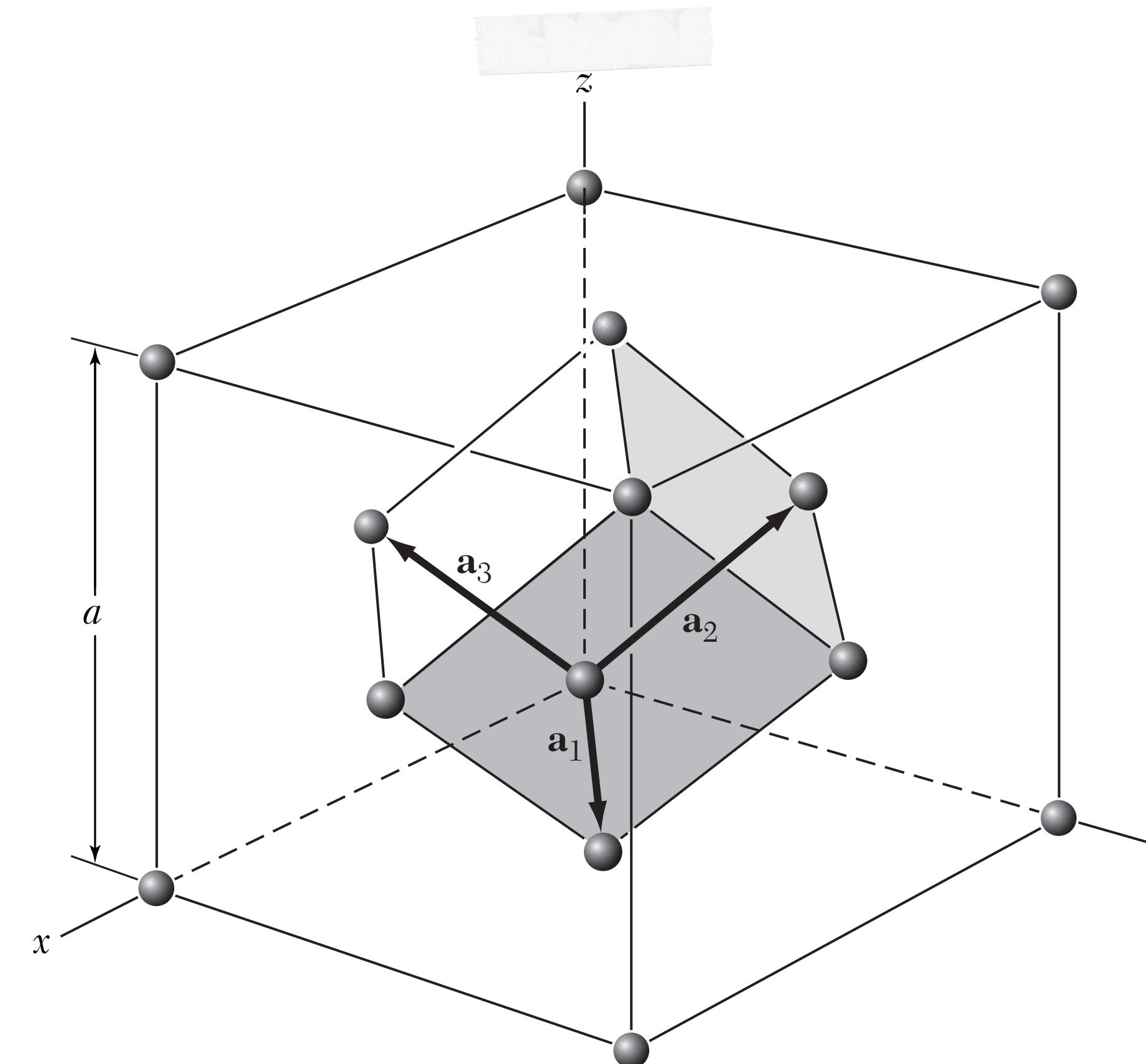


Figure 11 The rhombohedral primitive cell of the face-centered cubic crystal. The primitive translation vectors \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 connect the lattice point at the origin with lattice points at the face centers. As drawn, the primitive vectors are:

$$\mathbf{a}_1 = \frac{1}{2}a(\hat{\mathbf{x}} + \hat{\mathbf{y}}) ; \quad \mathbf{a}_2 = \frac{1}{2}a(\hat{\mathbf{y}} + \hat{\mathbf{z}}) ; \quad \mathbf{a}_3 = \frac{1}{2}a(\hat{\mathbf{z}} + \hat{\mathbf{x}}) .$$

The angles between the axes are 60° .

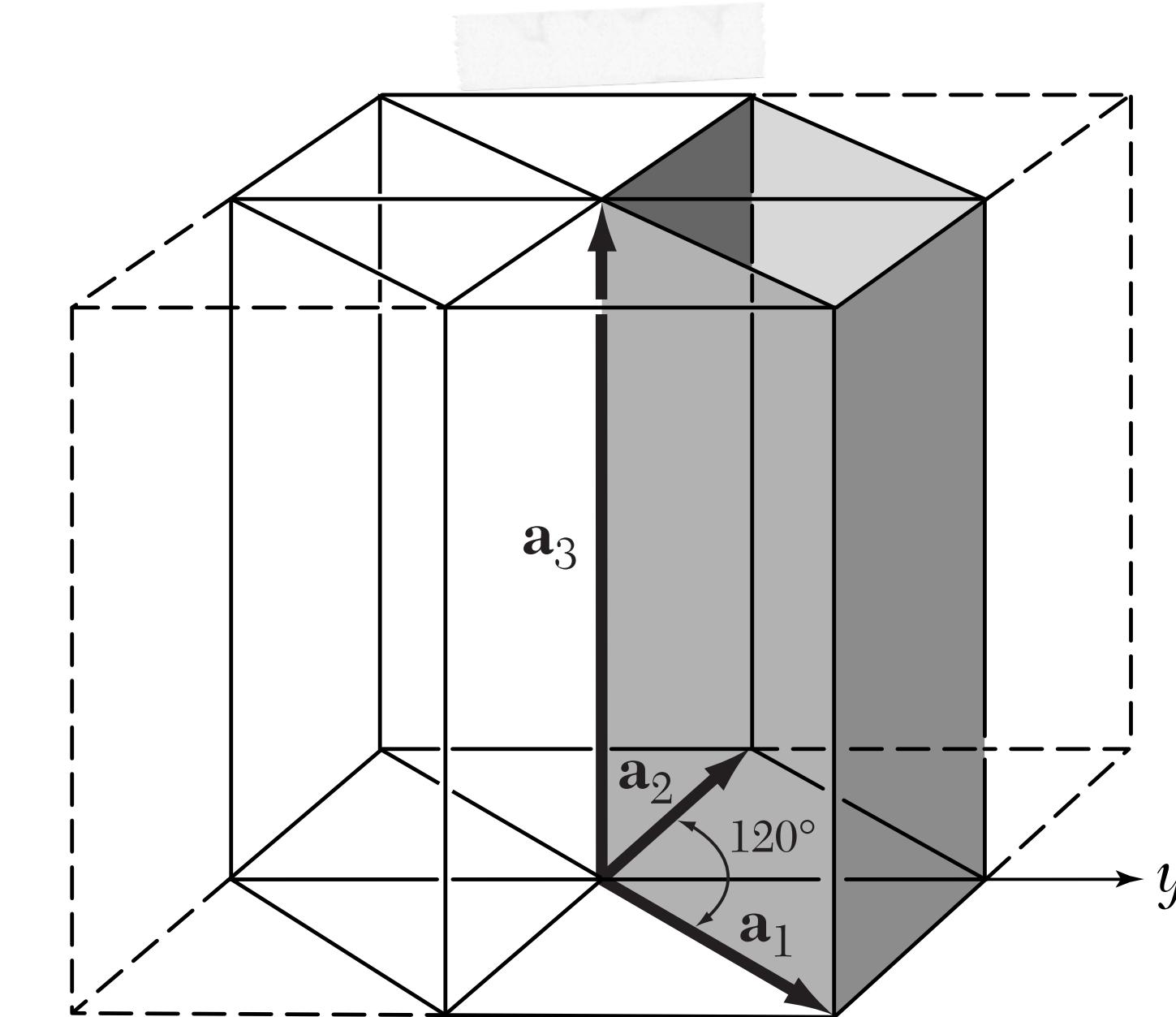
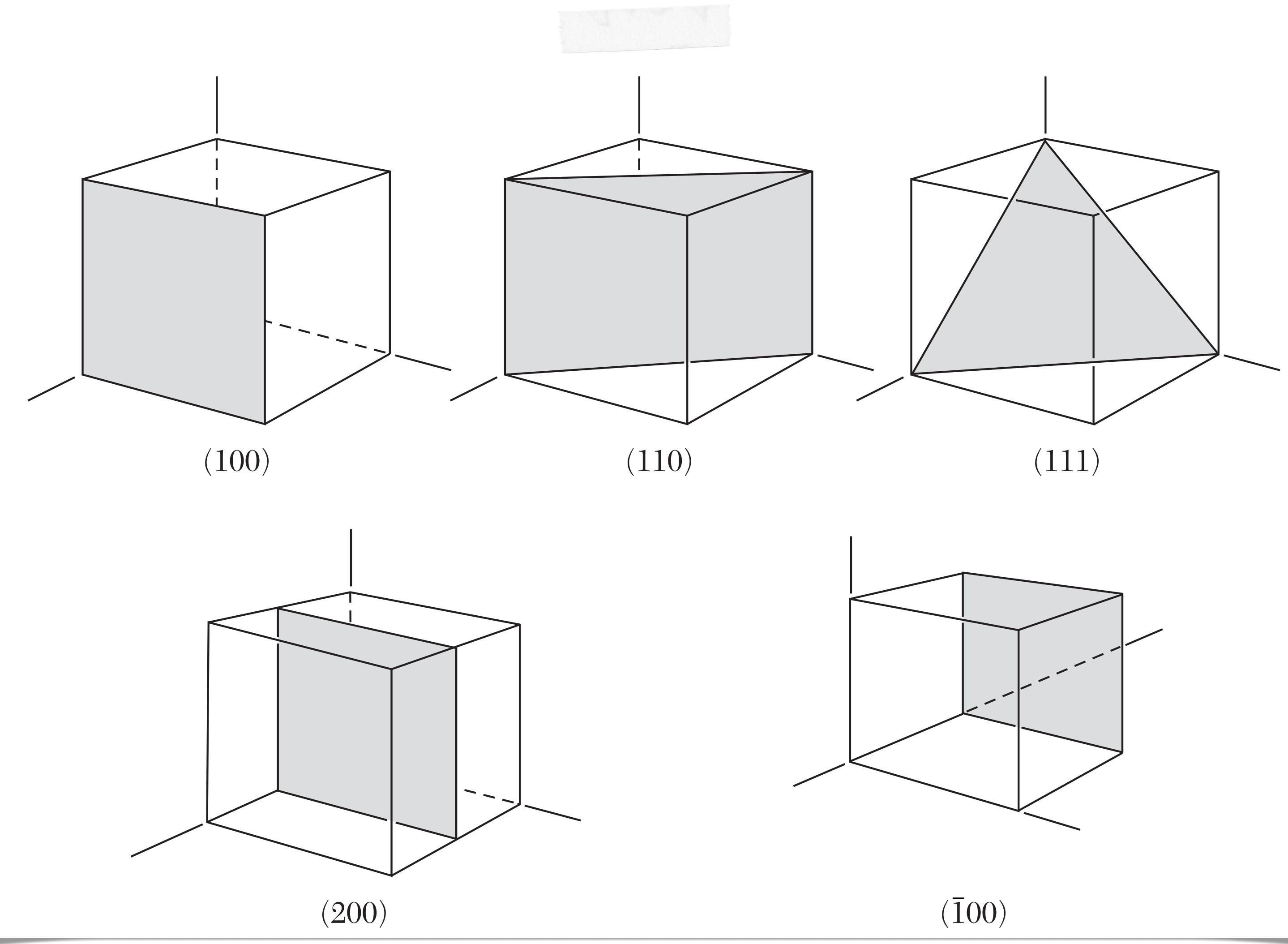
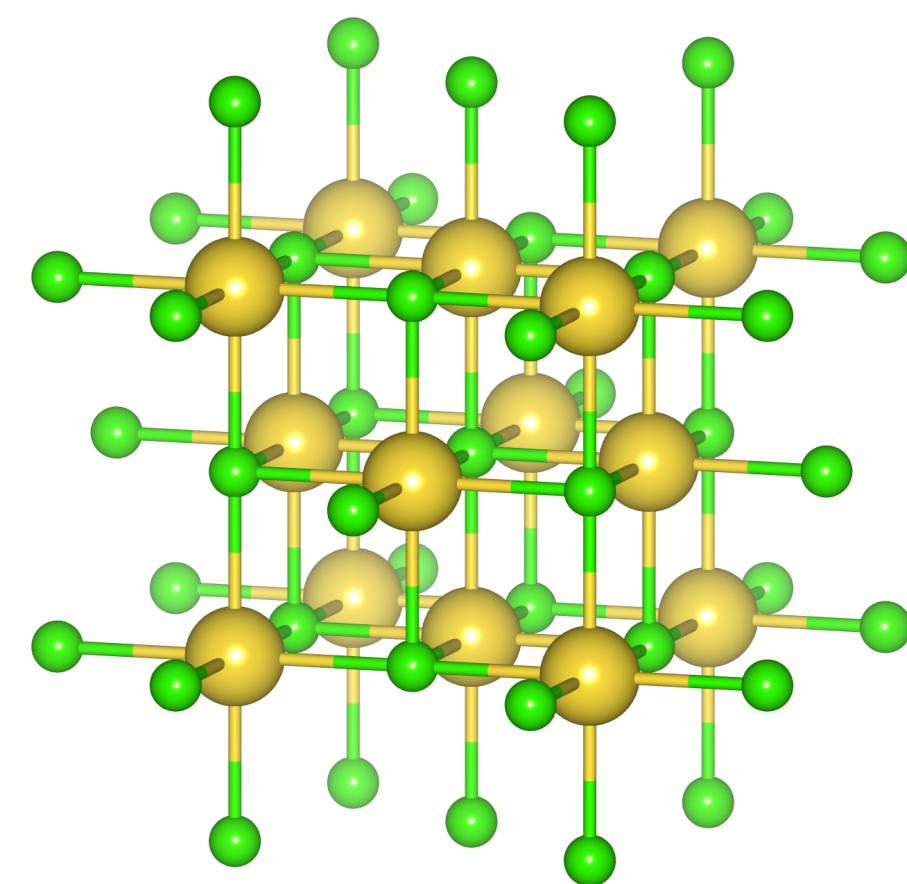


Figure 12 Relation of the primitive cell in the hexagonal system (heavy lines) to a prism of hexagonal symmetry. Here $a_1 = a_2 \neq a_3$.

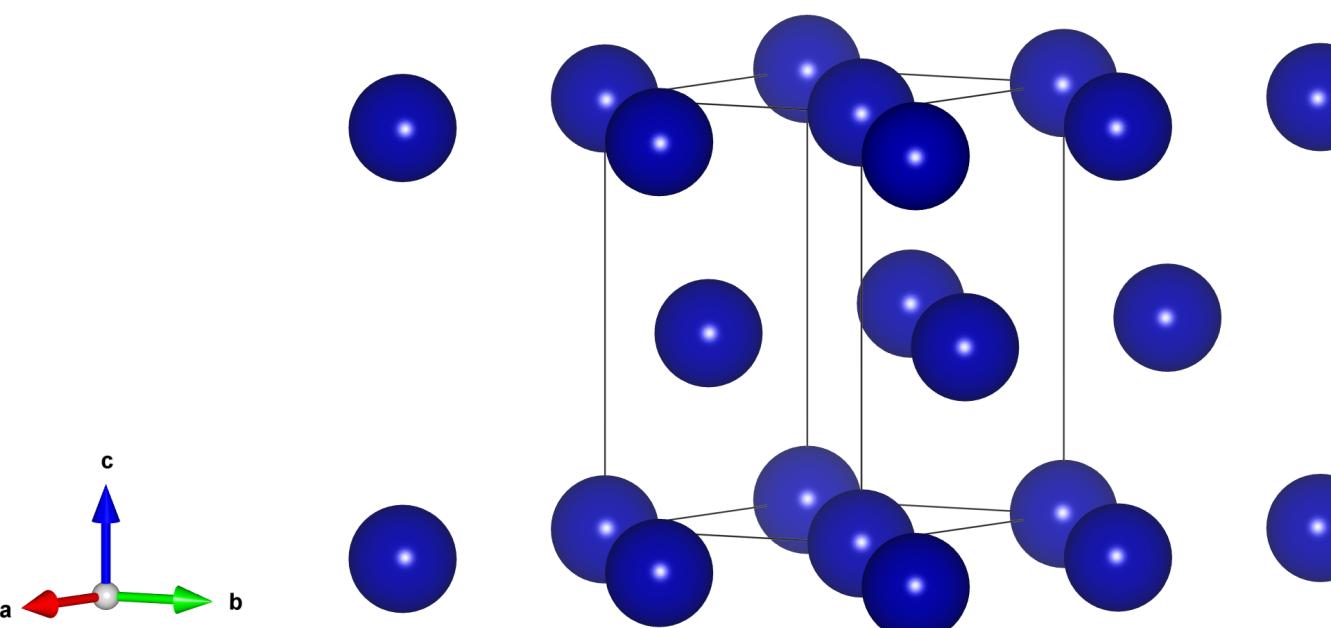
Primitive and unit-cells



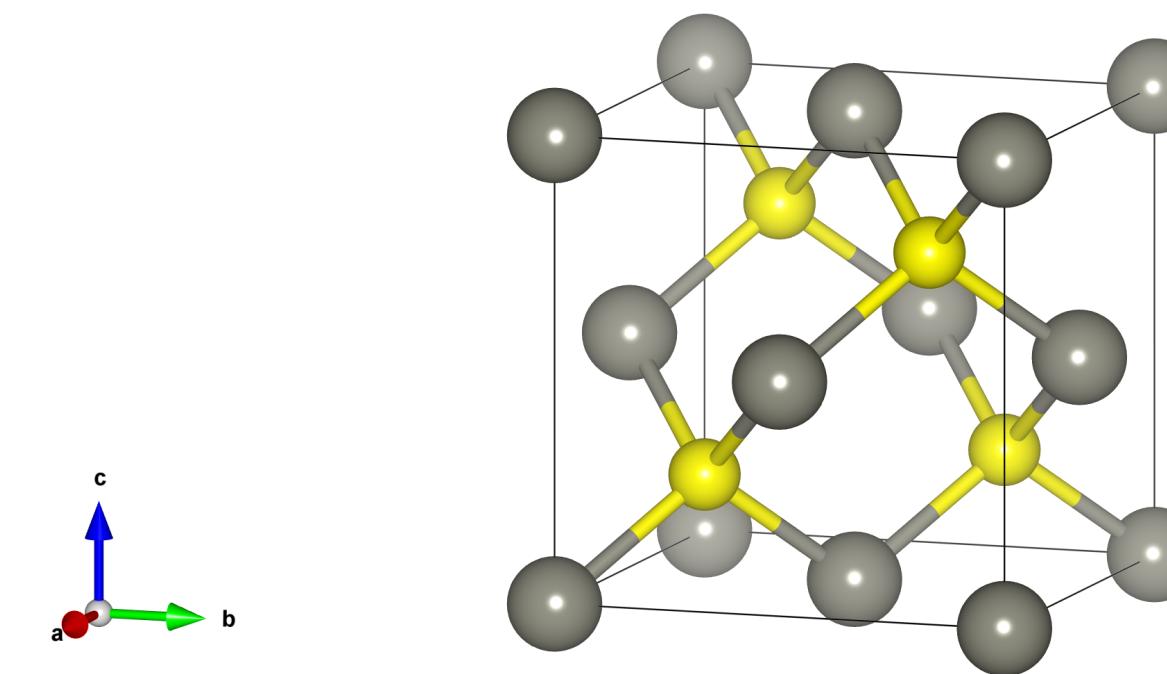
Lattice planes!



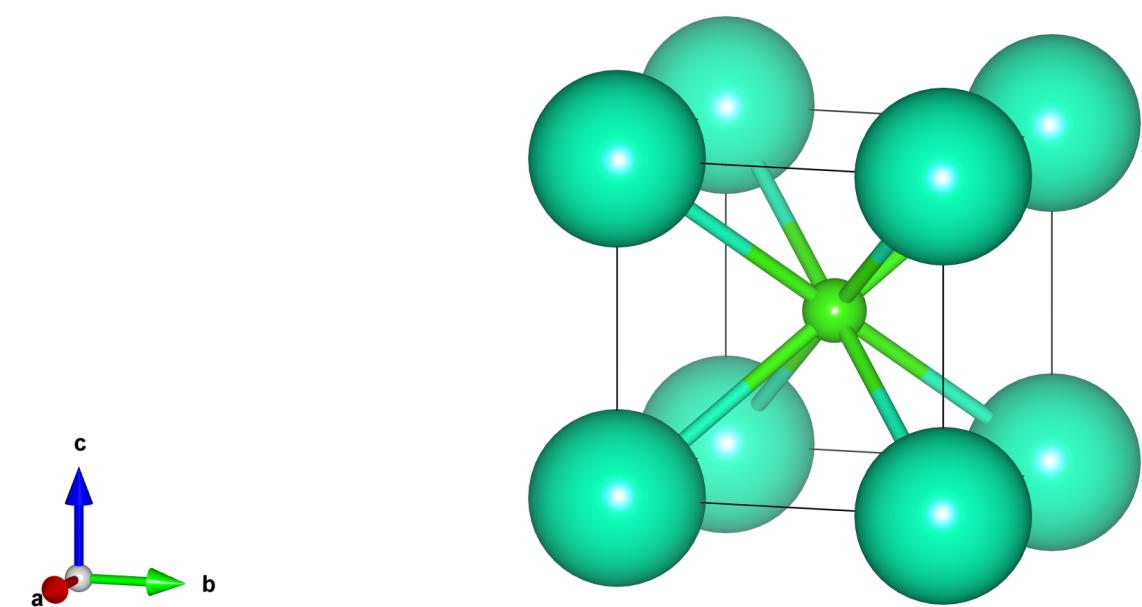
NaCl



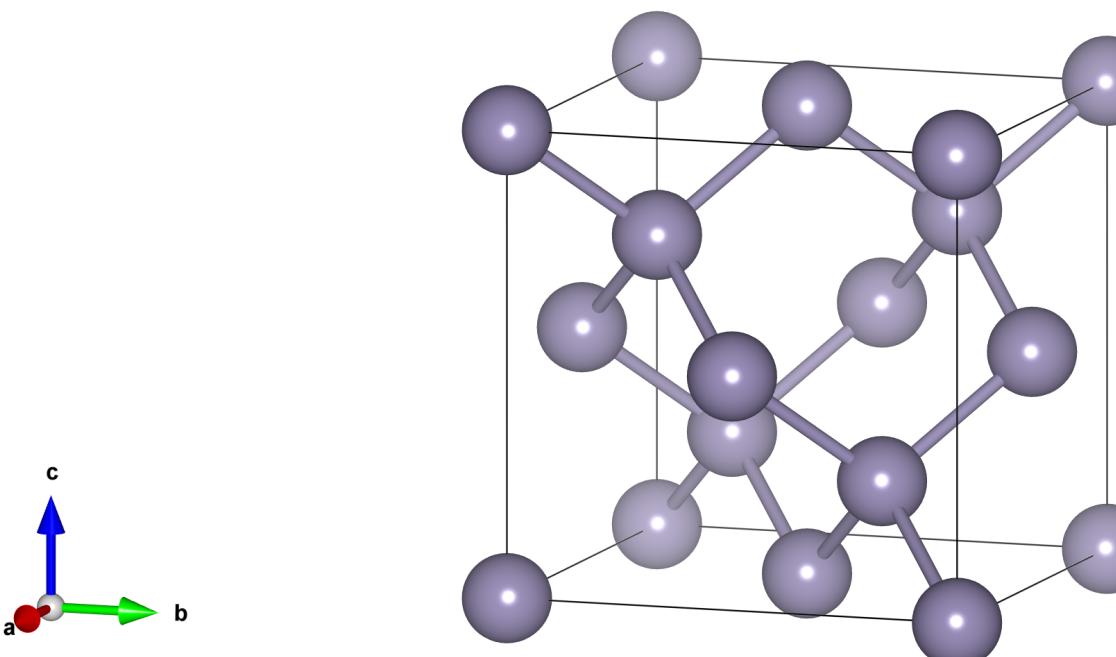
Co - hcp



ZnS - Diamond



CsCl



Si - Diamond

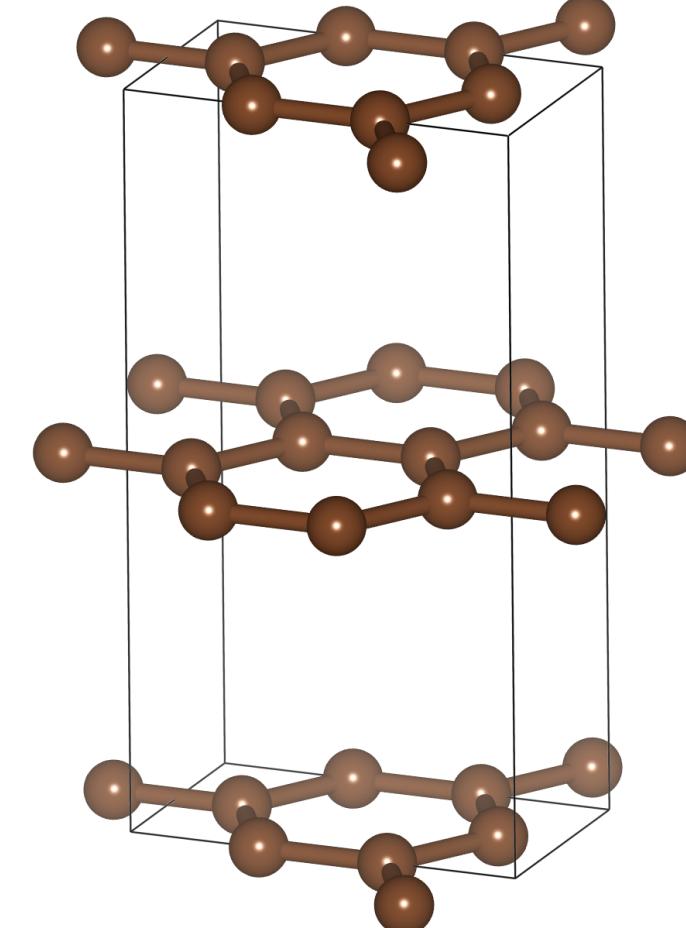
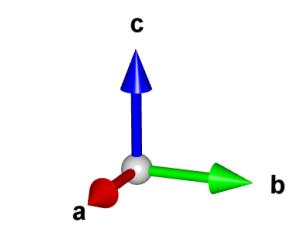
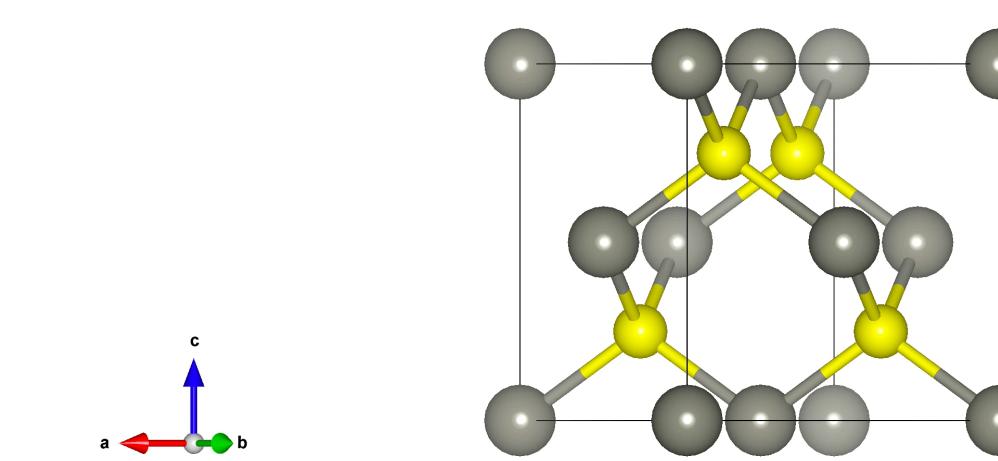




Table 3 Crystal structures of the elements

H ¹ 4K																He ⁴ 2K								
hcp																hcp								
3.75																3.57								
6.12																5.83								
Li 78K	Be															Ne 4K								
bcc	hcp															fcc								
3.491	2.27															4.46								
	3.59																							
Na 5K	Mg															Al 4K								
bcc	hcp															fcc								
4.225	3.21															4.05								
	5.21															5.430								
← Crystal structure. → a lattice parameter, in Å c lattice parameter, in Å																								
K 5K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr 4K							
bcc	fcc	hcp	hcp	bcc	bcc	cubic	bcc	hcp	fcc	fcc	hcp	complex	diamond	rhomb.	hex.	complex	fcc							
5.225	5.58	3.31	2.95	3.03	2.88	complex	2.87	2.51	3.52	3.61	2.66	5.658			(Br ₂)	5.64								
	5.27	4.68						4.07			4.95													
Rb 5K	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn (α)	Sb	Te	I	Xe 4K							
bcc	fcc	hcp	hcp	bcc	bcc	hcp	hcp	fcc	fcc	fcc	hcp	tetr.	diamond	rhomb.	hex.	complex	fcc							
5.585	6.08	3.65	3.23	3.30	3.15	2.74	2.71	3.80	3.89	4.09	2.98	3.25	6.49			(I ₂)	6.13							
	5.73	5.15				4.40	4.28				5.62	4.95												
Cs 5K	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn							
bcc	bcc	hex.	hcp	bcc	bcc	hcp	hcp	fcc	fcc	fcc	rhomb.	hcp	fcc	rhomb.	sc	—	—							
6.045	5.02	3.77	3.19	3.30	3.16	2.76	2.74	3.84	3.92	4.08	3.46	4.95		3.34	—	—								
		ABAC	5.05			4.46	4.32				5.52													
Fr	Ra	Ac																						
			fcc																					
			5.31																					
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu											
hcp	hex.	hex.	—	complex	bcc	hcp	hcp	hcp	hcp	hcp	hcp	fcc	hcp											
5.16	3.67	3.66			4.58	3.63	3.60	3.59	3.58	3.56	3.54	5.48	3.50											
	ABAC					5.78	5.70	5.65	5.62	5.59	5.56													
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr											
fcc	tetr.	complex	complex	complex	hex.	—	—	—	—	—	—	—	—											
5.08	3.92	3.24			3.64																			

