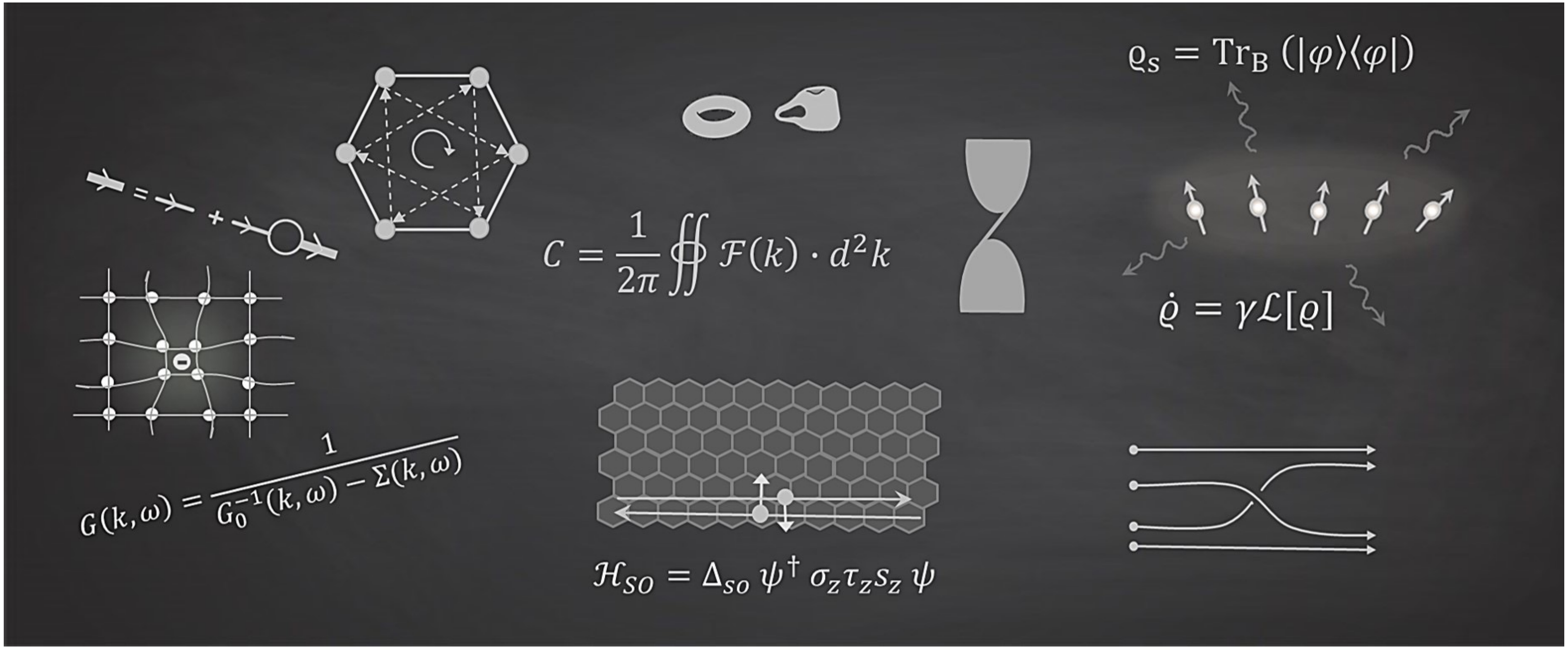
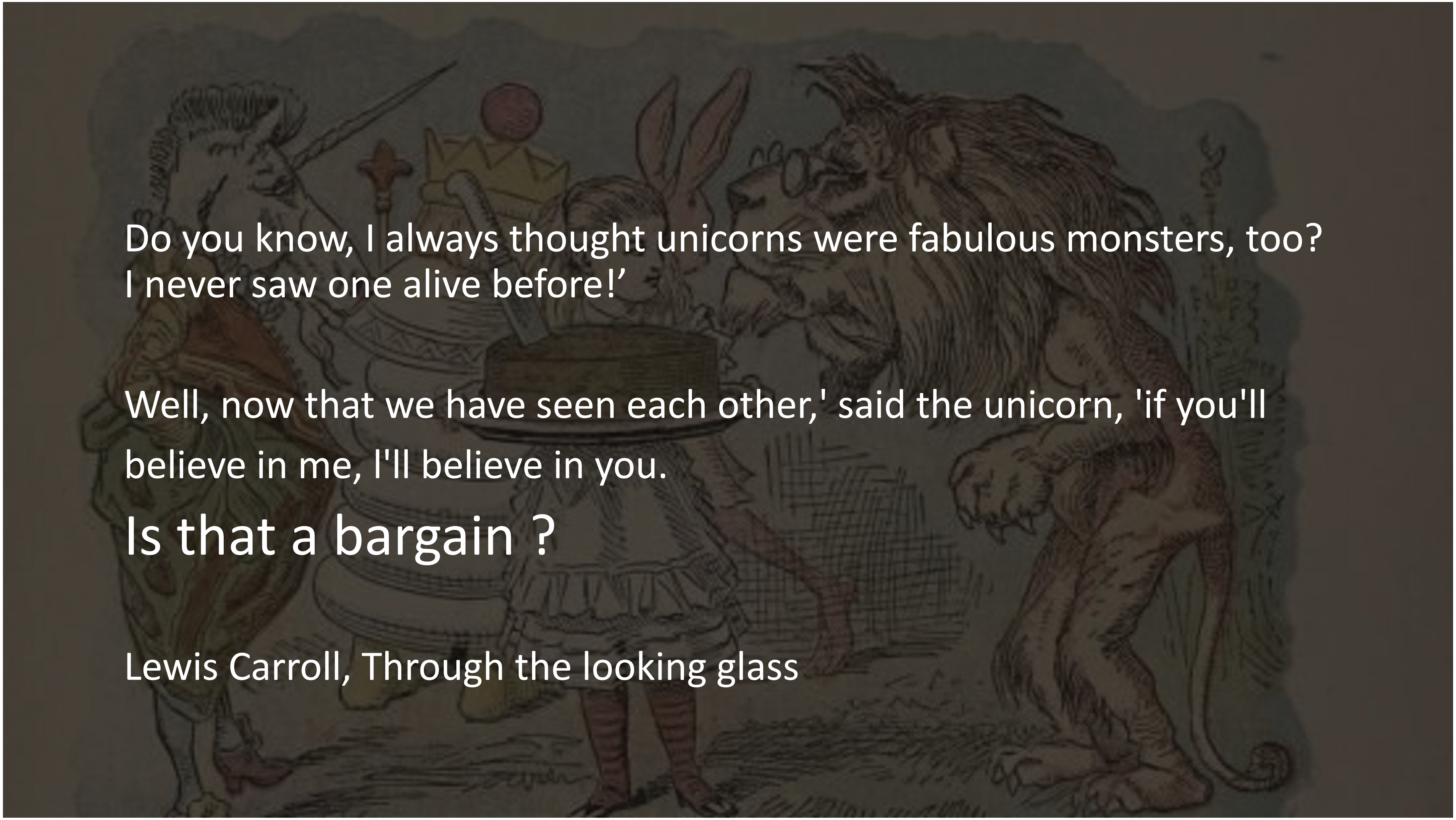
Física da Matéria Condensada

Margarida Telo da Gama





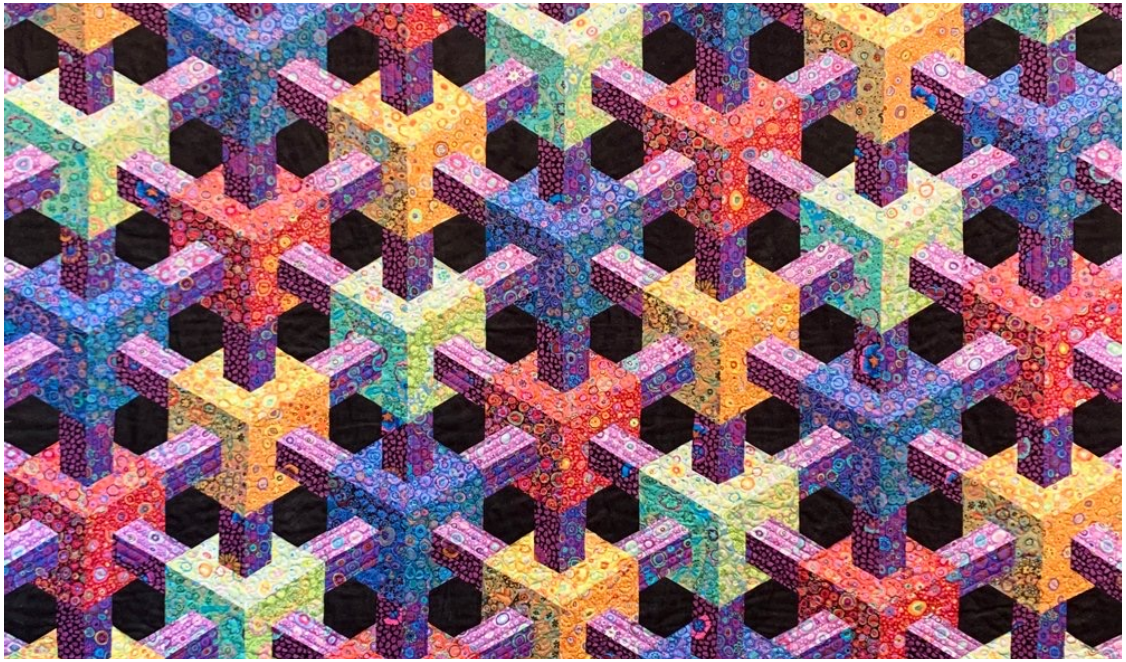
Do you know, I always thought unicorns were fabulous monsters, too?
I never saw one alive before!’

Well, now that we have seen each other,' said the unicorn, 'if you'll believe in me, I'll believe in you.

Is that a bargain ?

Lewis Carroll, Through the looking glass

PROGRAMA (OUTLINE)



1. INTRODUÇÃO
2. ESTRUTURA CRISTALINA
3. ESTRUTURAS DOS SÓLIDOS
4. DIFRAÇÃO E DIFUSÃO ELÁSTICA DE ONDAS
5. LIGAÇÕES QUIMICAS
6. VIBRAÇÕES ATÓMICAS
7. TERMODINÂMICA DE FONÕES
8. ESTADOS ELECTRÓNICOS
9. TERMODINÂMICA DE ELECTRÕES EM METAIS
10. CONDUTIVIDADE ELÉCTRICA E TÉRMICA
11. ELECTRÕES EM SEMICONDUTORES

BIBLIOGRAFIA

1. Fundamentals of Solid State Physics, J. R. Christman, Wiley, 1988.

2. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Holt, 1976.

3. Introduction to Solid State Physics, 5th ed., C. Kittel, Wiley, 1976.

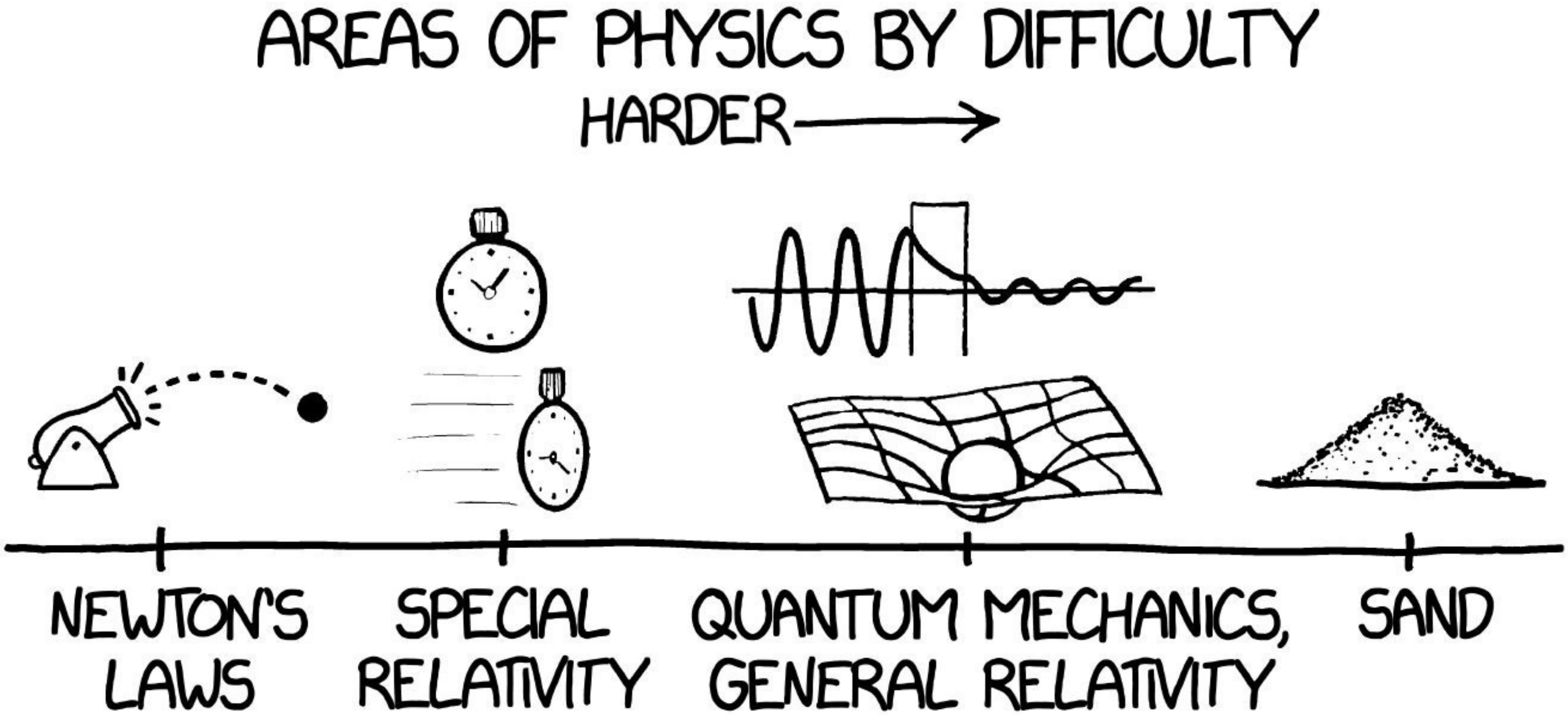
4. Solid State Physics, An Introduction to Principles of Materials Science, H. Ibach and H. Luth, Springer, 1995.

5. Solid State Physics, H. E. Hall, Wiley, 1974

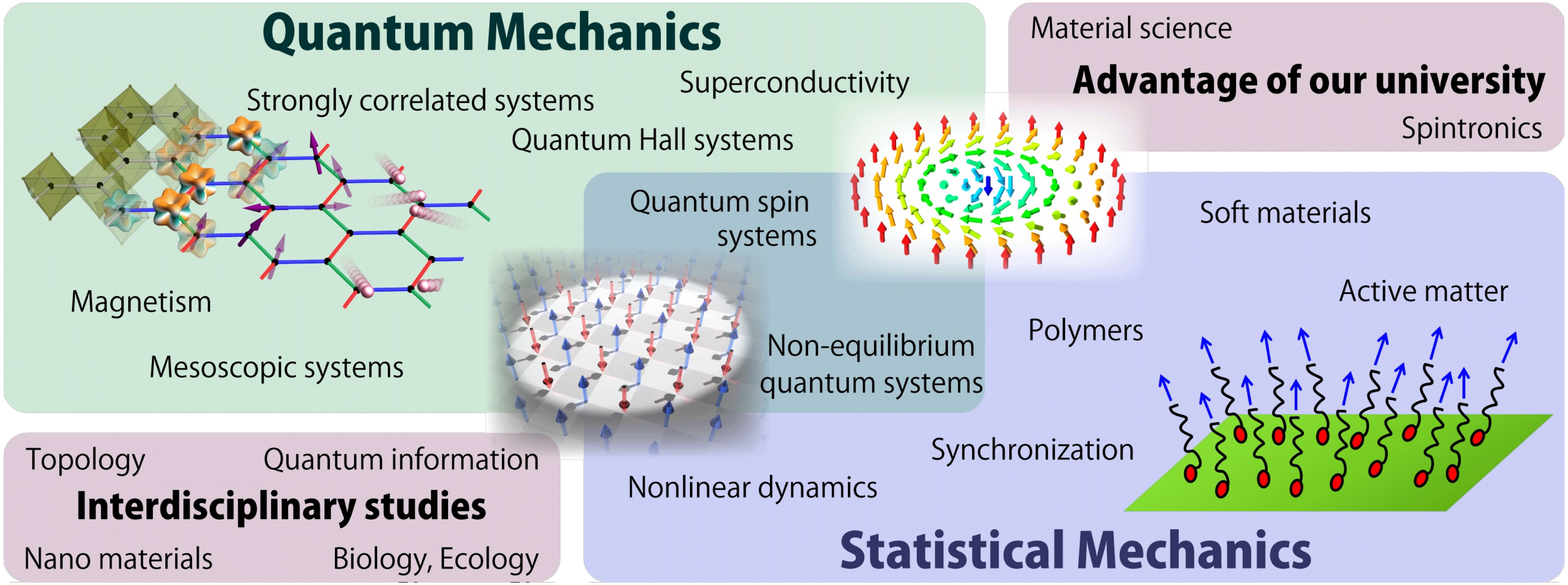
AVALIAÇÃO

- Exame

- Contínua: entrega da resolução escrita de 1-3 problemas das séries seguida da resolução no quadro durante as TPs (20%) e exame final (80%)


AREAS OF PHYSICS BY DIFFICULTY
HARDER
NEWTON'S LAWS
SPECIAL RELATIVITY
QUANTUM MECHANICS, GENERAL RELATIVITY
SAND

1. Introduction



What is condensed matter ?

Collective properties that emerge from the interactions of many particles:

- Quantum or classical Dynamics to calculate the energy spectrum (states) - E_N
- Statistical Mechanics to calculate the occupation probability of each state – $P(E_N)$

What is condensed matter physics ?

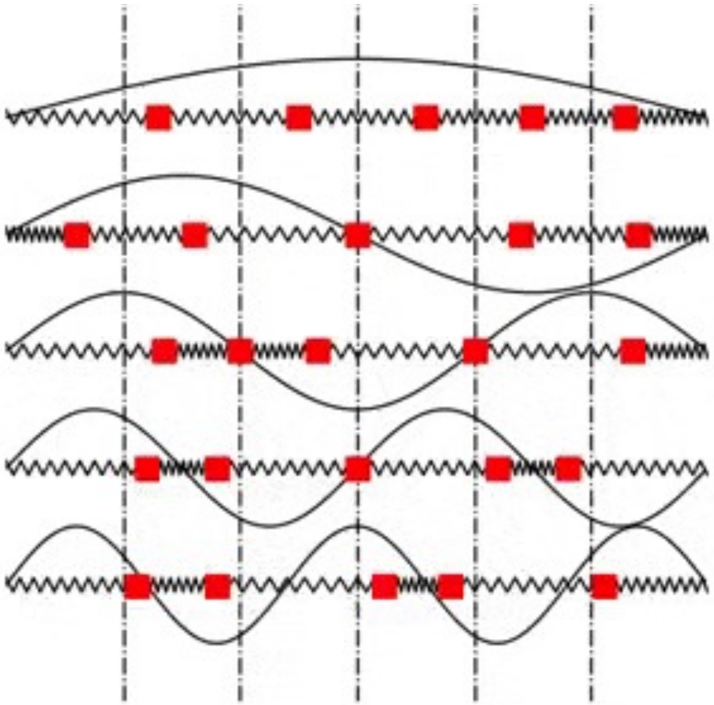
Properties of materials in terms of the interacting building blocks:

- Hard condensed matter: electrons & nuclei
- Soft condensed matter: polymers, colloids ...

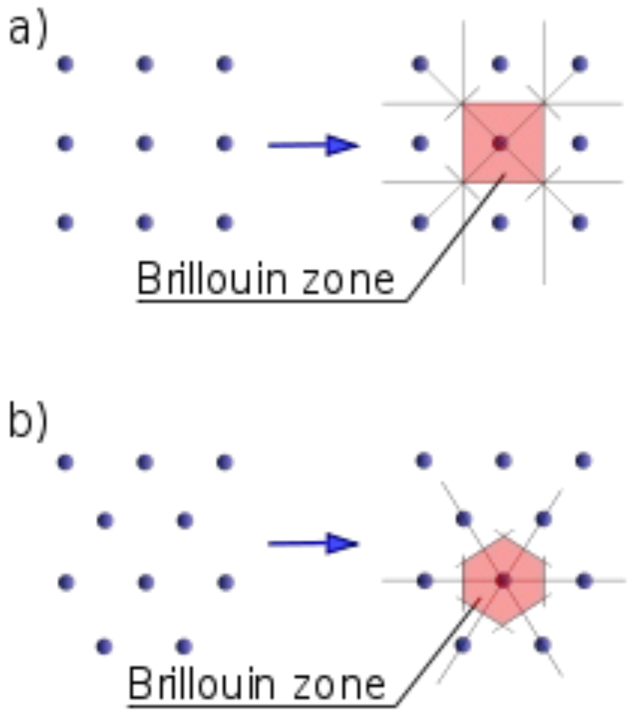
Response to external fields:

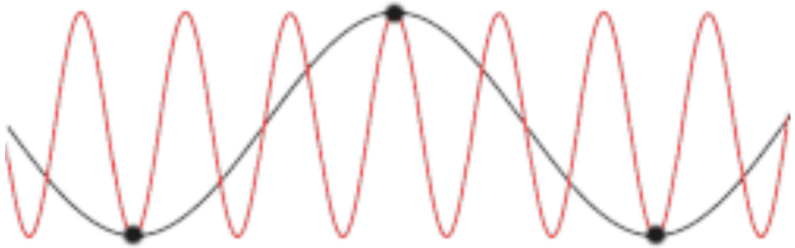
- Linear
- Non-linear

6. Vibraçoes atómicas

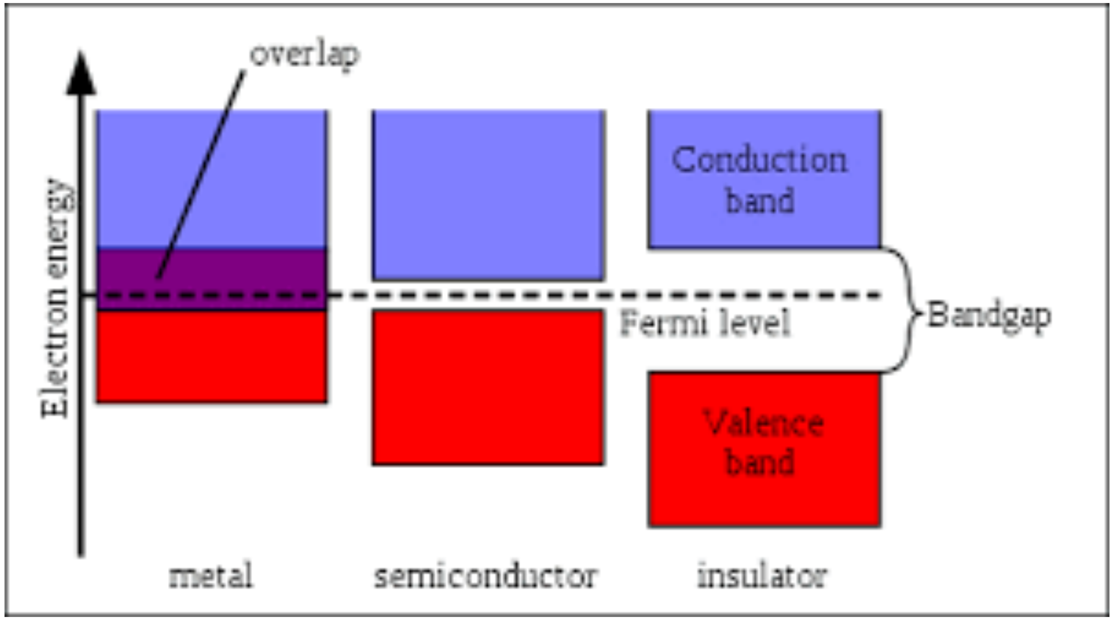


7. Termodinâmica de fonões

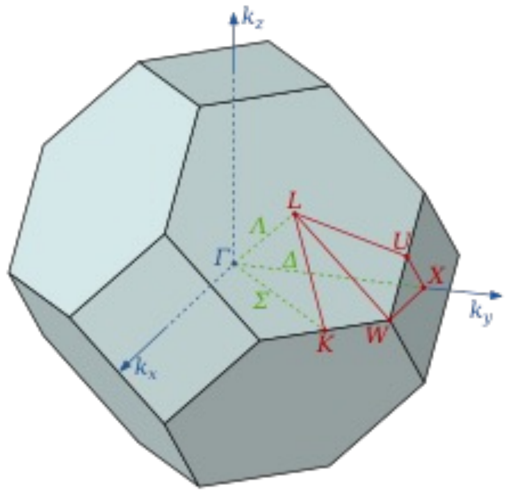


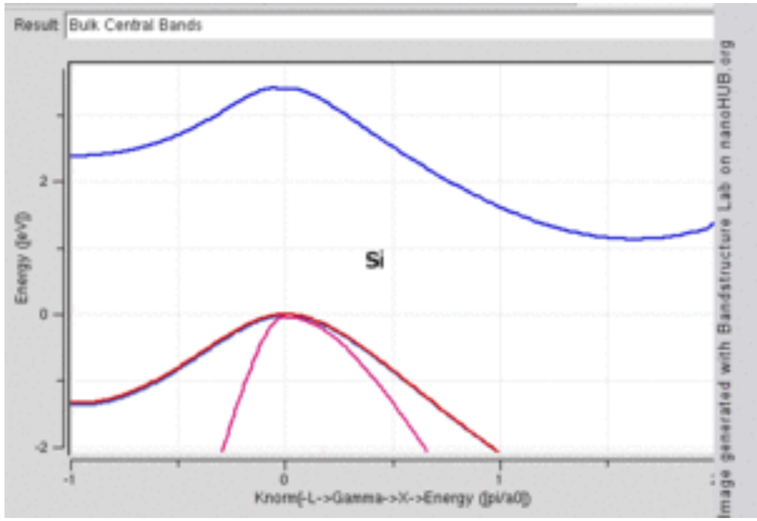


8. Estados electrónicos



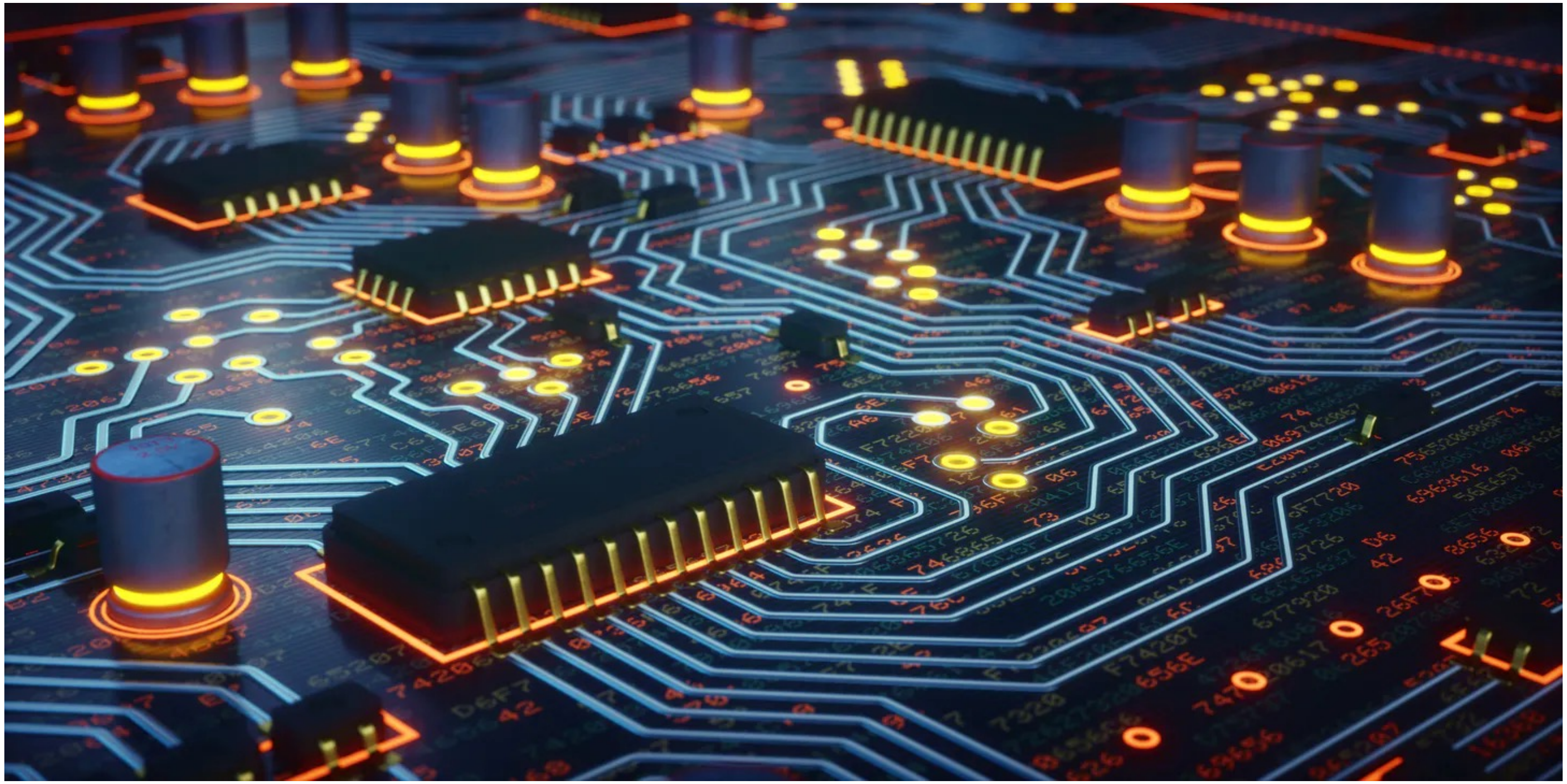
9. Termodinâmica de electrões



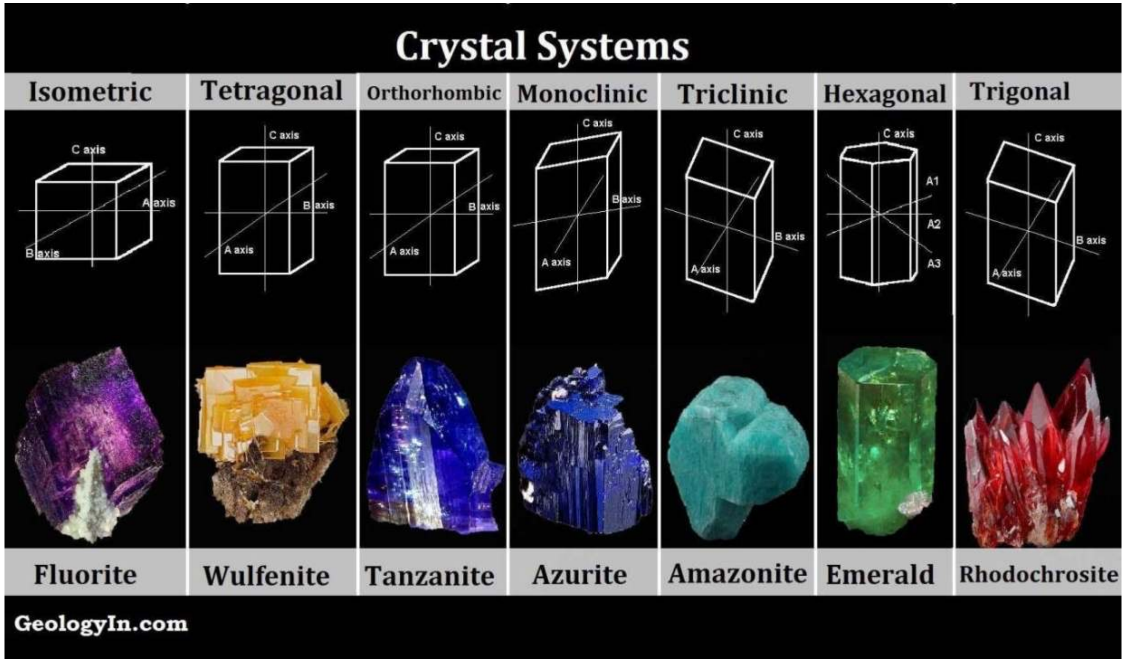


10. Condutividade elétrica e térmica

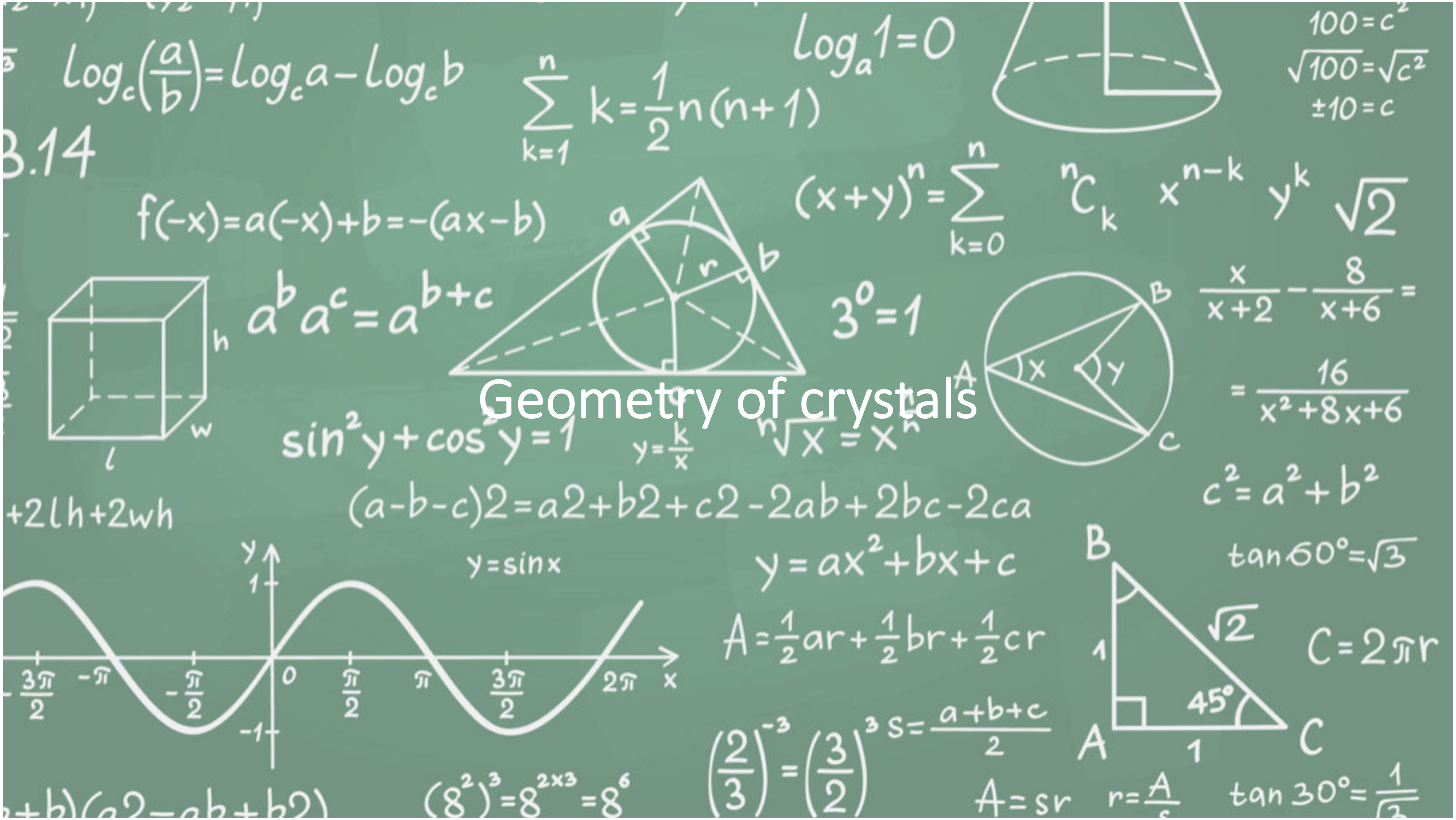
11. Electrões em semi-condutores



1. Crystal structure: Lattices



Geometry of crystals



Ideal solid

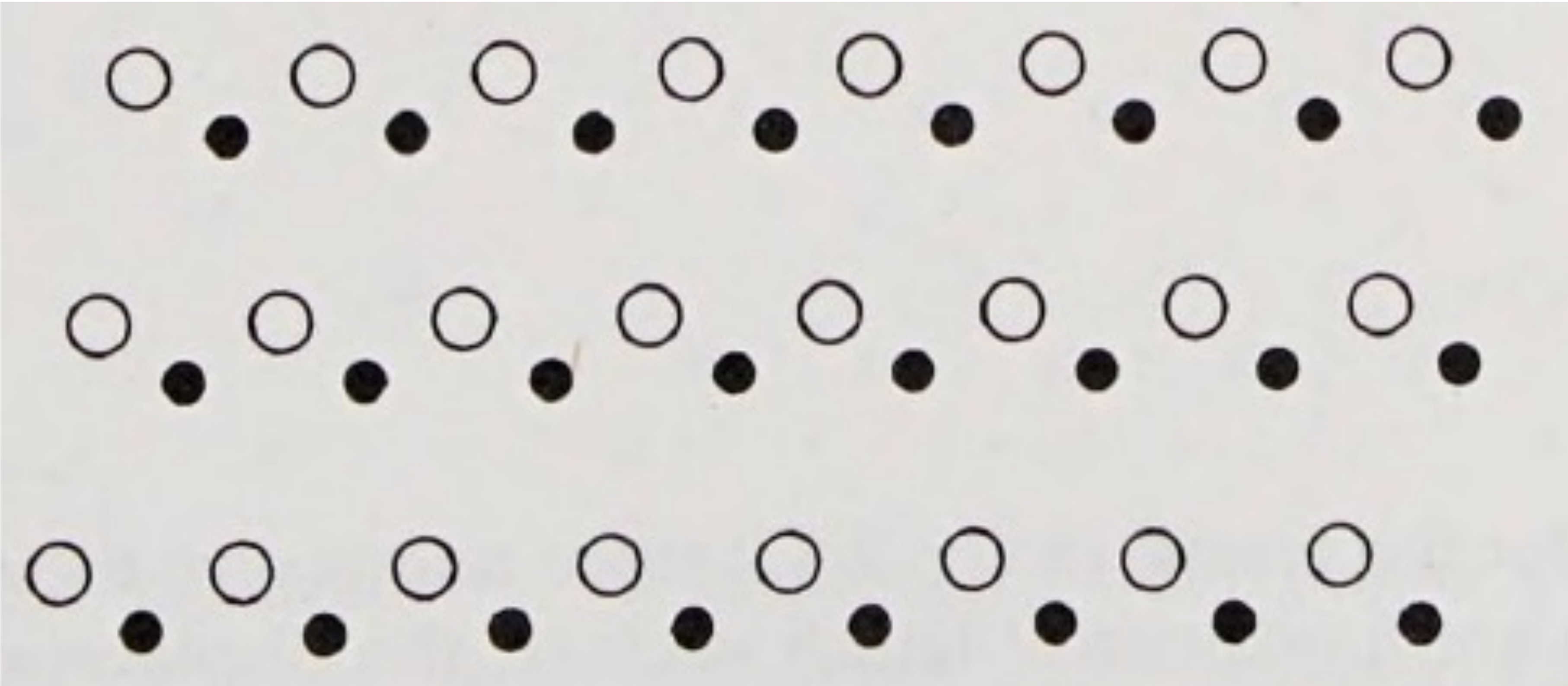
Periodic structure where the atoms are placed regularly with the medium exhibiting symmetry of translation.

Mathematically, there is symmetry of translation, in 3d, when there are, 3 no coplanar, vectors such that the medium is invariant for a translation

$$T = n_1\mathbf{a}+n_2\mathbf{b}+n_3\mathbf{c}$$

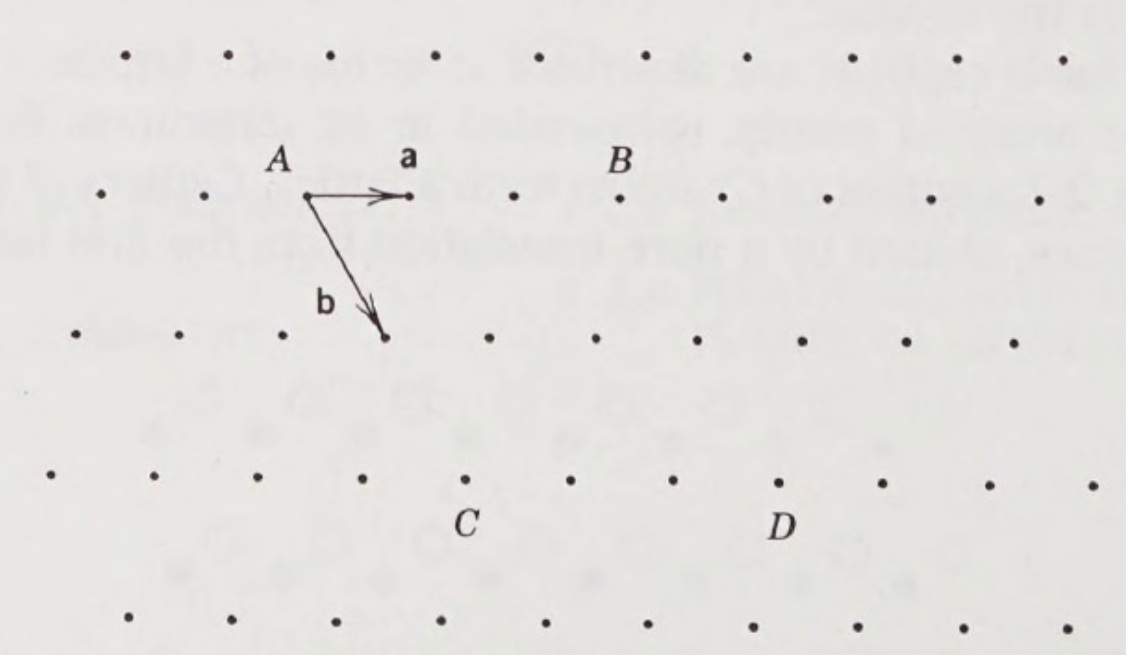
for all integers n_i

2D crystalline solid: the basis of two atoms is repeated periodically

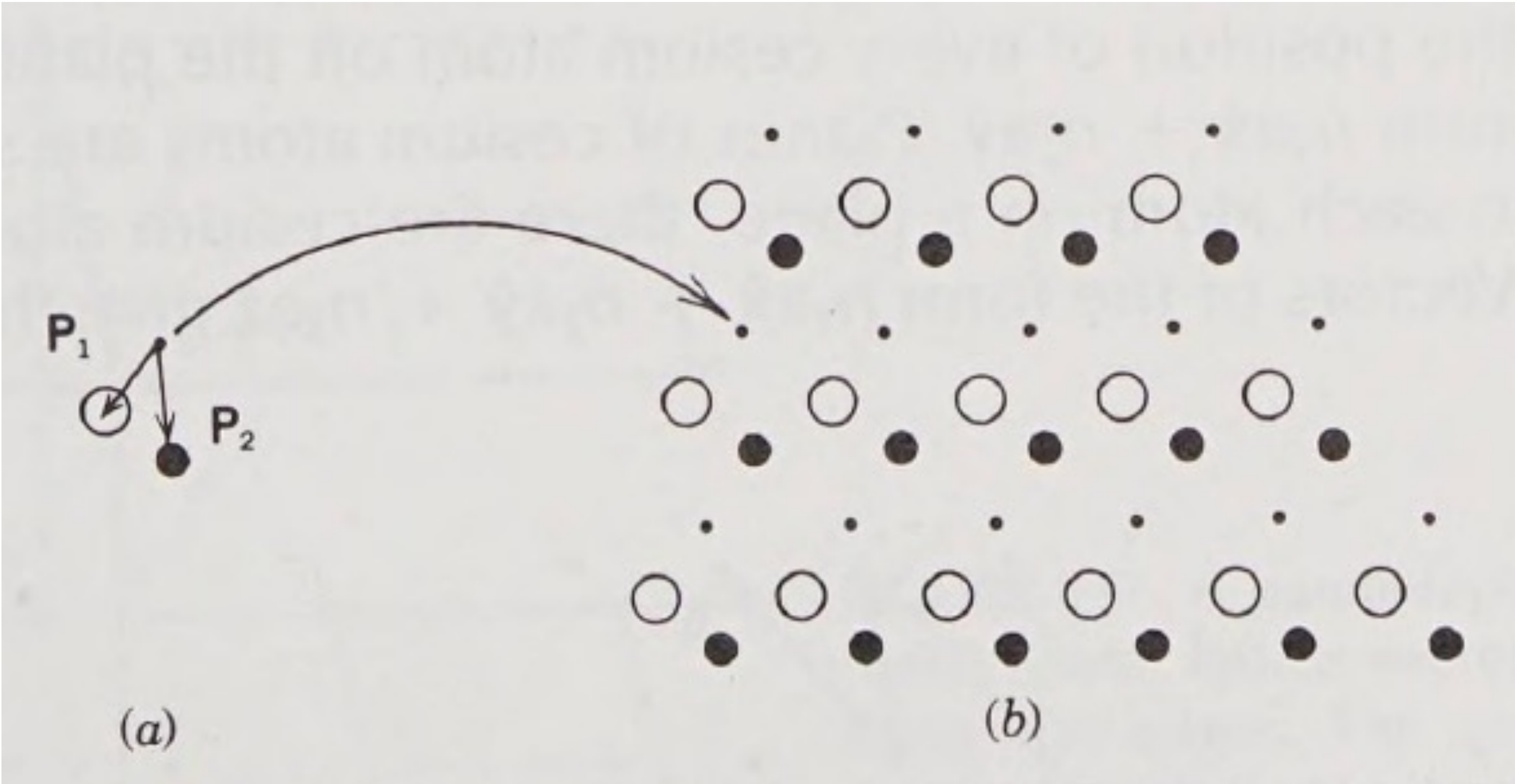


Lattice points give the positions of the basis
a and **b** are fundamental lattice vectors

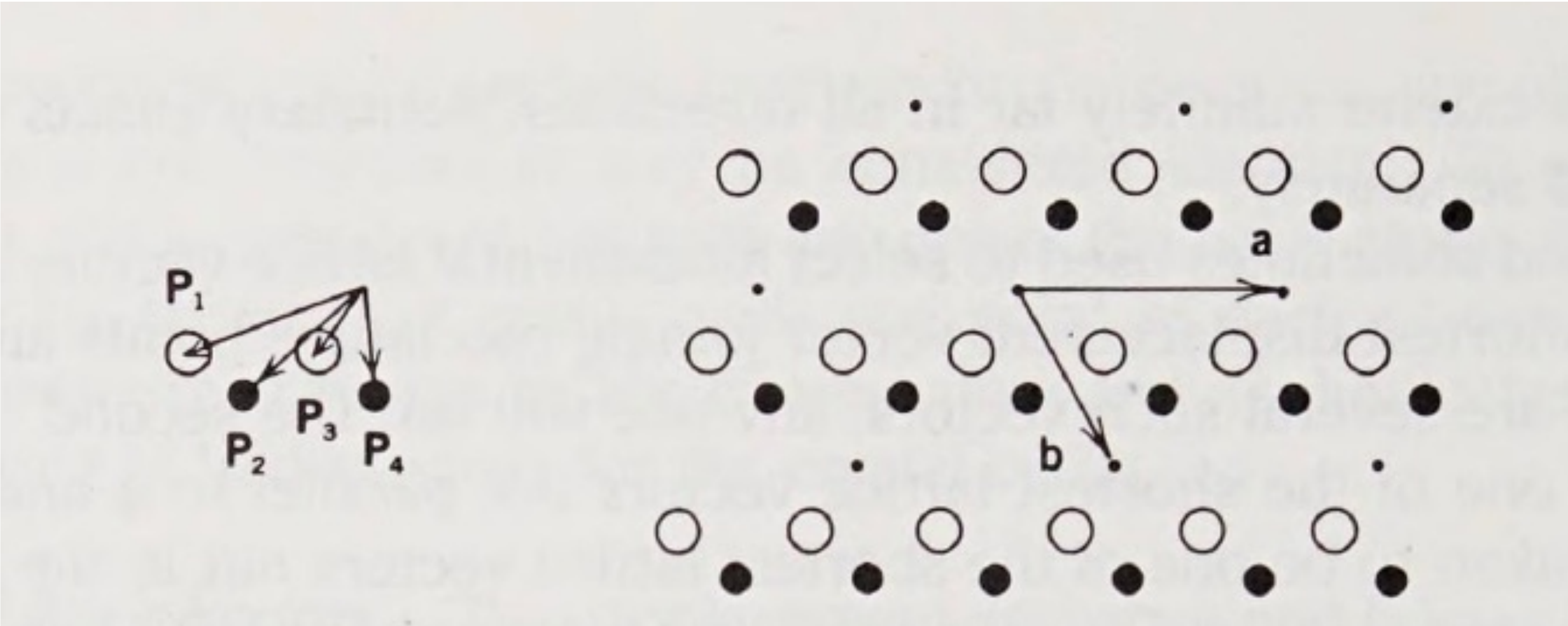
Displacement of any lattice point is $n_1\mathbf{a}+n_2\mathbf{b}$



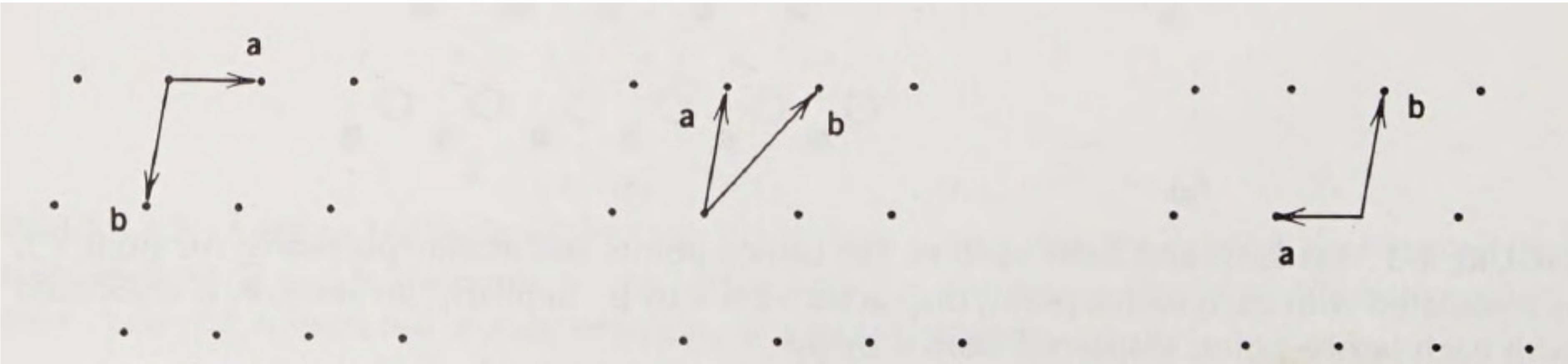
Basis and basis vectors (a) lattice points and atomic positions (b)



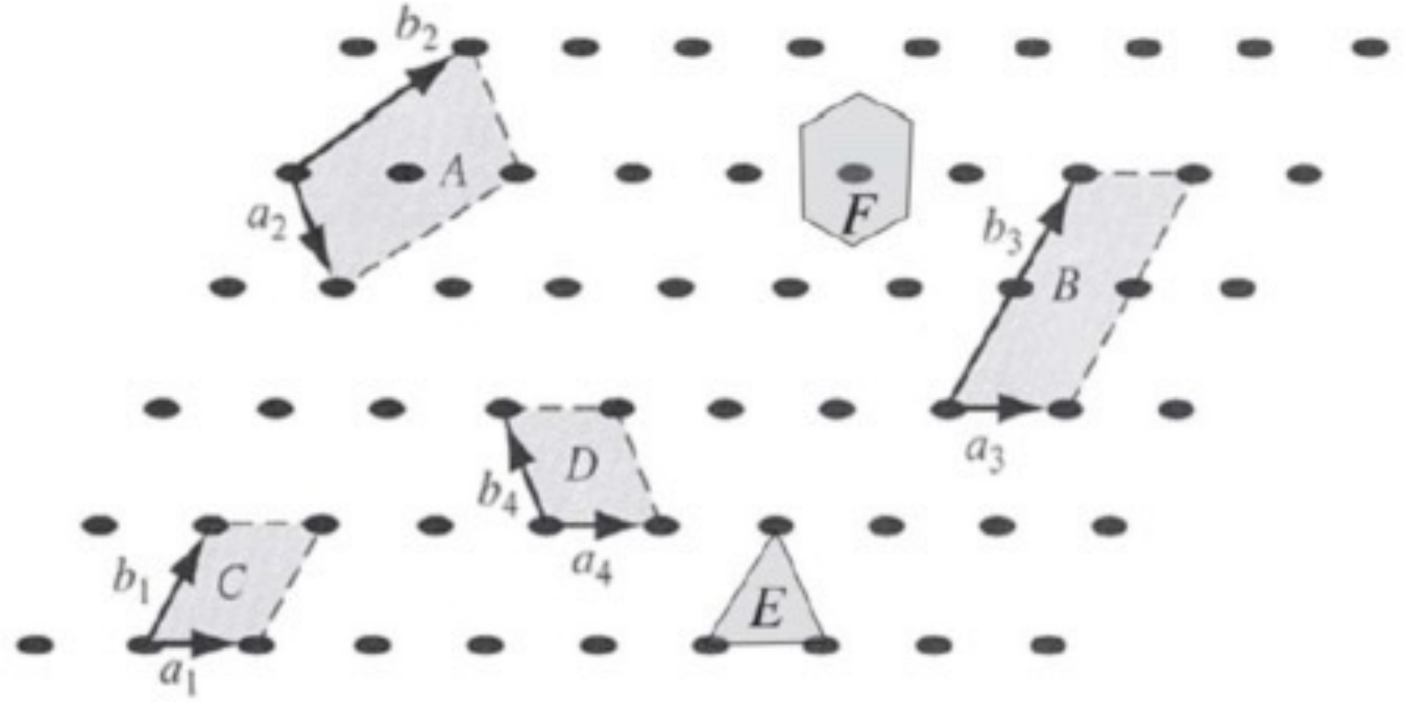
Another basis and the same lattice



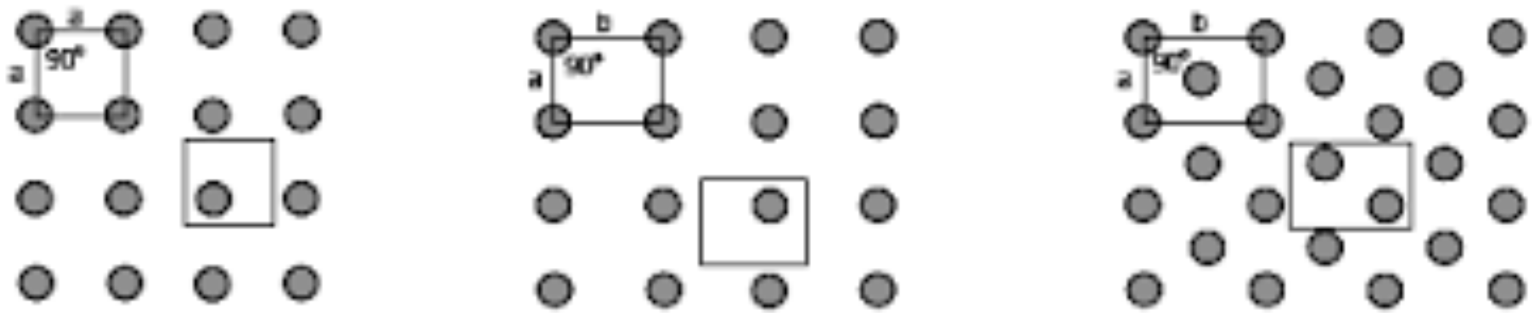
Primitive lattice vectors correspond to the smallest possible basis



Lattice vectors and unit cells



Unit cells

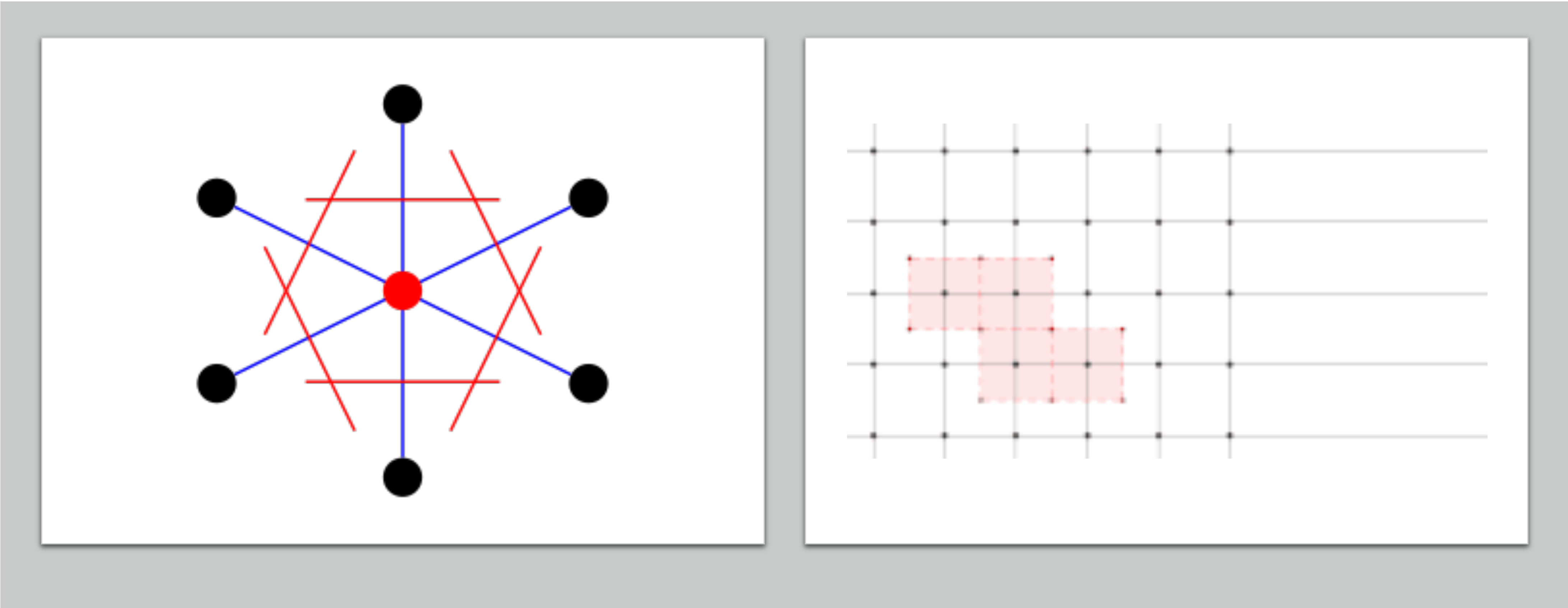


square lattice
square unit cell

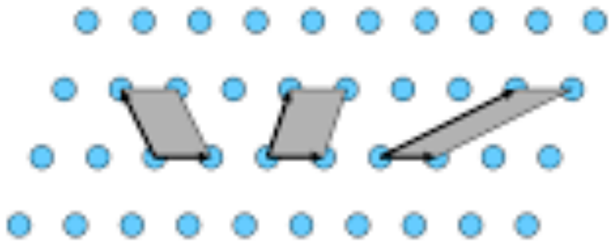
rectangular lattice
rectangular unit cell

rectangular lattice
centered rectangular unit cell

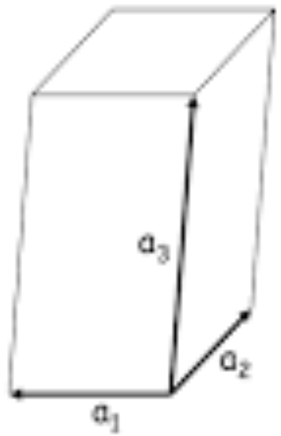
Wigner-Seitz cell



Volume of a unit cell



There is more than one choice for a primitive unit cell

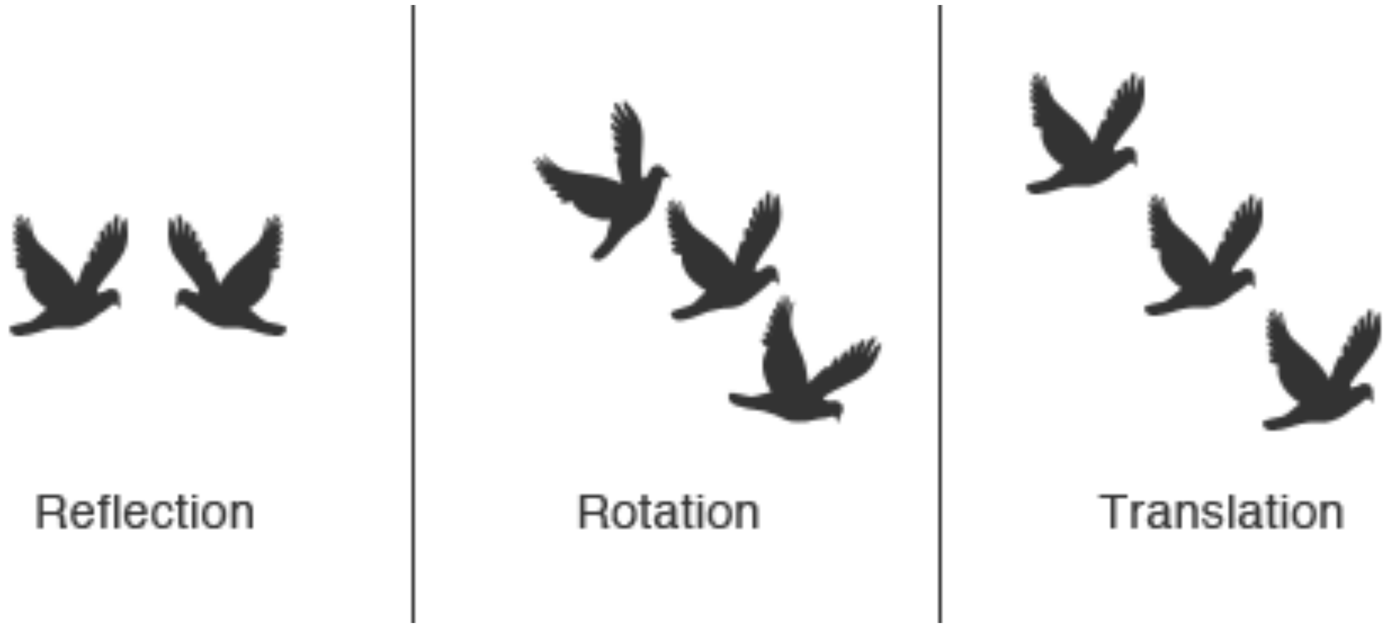


Primitive unit cell

Volume of a unit cell

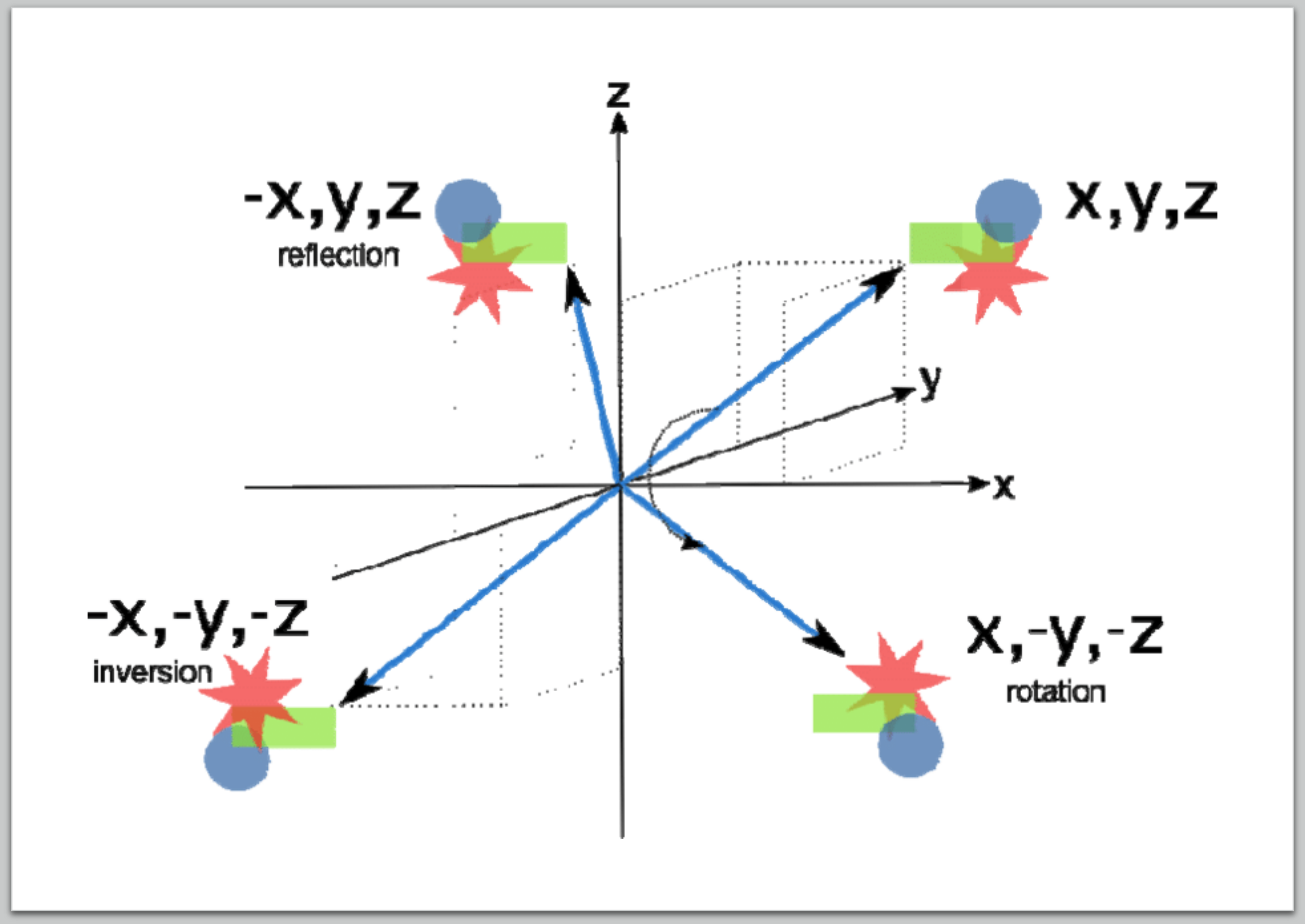
|**c** . **a** x b|

Rigid symmetry operations: Point & spatial

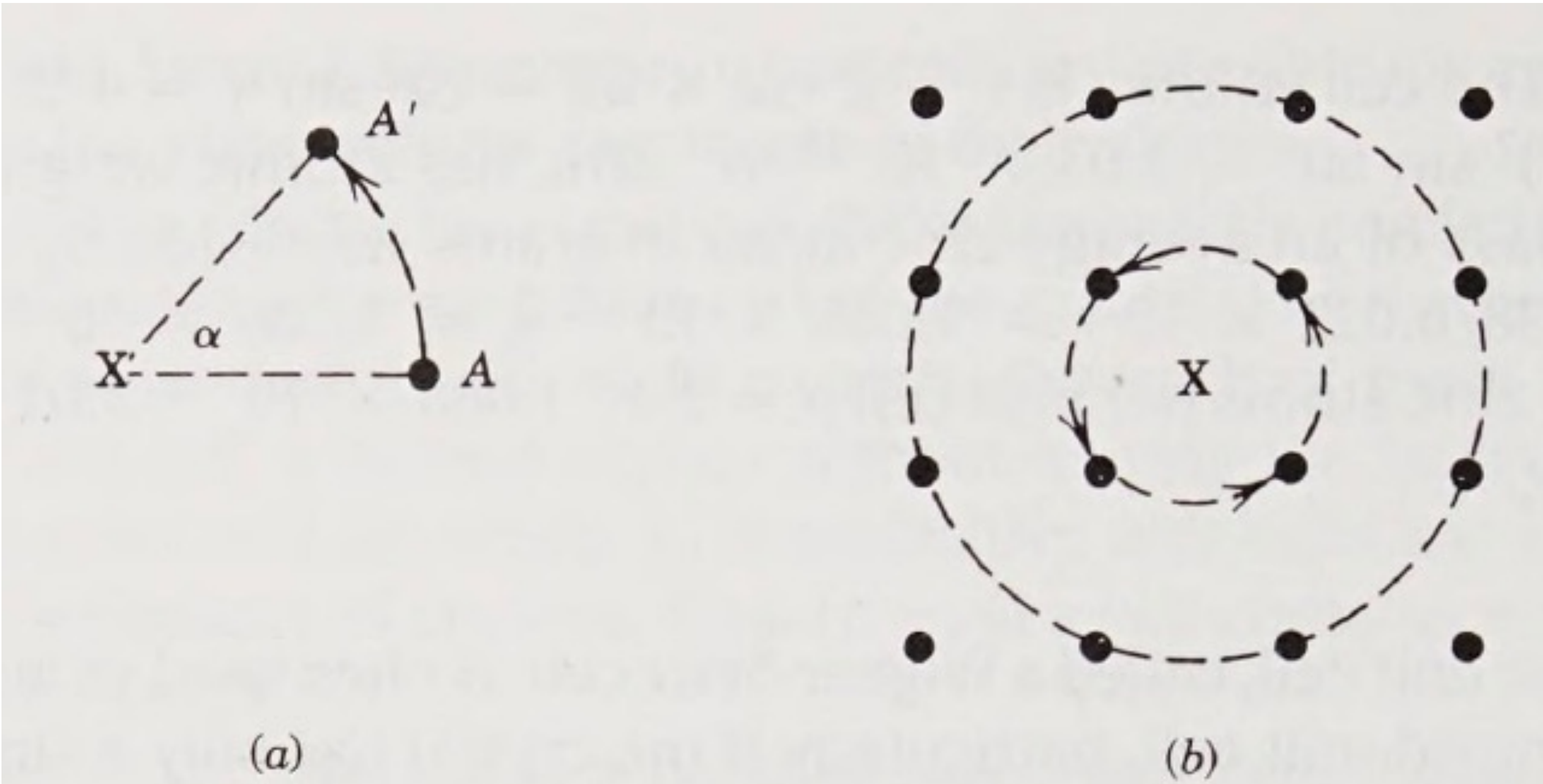


Point symmetries

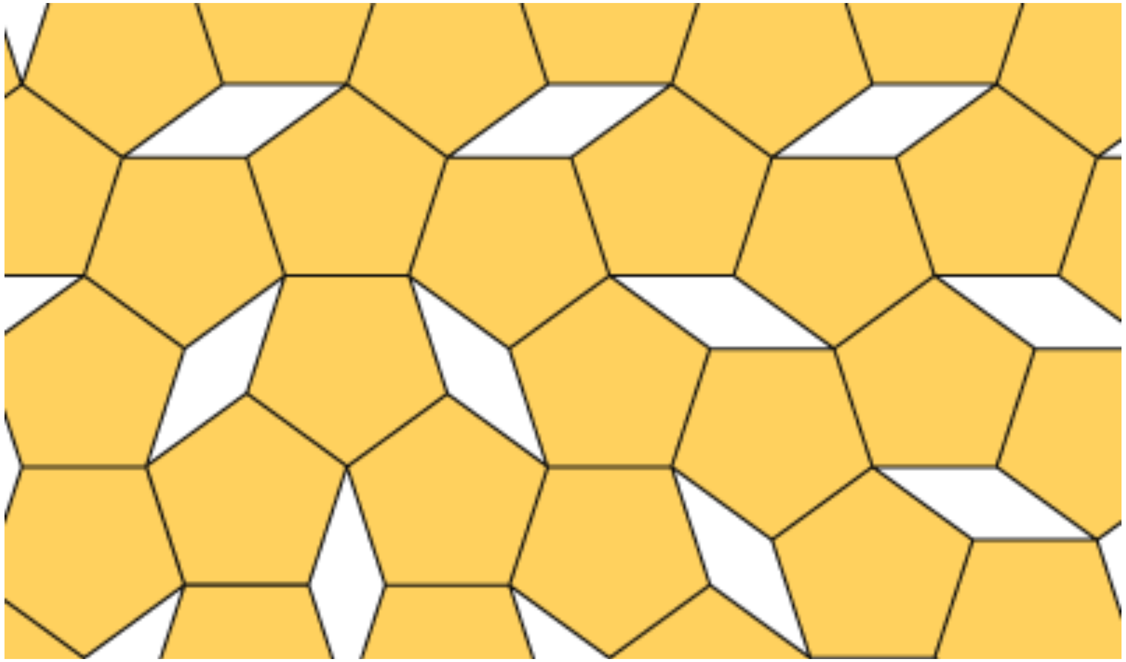
Mirror, rotation and inversion

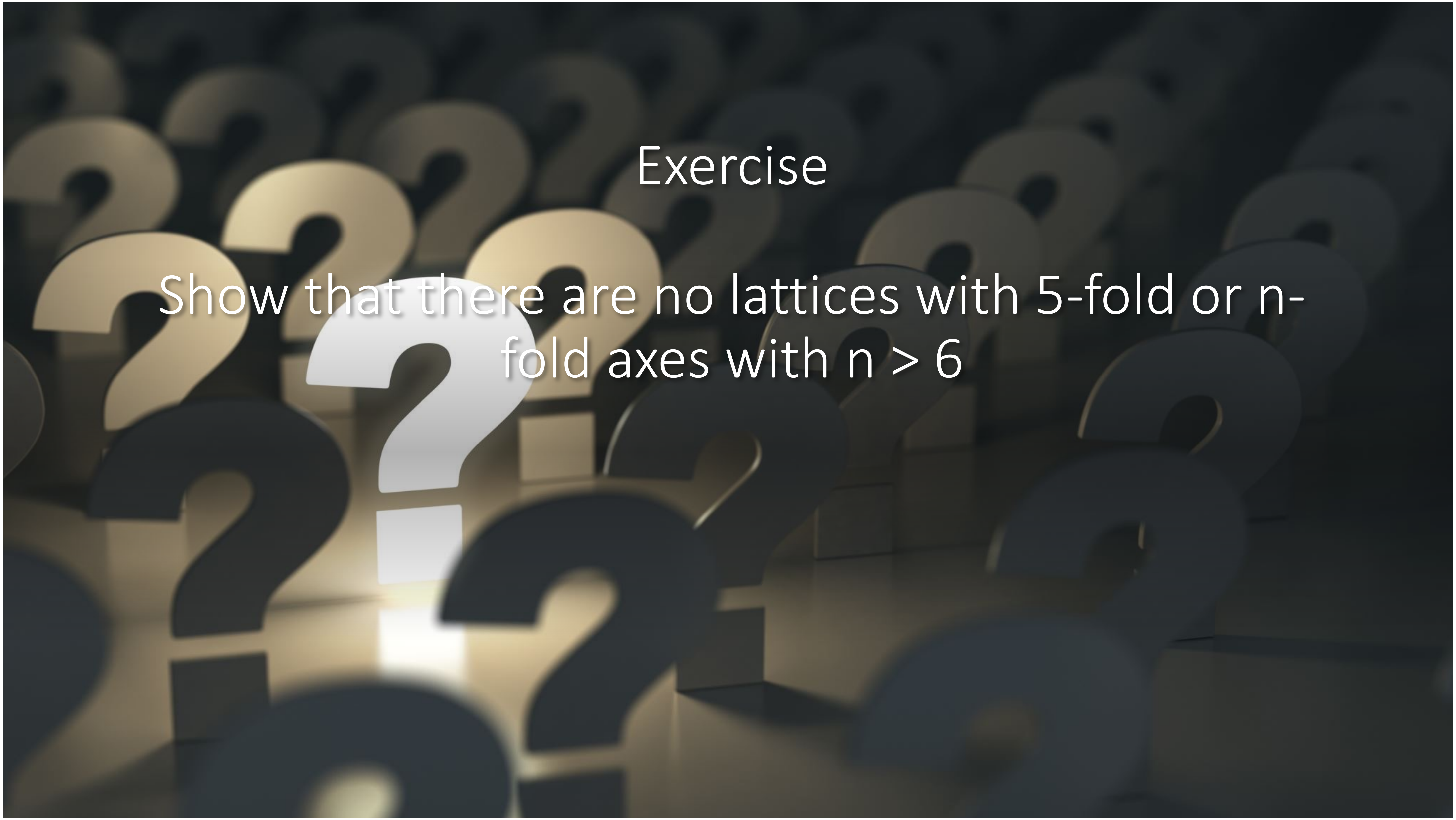


Rotational symmetry

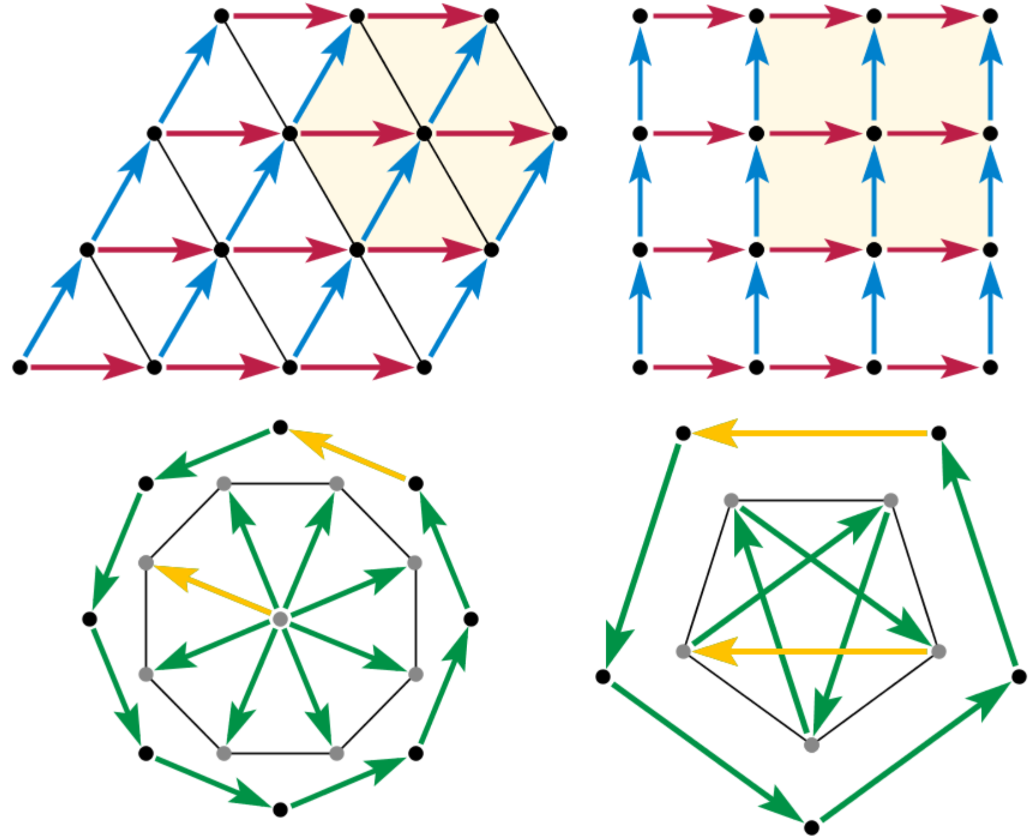


Crystals do not have 5-fold rotational axes

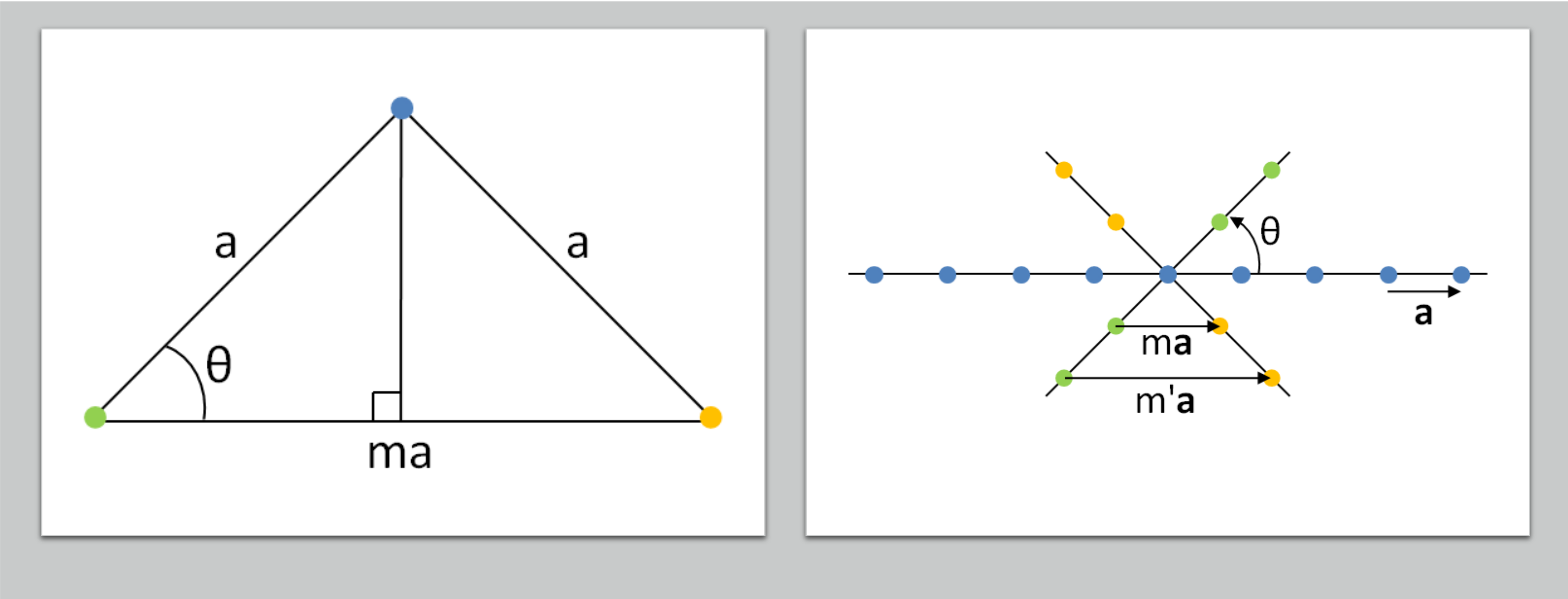



Exercise
Show that there are no lattices with 5-fold or n-fold axes with n > 6

Lattice proof



Geometric proof



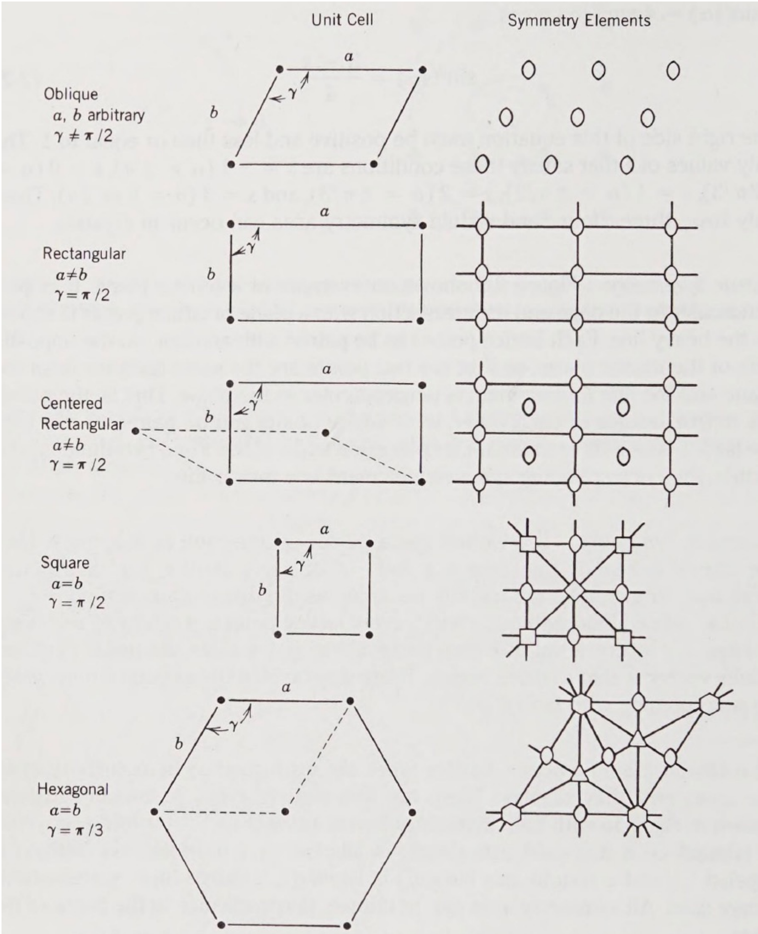
Rigid symmetries are not independent

For example, a 2-fold axis perpendicular to a mirror plane implies inversion symmetry (prove this).

Small number of symmetry groups in 2 and 3 dimensions.

Point symmetry groups: Crystallographic systems

Spatial symmetry groups: Bravais lattices

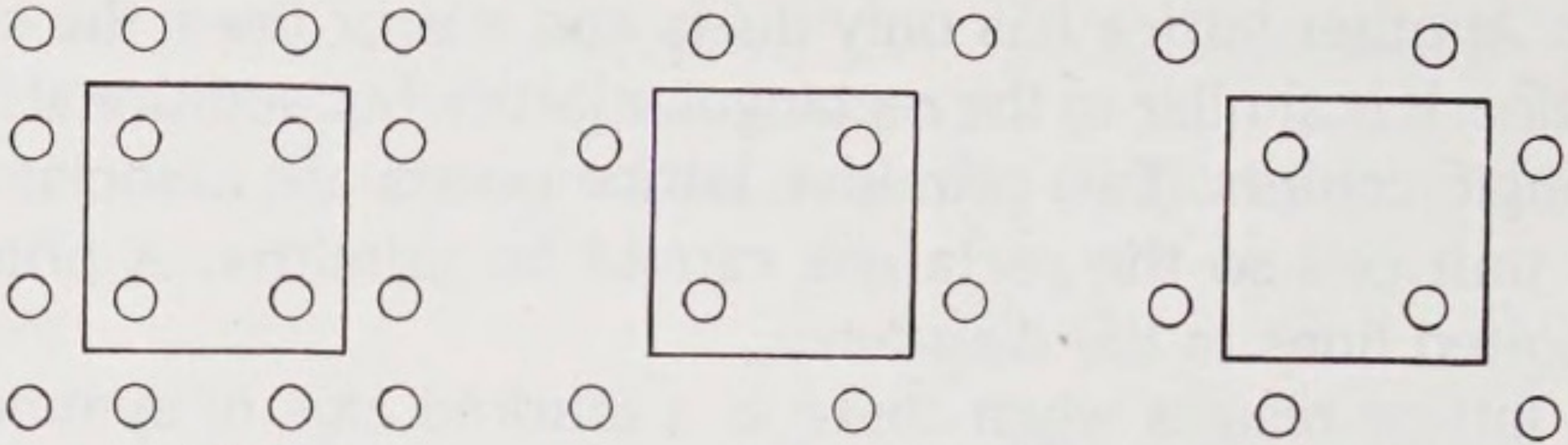


2D

Unit cells and symmetry groups

5 Bravais lattices

4 crystallographic systems



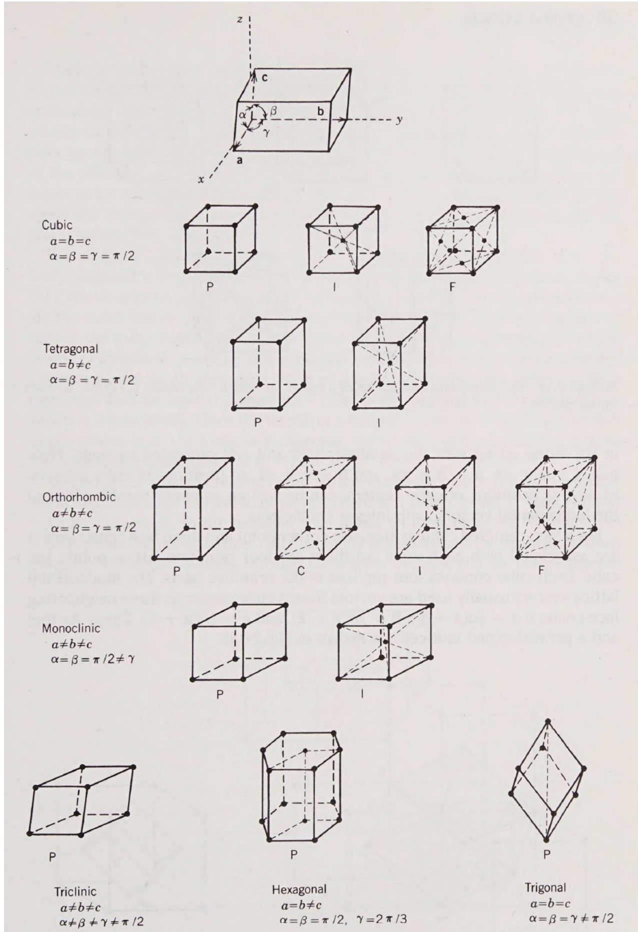
(a) (b) (c)

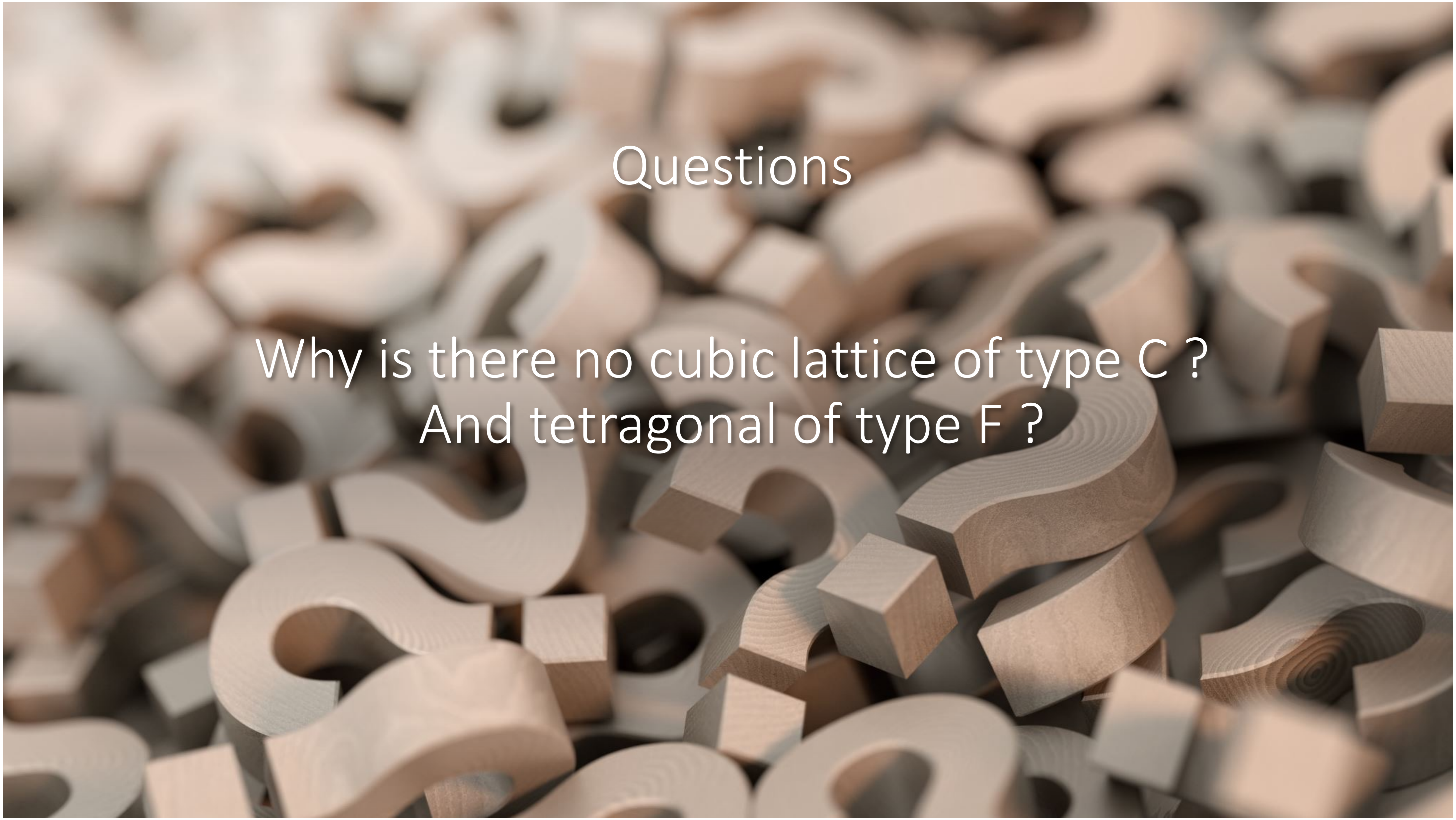
3D

Unit cells and symmetry groups

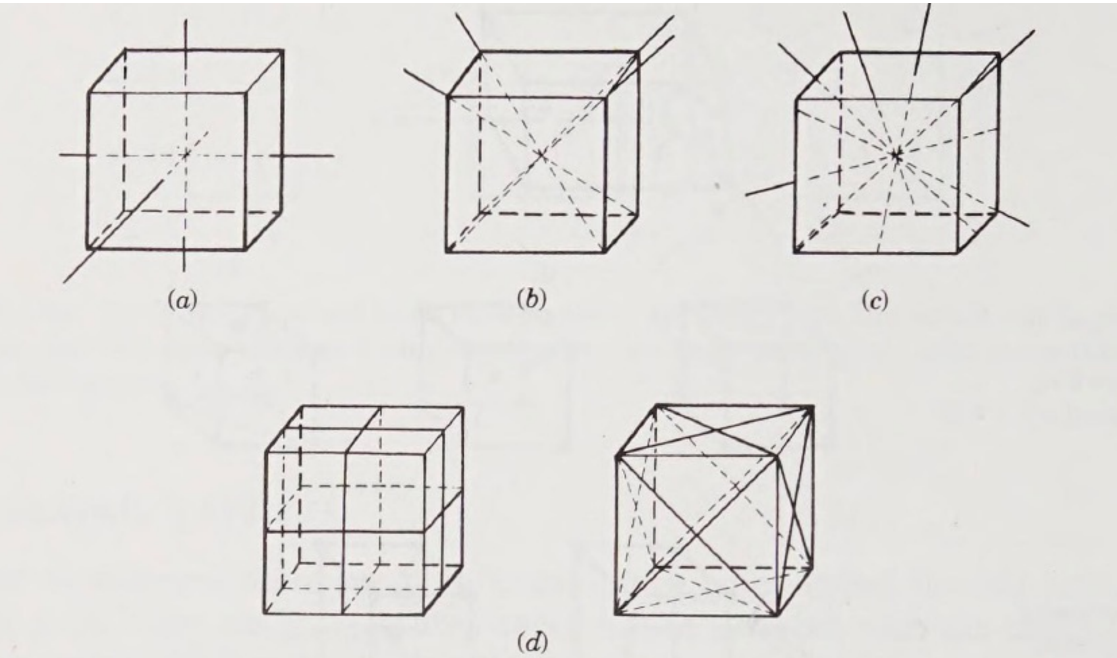
14 Bravais lattices

7 crystallographic systems

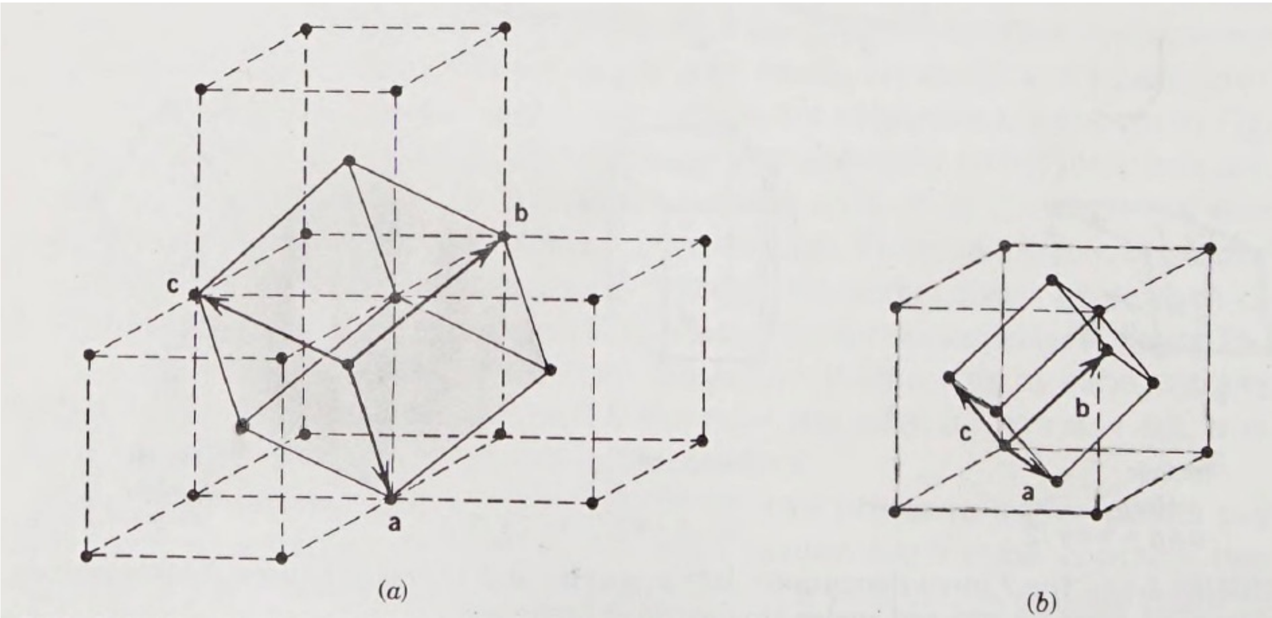



Questions
Why is there no cubic lattice of type C ?
And tetragonal of type F ?

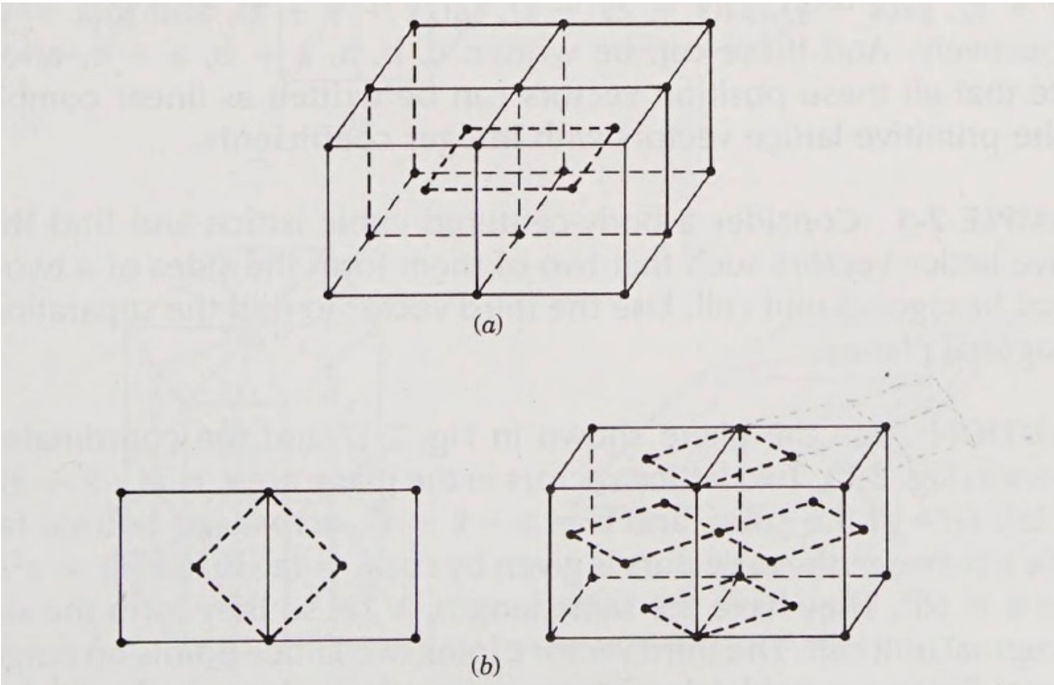
Symmetry axes and planes of a cube



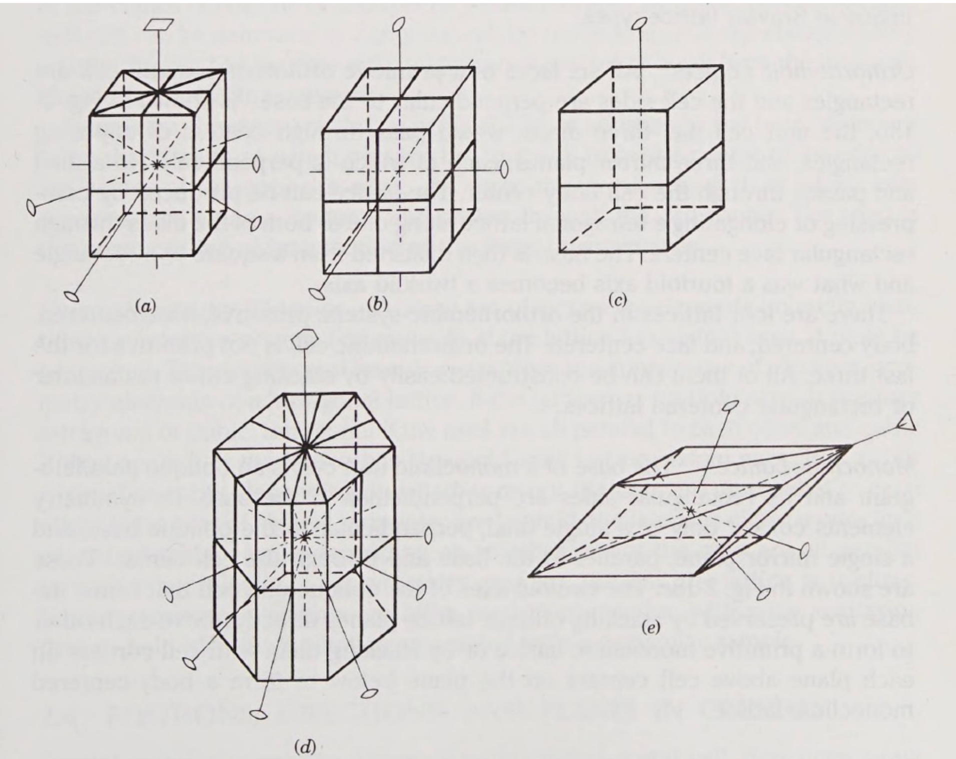
Primitive translation vectors and primitive cells for bcc and fcc



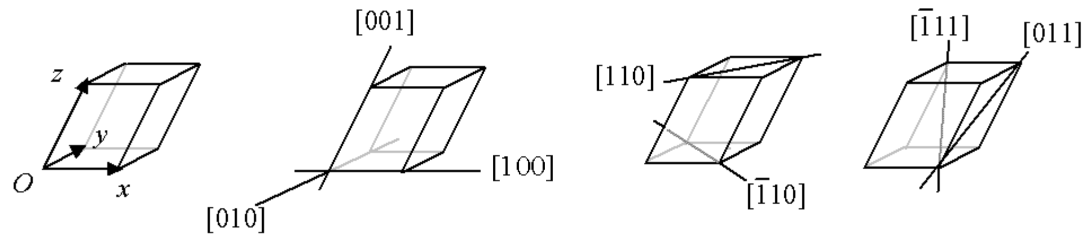
Stacking of square lattices to form bcc and fcc



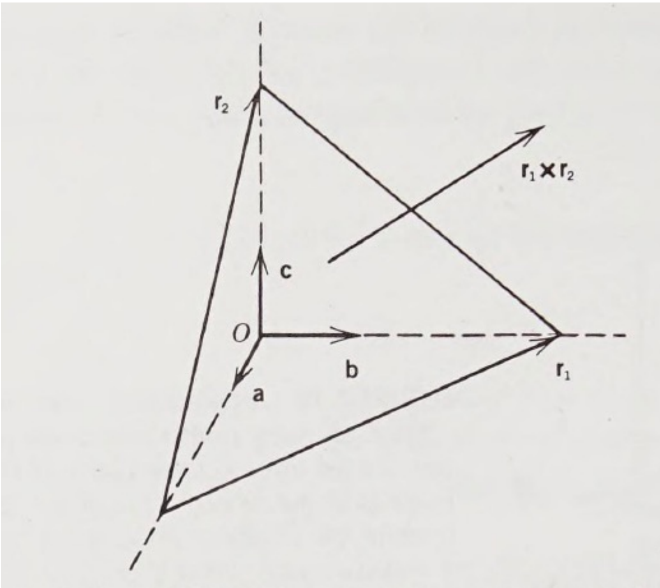
Symmetry elements of unit cells

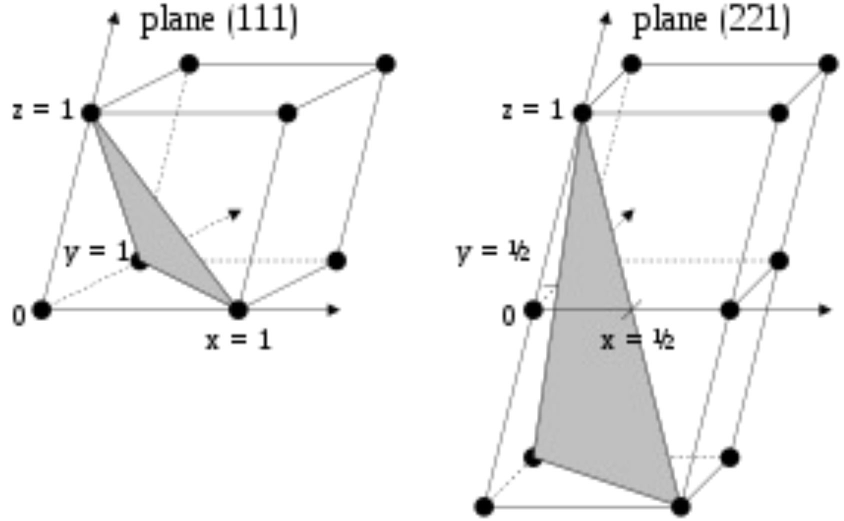


Directions

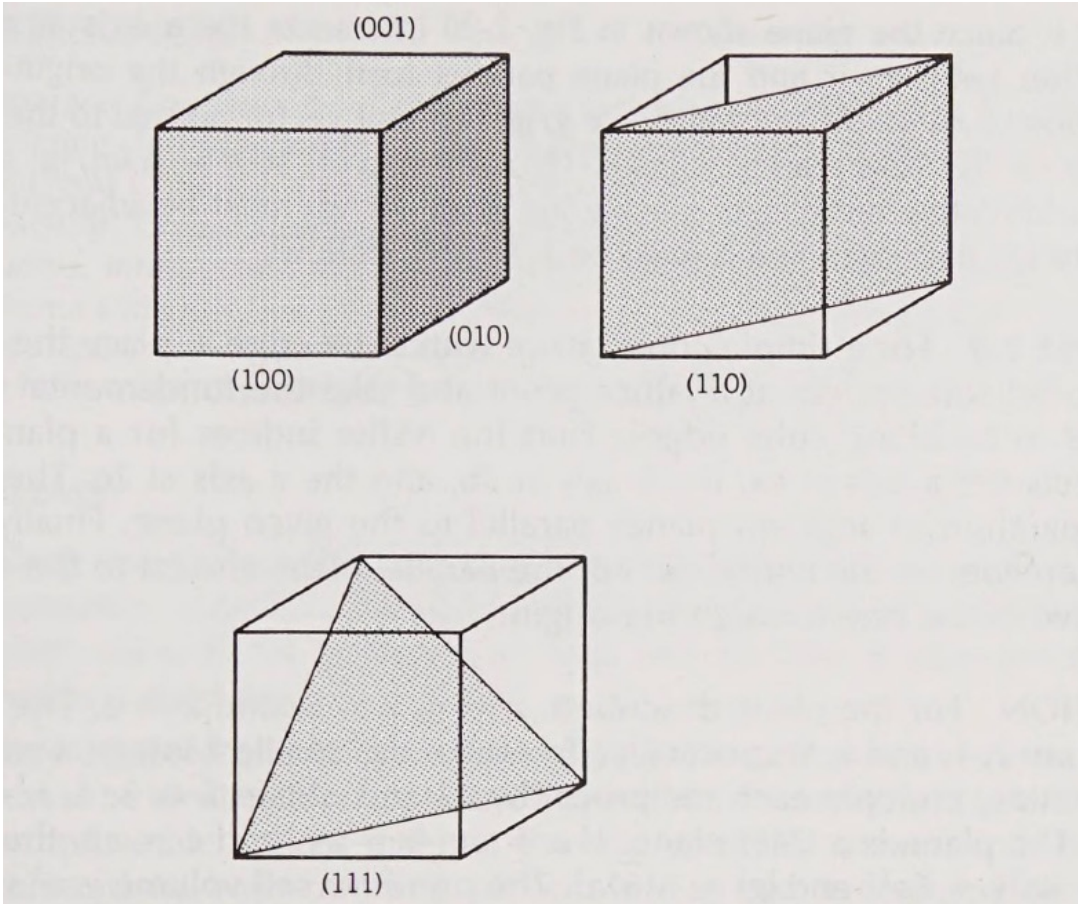


Crystallograpic planes: Miller indices

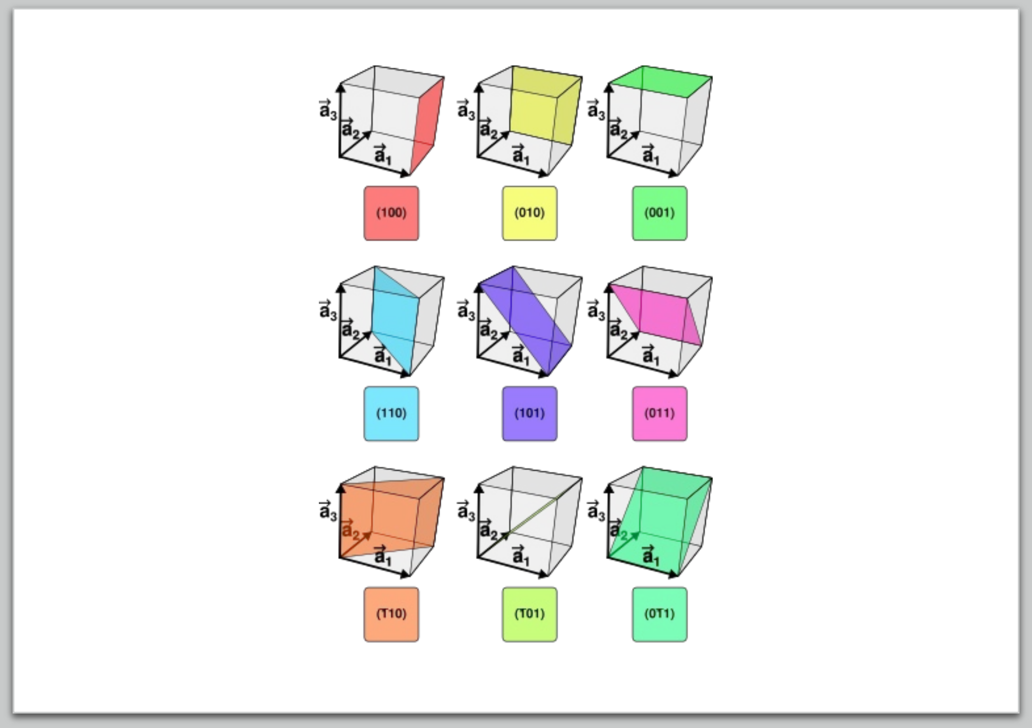


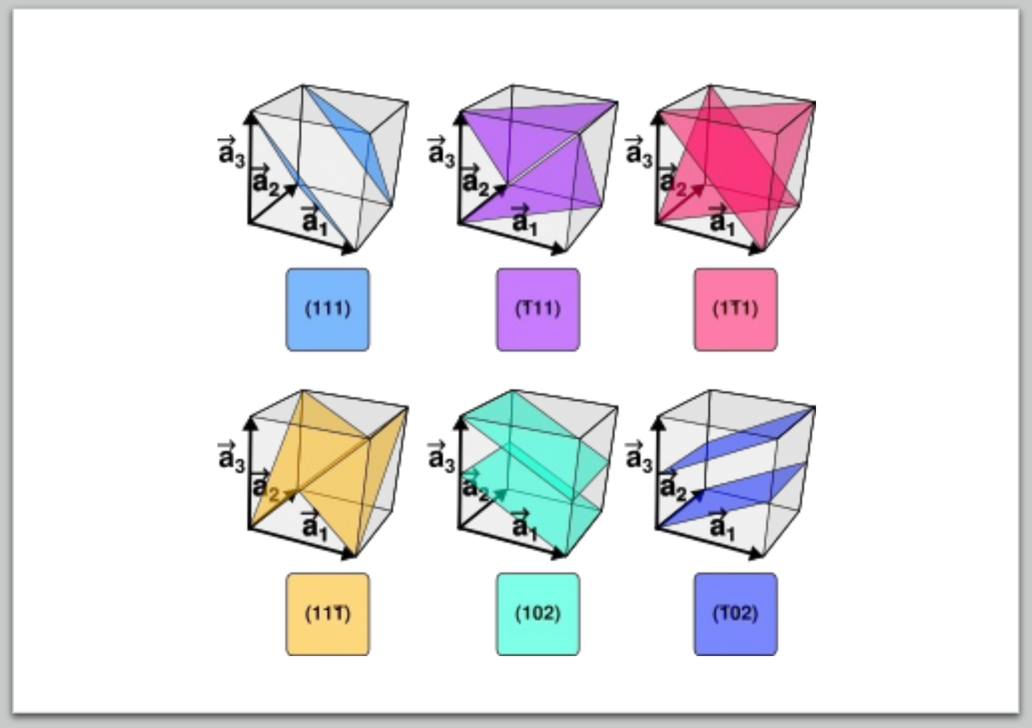


Planes of cubic lattices

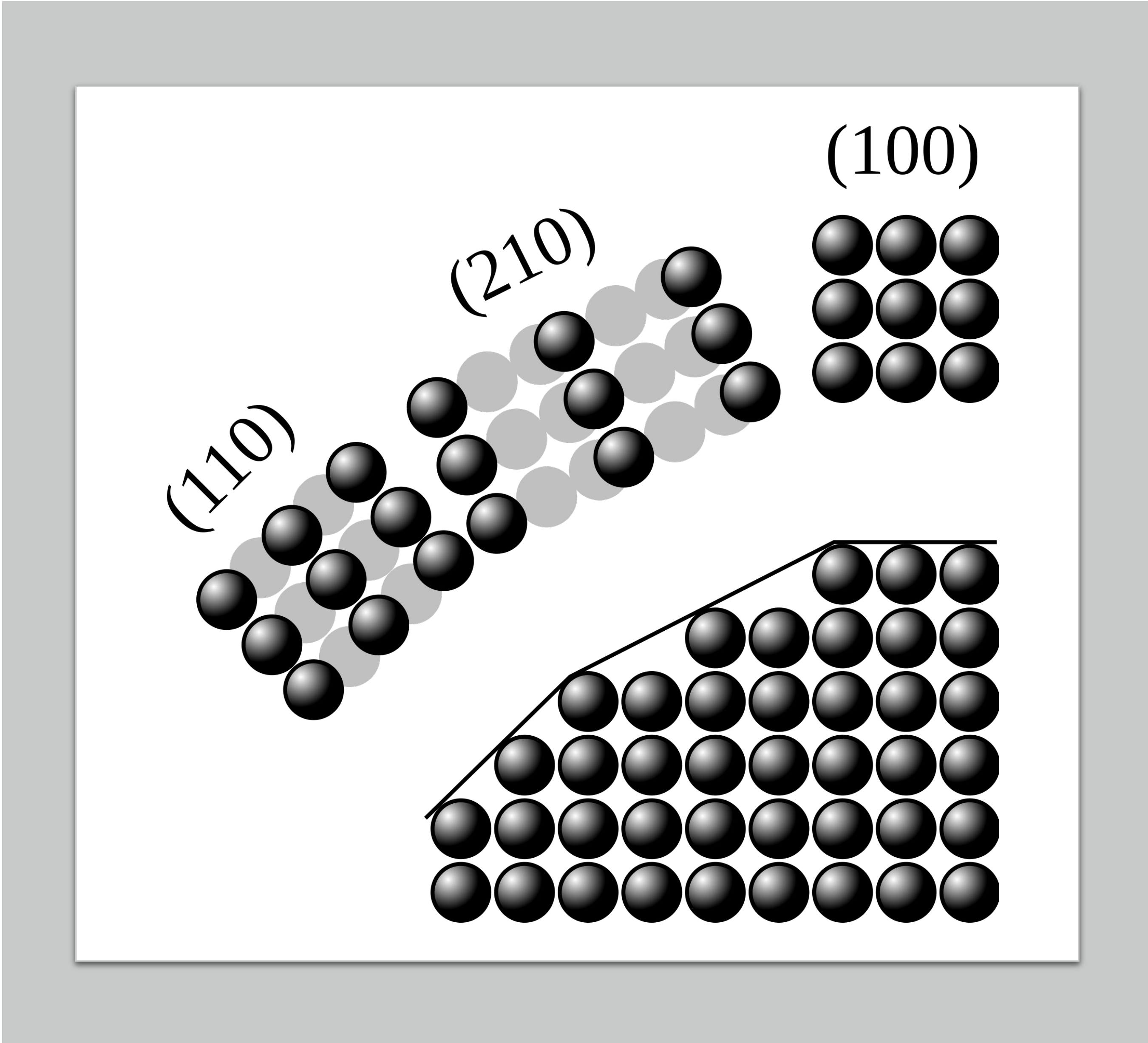


Planes of cubic lattices

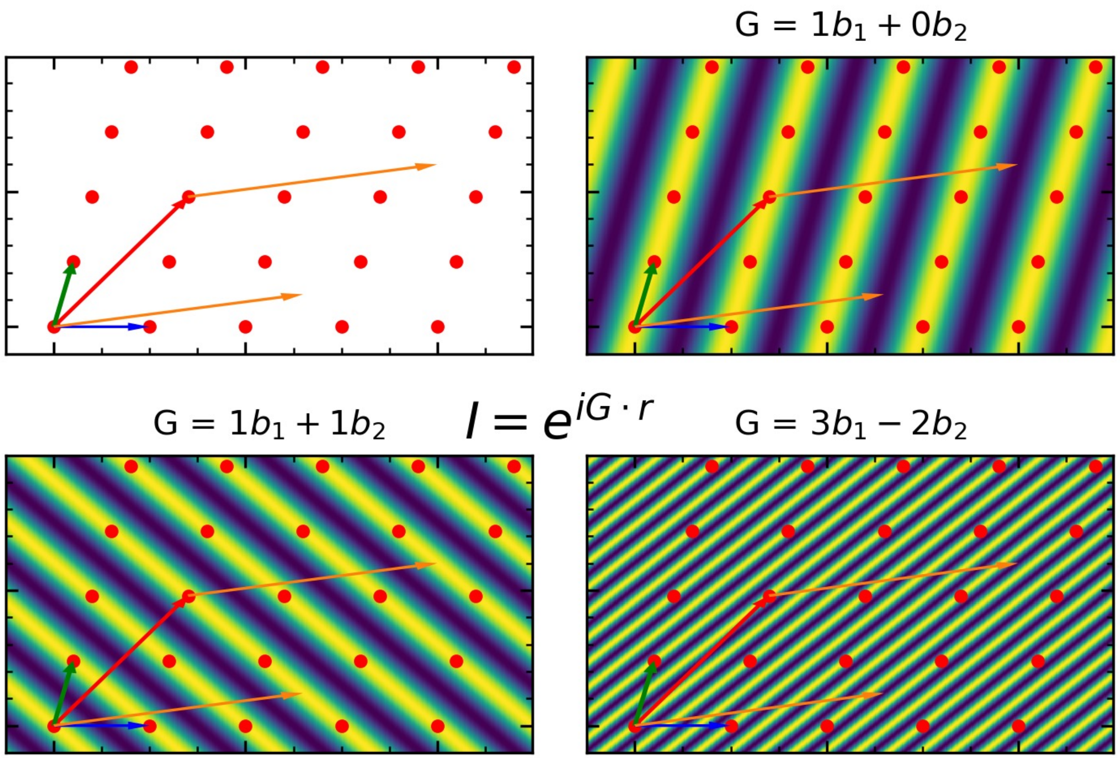




Dense crystallographic planes



Reciprocal lattice



$$I = e^{iG \cdot r}$$

Reciprocal lattice vectors

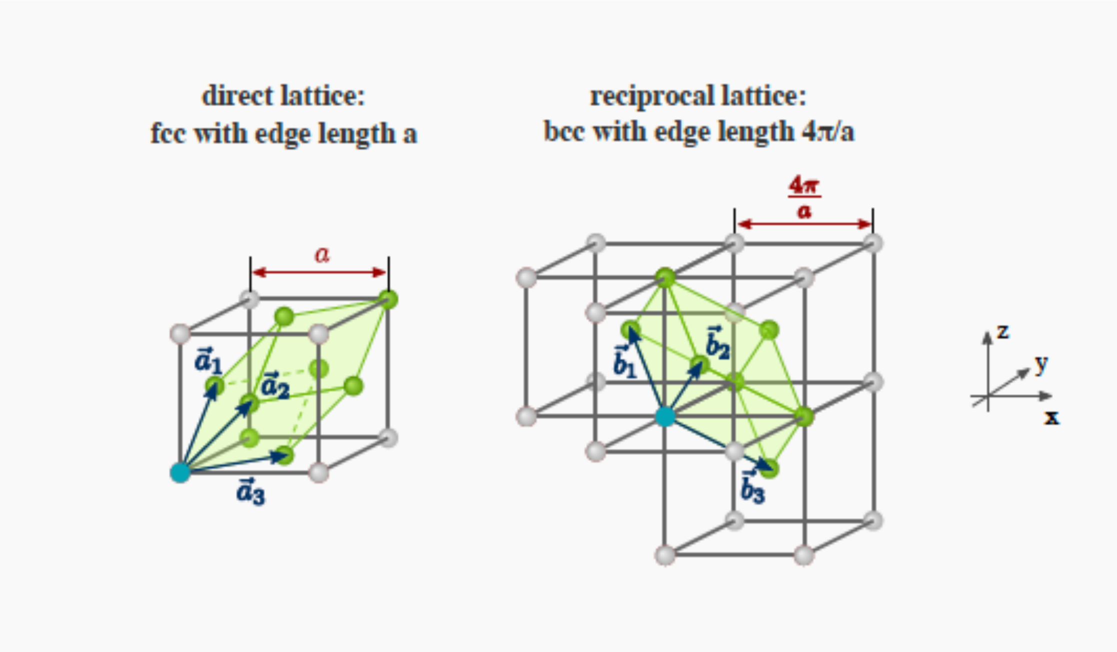
$$\vec{b}_1 = 2\pi \cdot \frac{\vec{a}_2 \times \vec{a}_3}{V}$$

$$\vec{b}_2 = 2\pi \cdot \frac{\vec{a}_3 \times \vec{a}_1}{V}$$

$$\vec{b}_3 = 2\pi \cdot \frac{\vec{a}_1 \times \vec{a}_2}{V}$$

- As we have seen above, the reciprocal lattice of a Bravais lattice is again a Bravais lattice.
- The reciprocal latticeof a reciprocal lattice is the (original) direct lattice.
- The length of the reciprocal lattice vectors is proportional to the reciprocal of the length of the direct lattice vectors. This is where the term reciprocal lattice arises from.

Reciprocal lattice of an fcc lattice



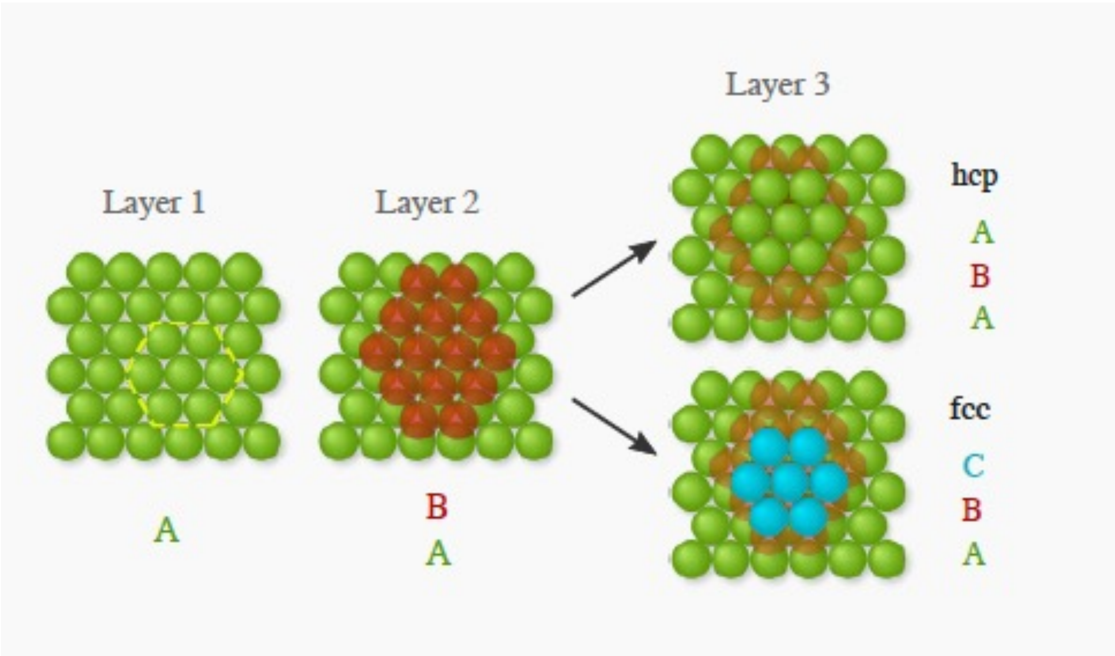
$$\vec{b}_1 = \frac{8\pi}{a^3} \cdot \vec{a}_2 \times \vec{a}_3 = \frac{4\pi}{a} \cdot \left(-\frac{\hat{x}}{2} + \frac{\hat{y}}{2} + \frac{\hat{z}}{2} \right)$$

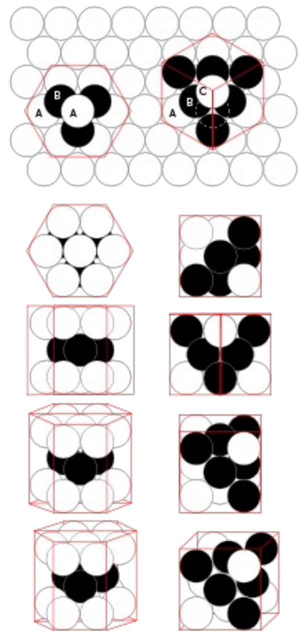
$$\vec{b}_2 = \frac{8\pi}{a^3} \cdot \vec{a}_3 \times \vec{a}_1 = \frac{4\pi}{a} \cdot \left(\frac{\hat{x}}{2} - \frac{\hat{y}}{2} + \frac{\hat{z}}{2} \right)$$

$$\vec{b}_3 = \frac{8\pi}{a^3} \cdot \vec{a}_1 \times \vec{a}_2 = \frac{4\pi}{a} \cdot \left(\frac{\hat{x}}{2} + \frac{\hat{y}}{2} - \frac{\hat{z}}{2} \right)$$

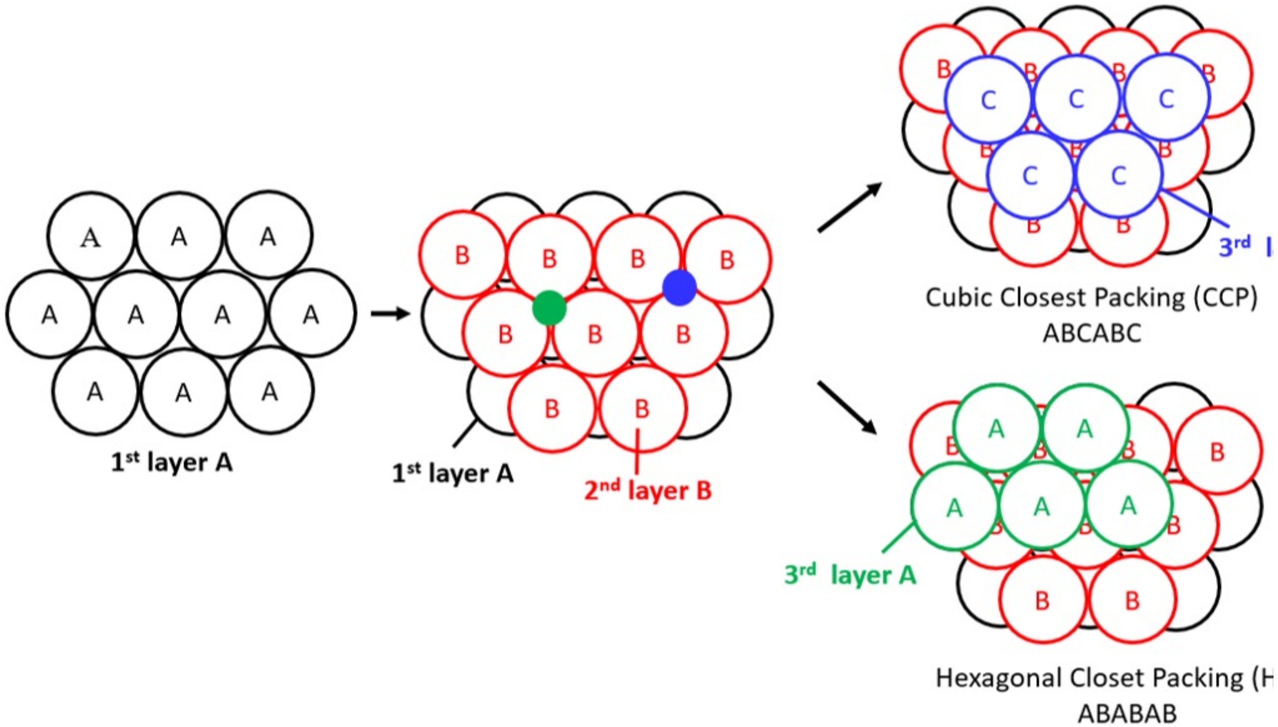
3. Structures of solids

Close packed structures





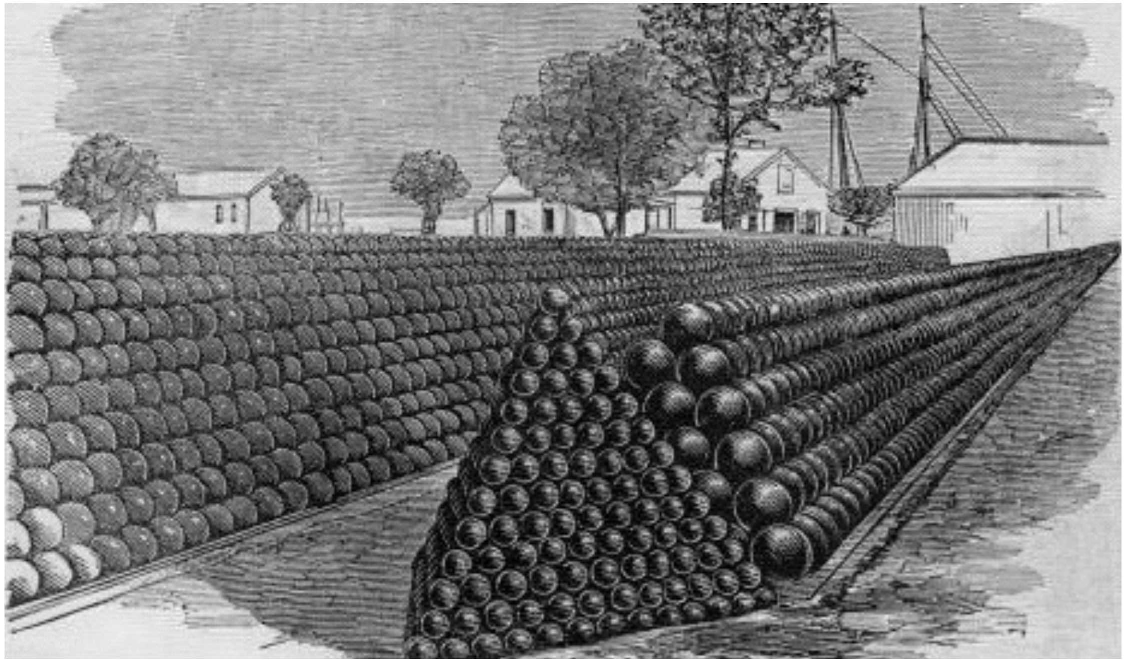
Close packed structures



Close packed structures

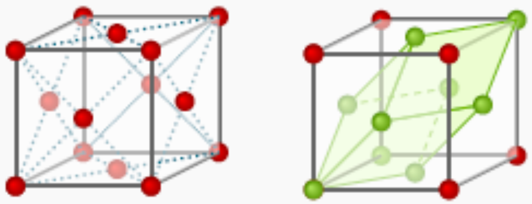
Snowballs stacked in preparation for a snowball fight. The front pyramid is hexagonal close - packed and rear is face-centered cubic.

The cannon ball mathematical problem (1587)



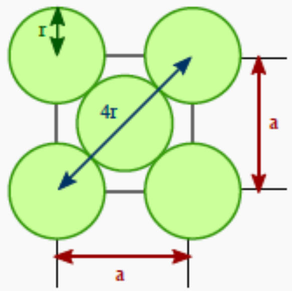
Cannonballs piled on a triangular *(front)* and rectangular *(back)* base, both fcc lattices.

Close packed density: fcc lattice



(a) conventional unit cell

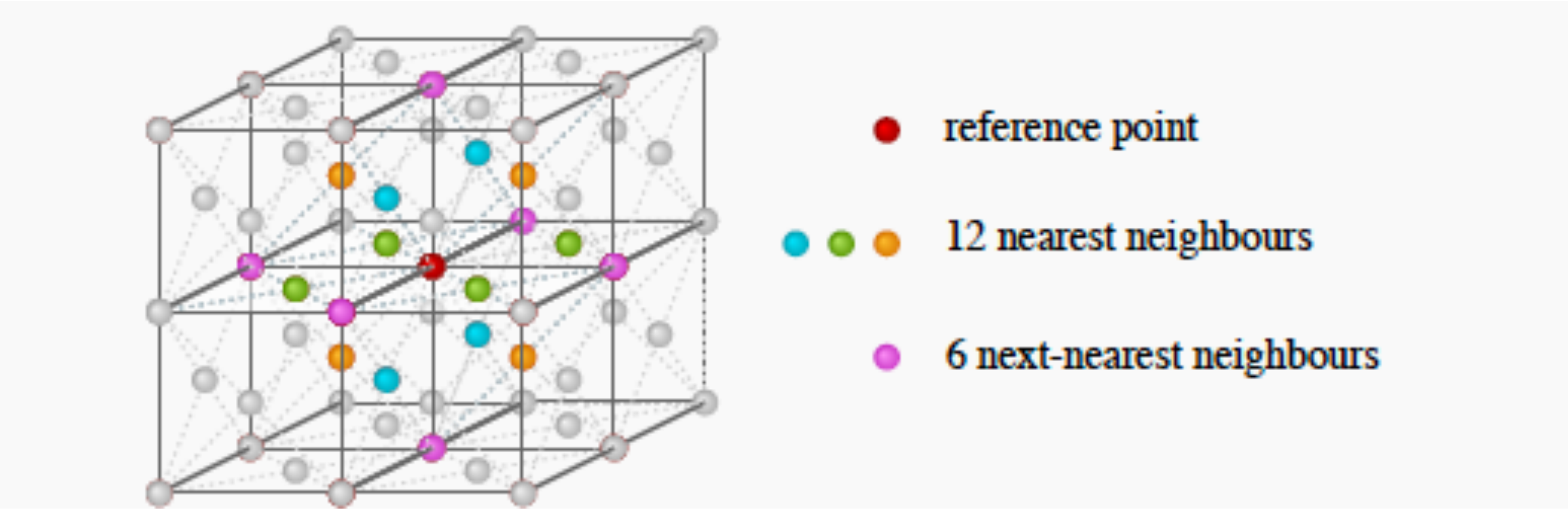
(b) primitive unit cell



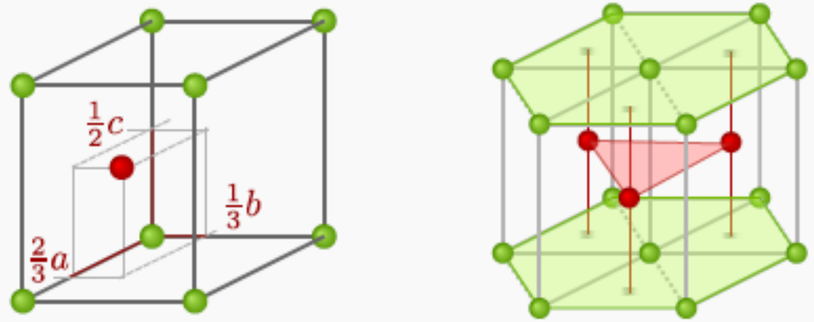
$$\varrho = \frac{n \cdot V_{\mathrm{sph}}}{V_{\mathrm{uc}}} = \frac{4 \cdot \frac{4}{3}\pi \cdot \left(\frac{\sqrt{2}}{4}\right)^3 a^3}{a^3}$$

$$= \frac{\sqrt{2}\pi}{6} \approx 74\%$$

Nearest-neighbours

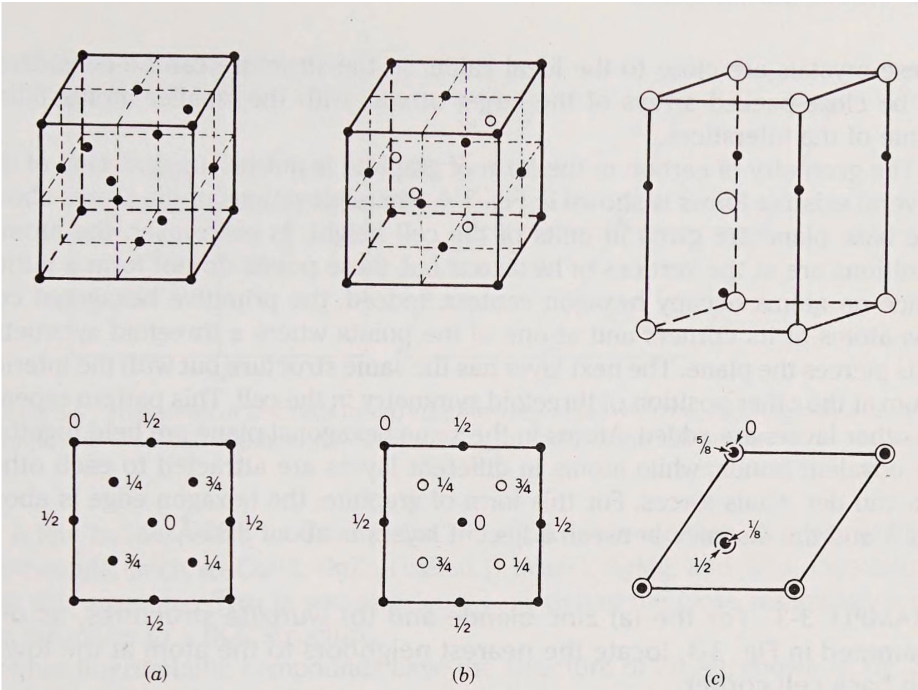


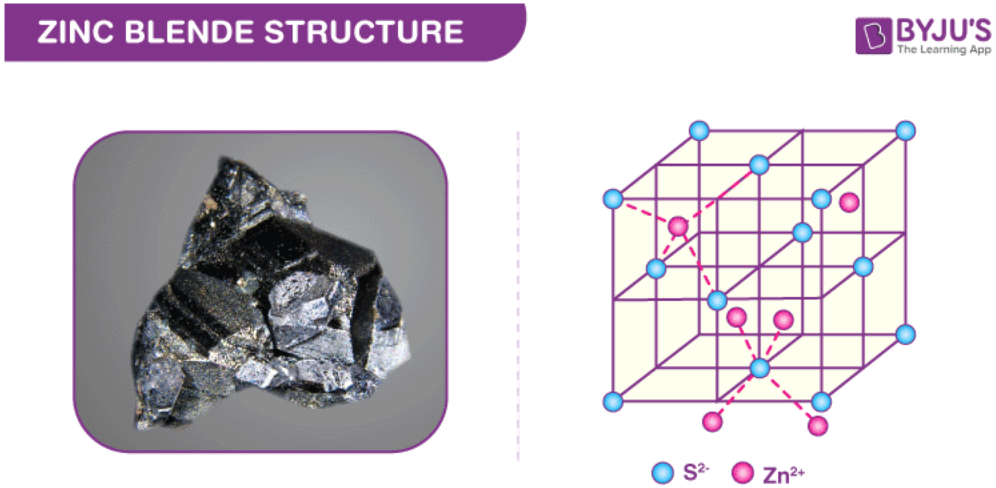
Second periodic close packed density: hcp structure

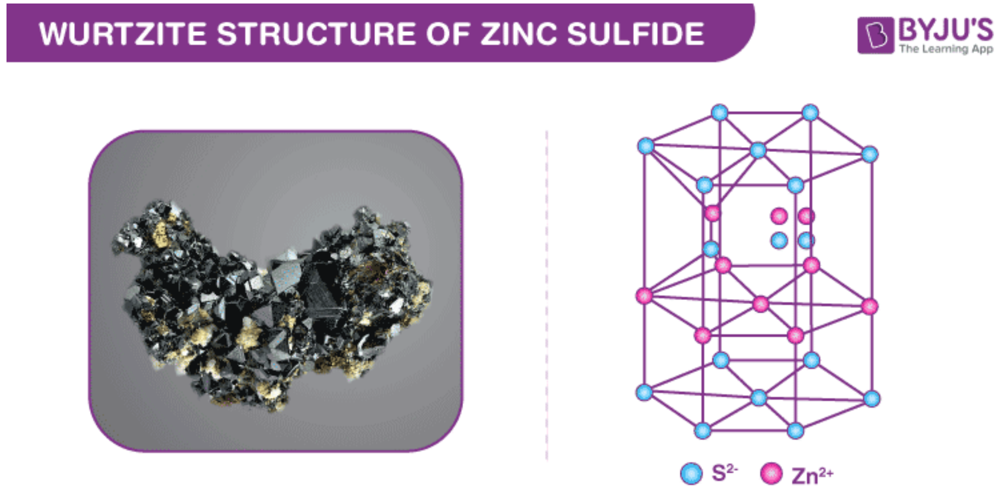


(a) (b)

Other crystal structures: diamond, zinc blende and wurzite

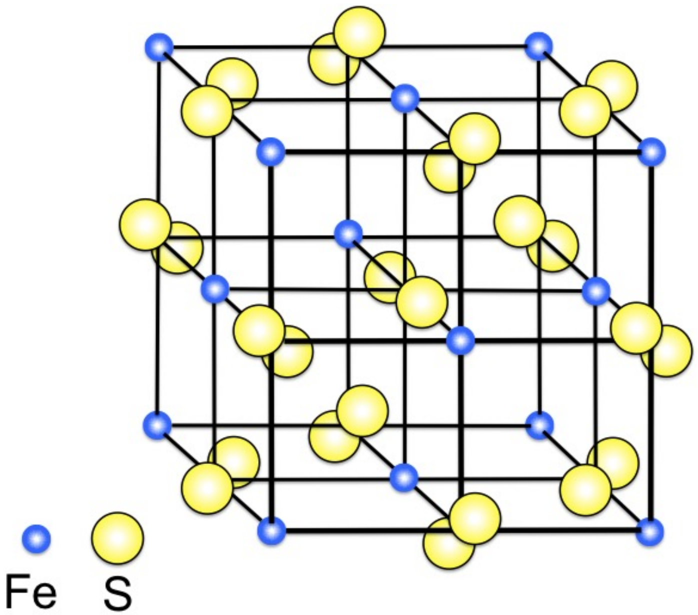


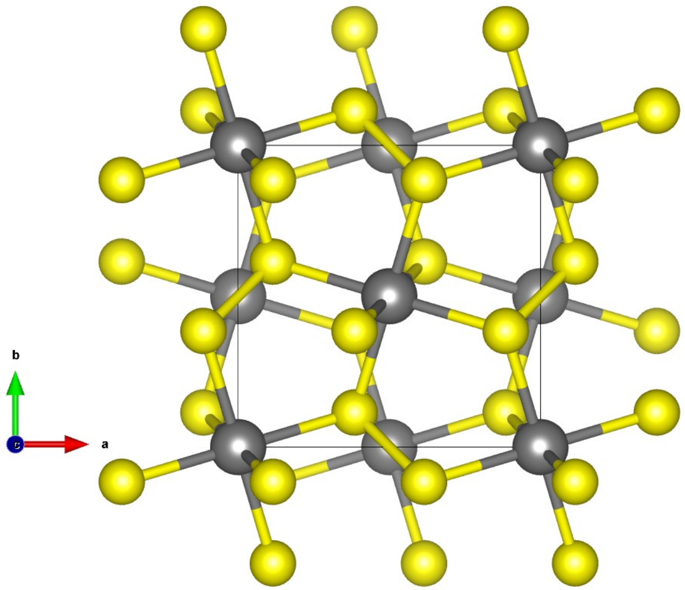




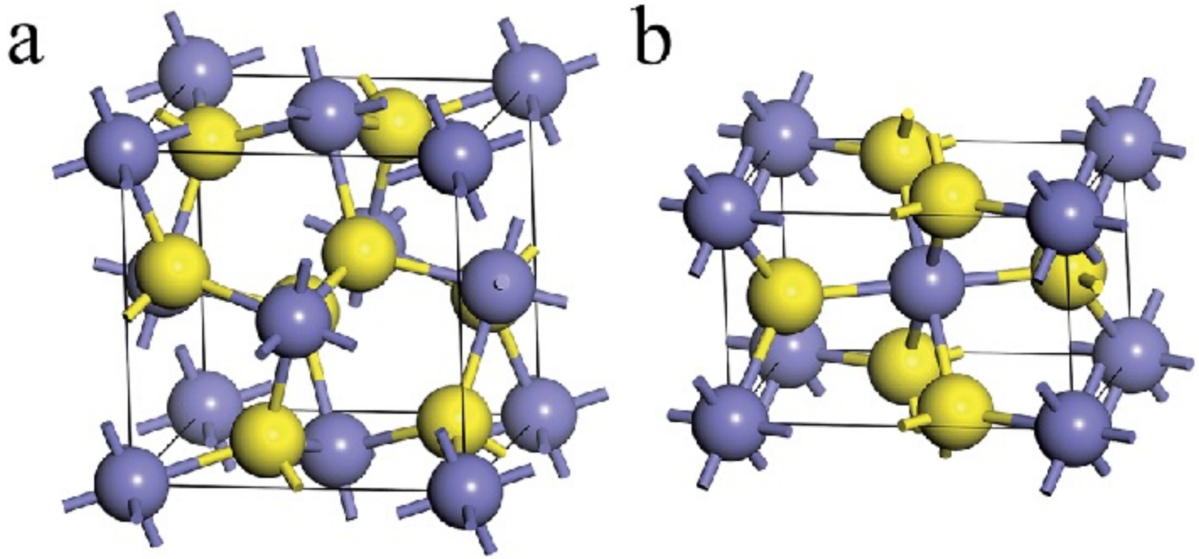
Zinc blende and wurzite
(Zinc sulfide)

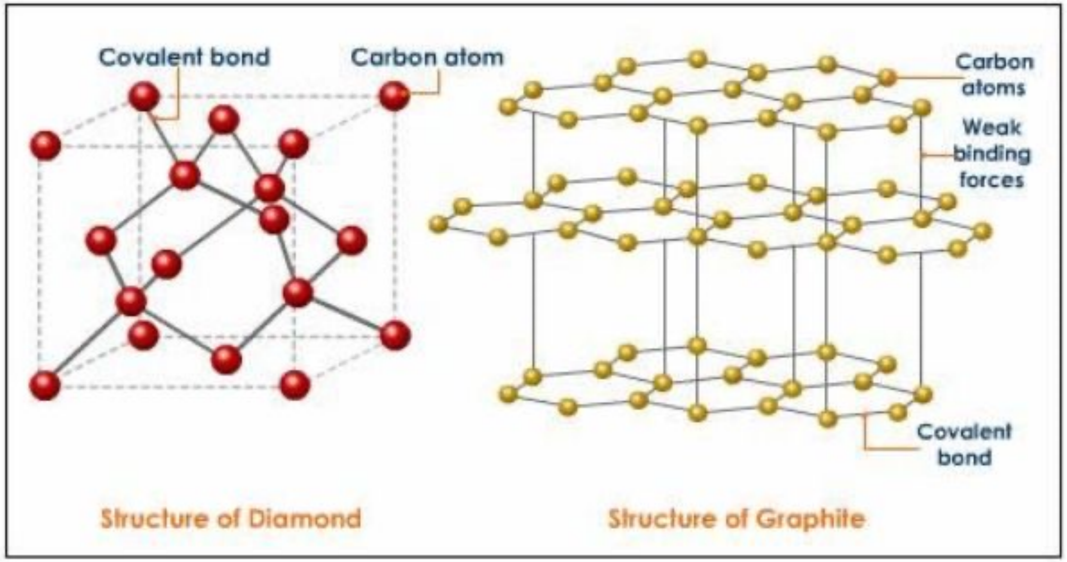
Pyrite (Fools Gold)



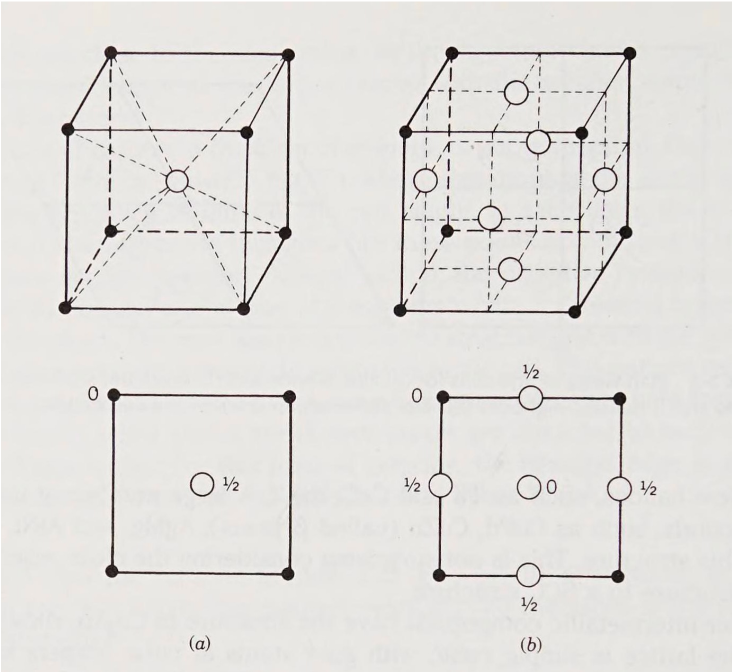


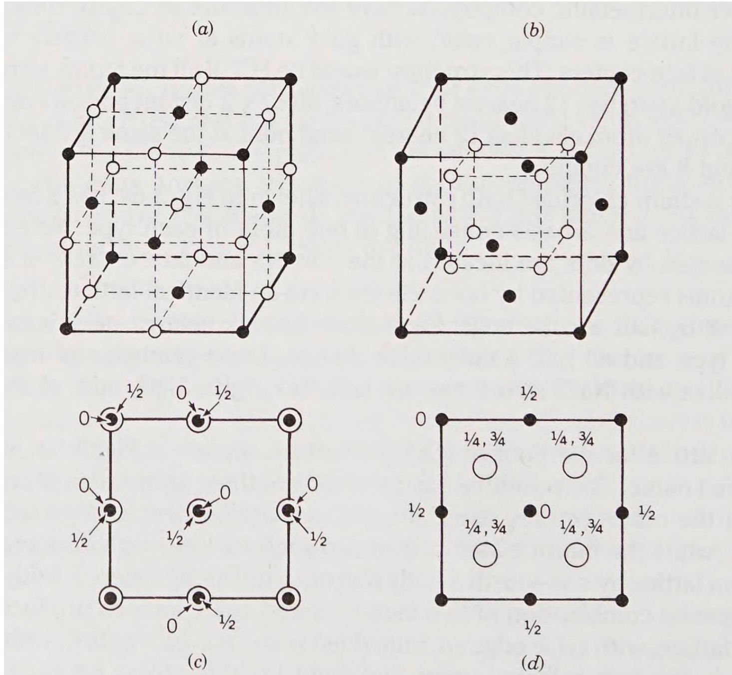
Pyrite and marcasite (Iron sulfide)





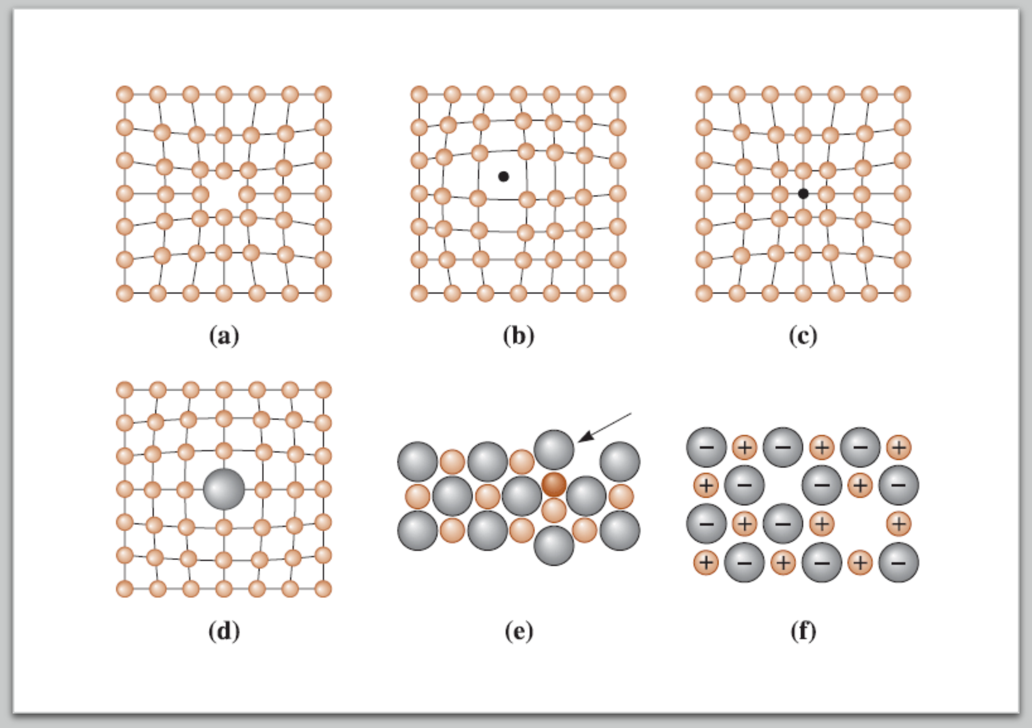
Diamond and graphite

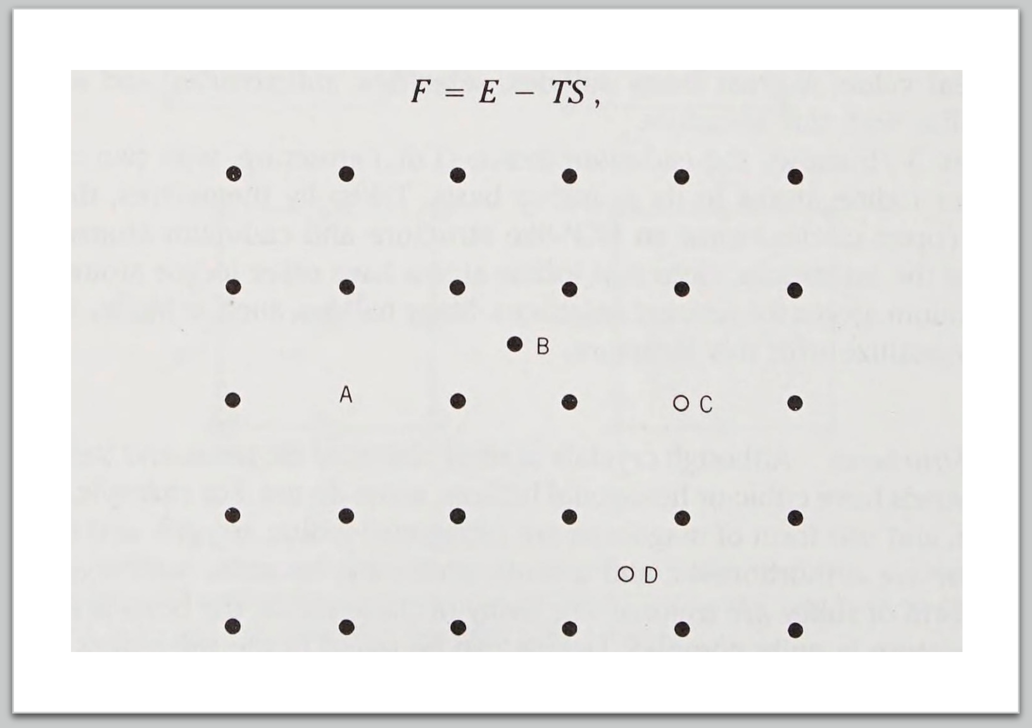


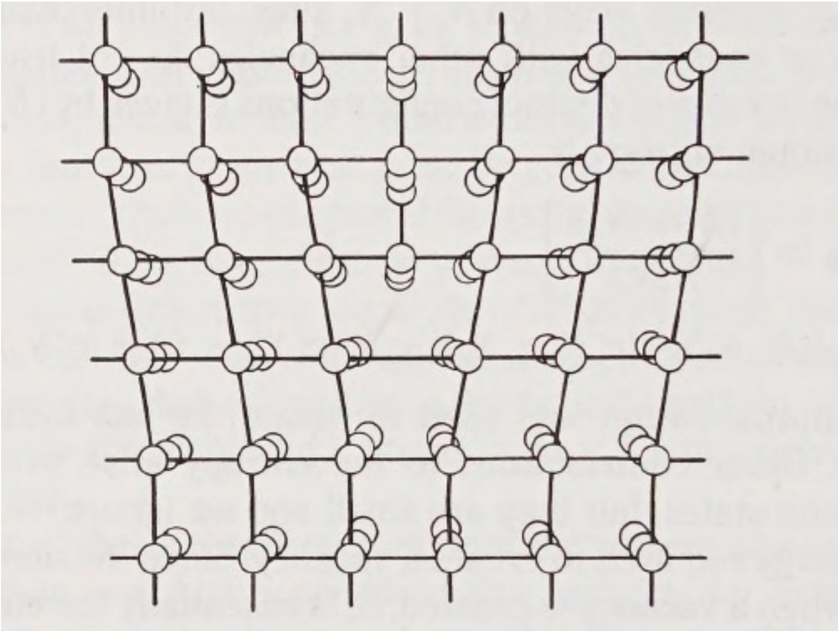


Other cubic structures: CsCl, Cu_3Au, NaCl, $CuFe_2$

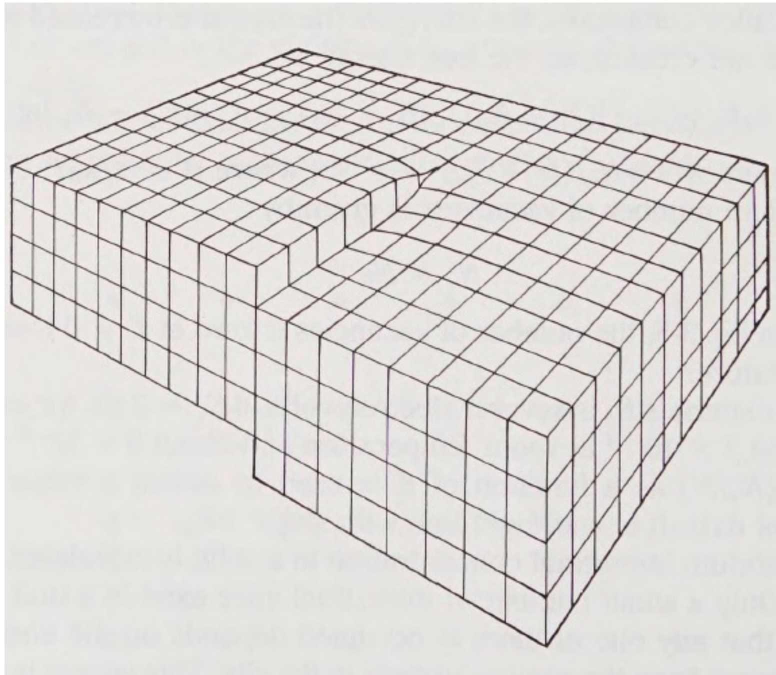
Point defects: A vacancy, B interstitial, C substitutional impurity, D interstitial impurity





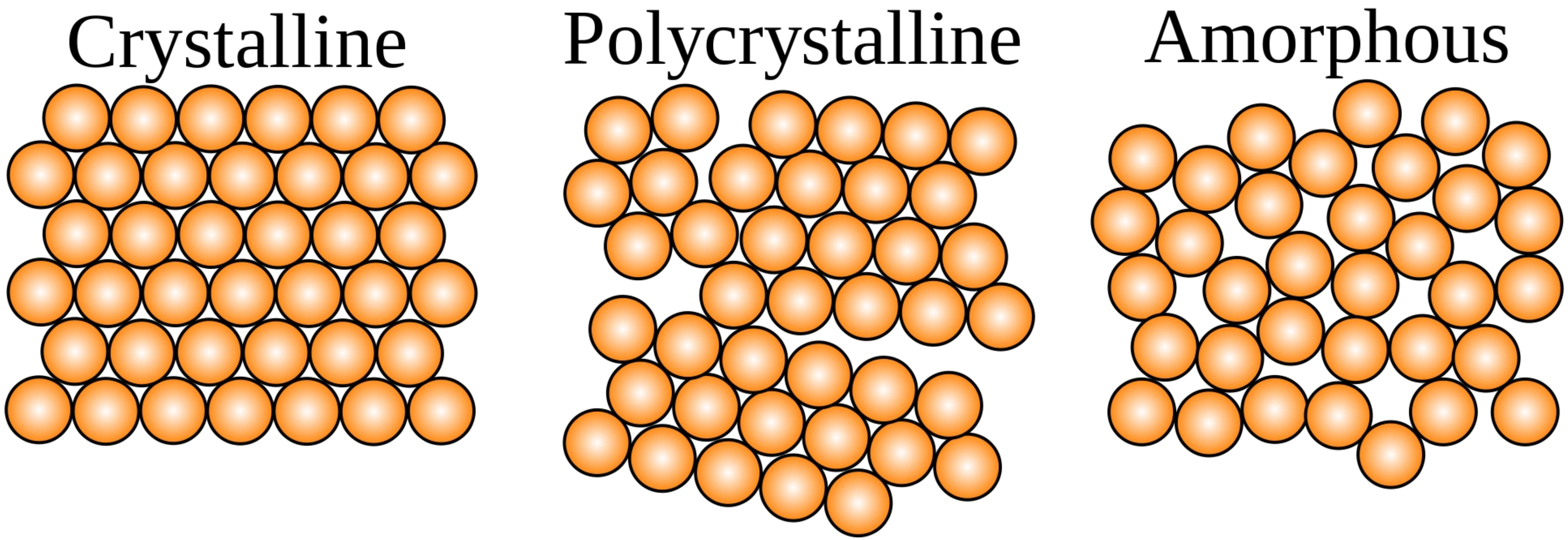


(a)

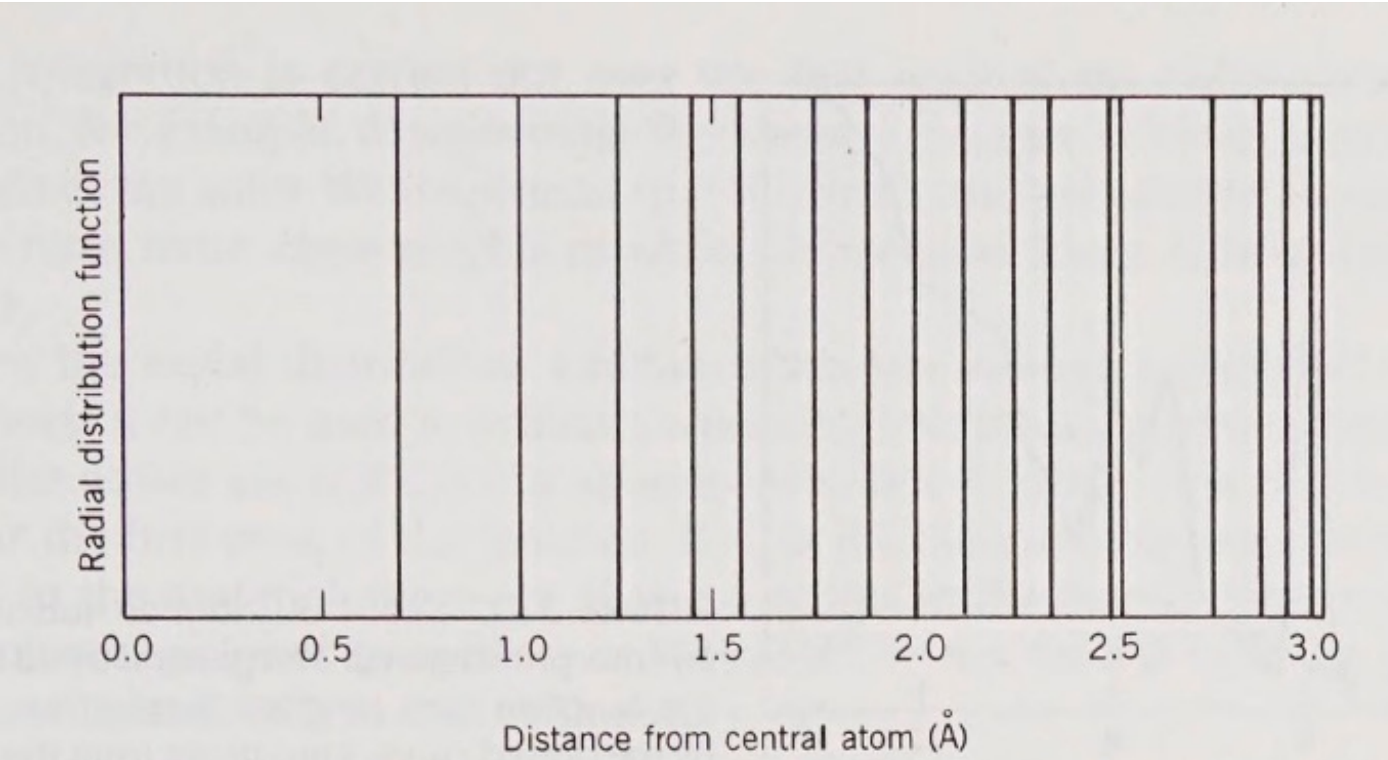


Dislocations: Edge (a) and screw (b)

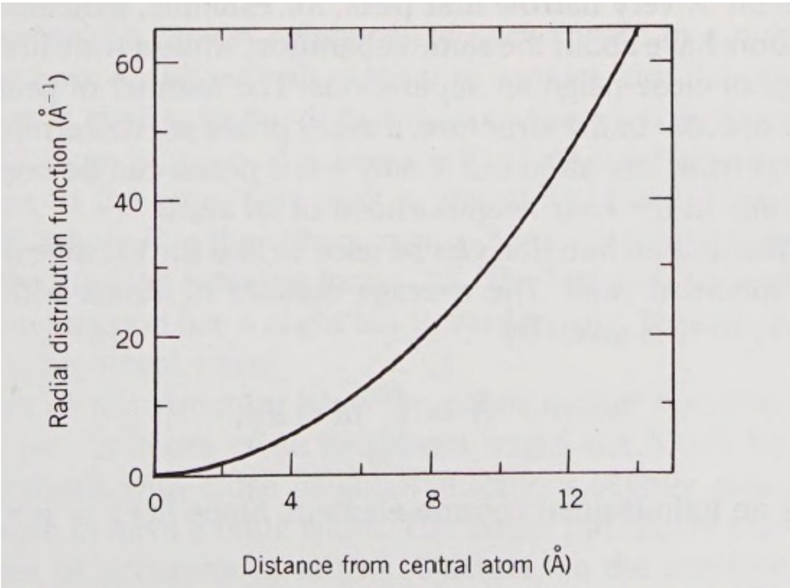
Amorphous structures

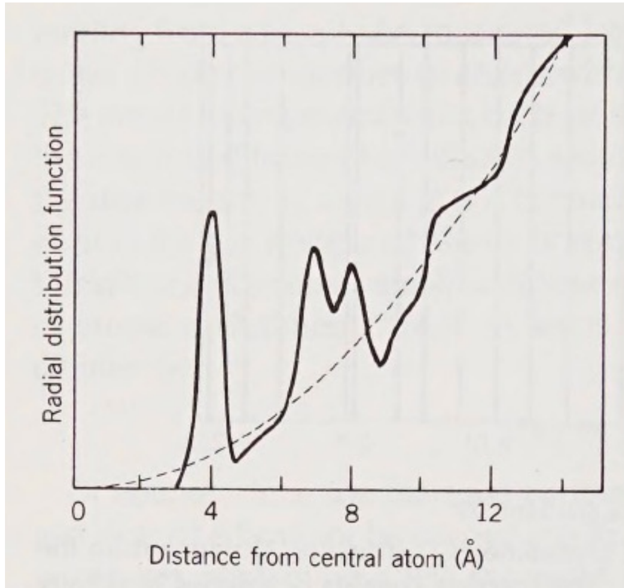


Radial distribution function of crystalline fcc structure



Radial distribution function of amorphous structures





Liquid crystalline order