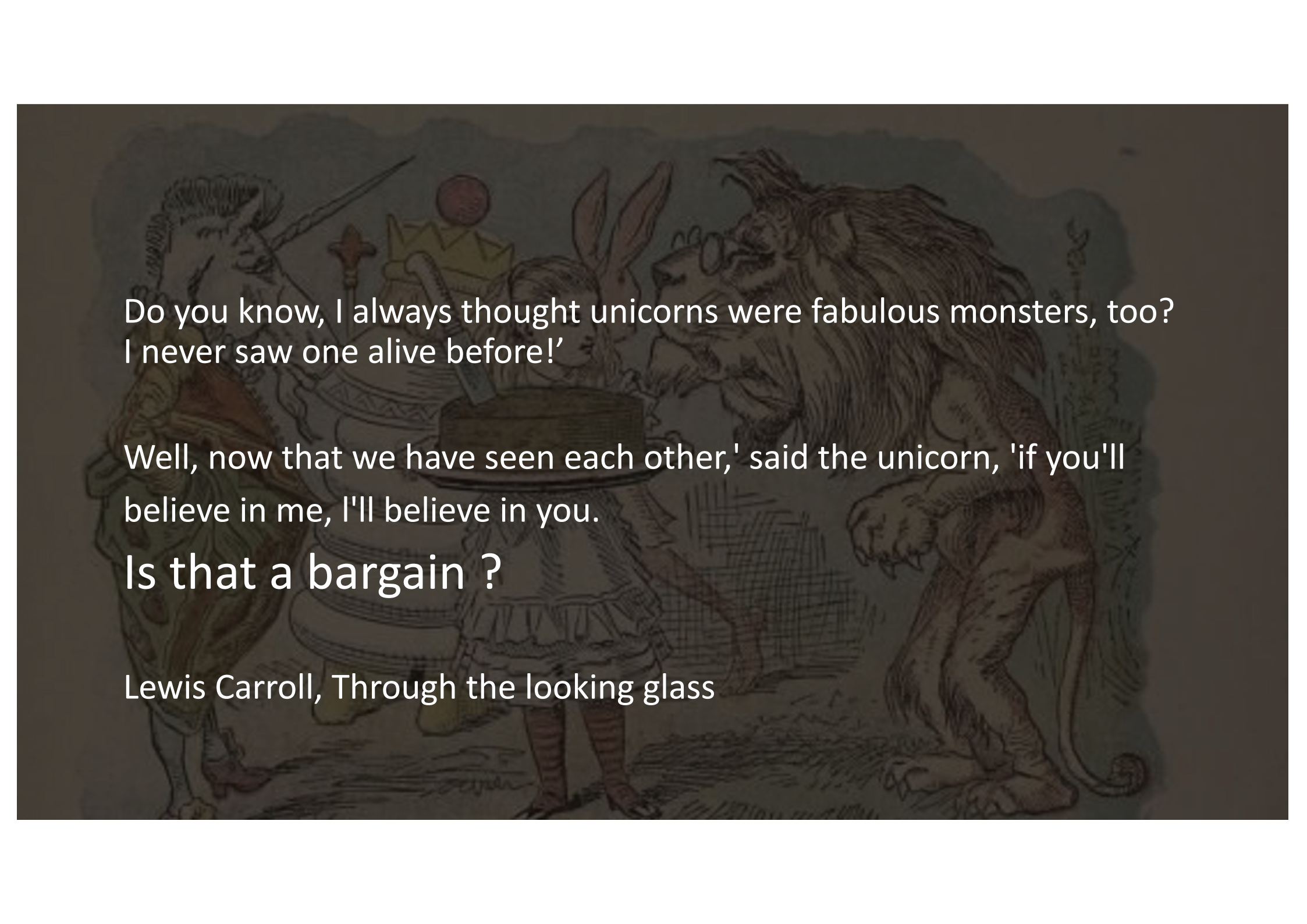


# Física da Matéria Condensada

Margarida Telo da Gama

The image is a collage of various physics concepts and equations in condensed matter physics:

- Top Left:** A diagram showing a lattice structure with a central site and surrounding sites, with arrows indicating interactions. Below it is a diagram of a hexagonal lattice with a central site and surrounding sites, with arrows indicating interactions.
- Top Center:** A diagram of a hexagonal lattice with a central site and surrounding sites, with arrows indicating interactions.
- Top Right:** A diagram of a torus (donut shape) and a sphere, representing topological states.
- Middle Left:** A diagram of a lattice structure with a central site and surrounding sites, with arrows indicating interactions.
- Middle Center:** The equation 
$$C = \frac{1}{2\pi} \oint \mathcal{F}(k) \cdot d^2k$$
- Middle Right:** A diagram of a lattice structure with a central site and surrounding sites, with arrows indicating interactions.
- Bottom Left:** The equation 
$$G(k, \omega) = \frac{1}{G_0^{-1}(k, \omega) - \Sigma(k, \omega)}$$
- Bottom Center:** A diagram of a honeycomb lattice with a central site and surrounding sites, with arrows indicating interactions. Below it is the equation 
$$\mathcal{H}_{SO} = \Delta_{SO} \psi^\dagger \sigma_z \tau_z s_z \psi$$
- Bottom Right:** A diagram of a lattice structure with a central site and surrounding sites, with arrows indicating interactions. Above it is the equation 
$$Q_s = \text{Tr}_B (|\varphi\rangle\langle\varphi|)$$
 and below it is the equation 
$$\dot{q} = \gamma \mathcal{L}[q]$$



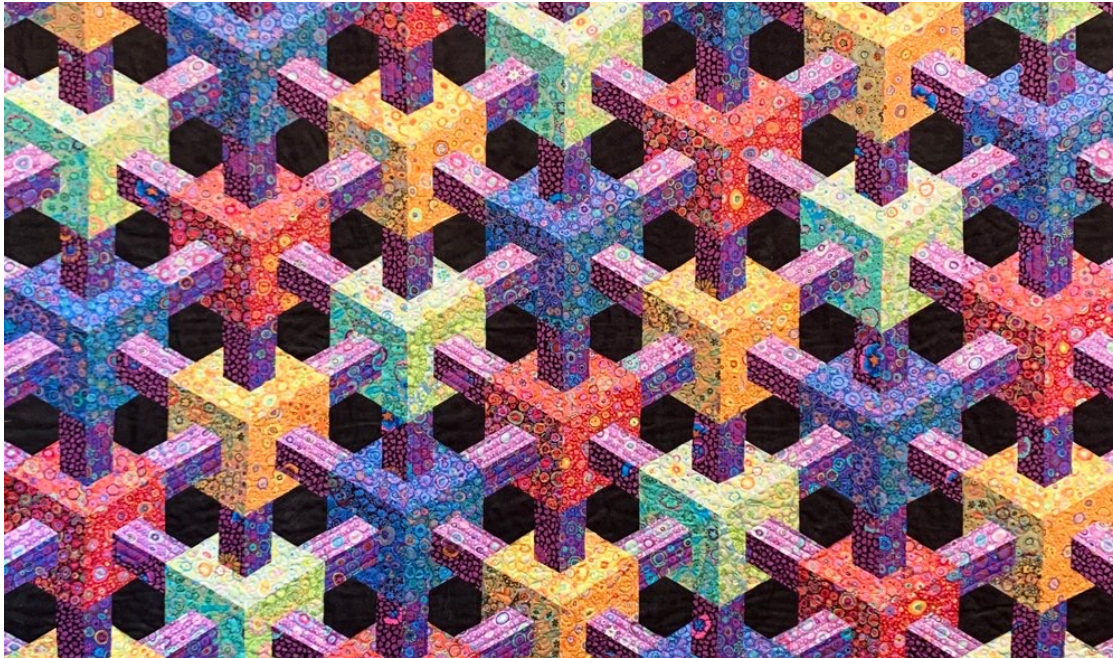
Do you know, I always thought unicorns were fabulous monsters, too?  
I never saw one alive before!

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 QUÍMICAS
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

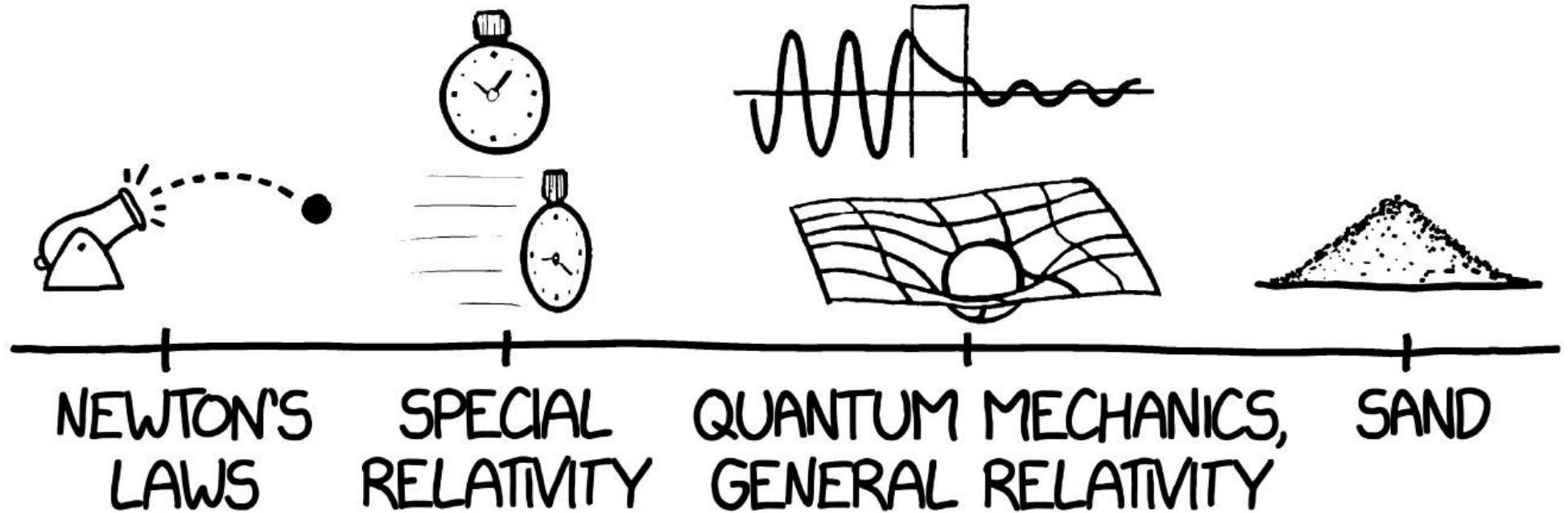
1. Fundamentals of Solid State Physics, J. R. Christman, Wiley, 1988.
2. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Holt, 1976.
3. Introduction to Solid State Physics, 5th ed., C. Kittel, Wiley, 1976.
4. Solid State Physics, An Introduction to Principles of Materials Science, H. Ibach and H. Luth, Springer, 1995.
5. Solid State Physics, H. E. Hall, Wiley, 1974

# AVALIAÇÃO

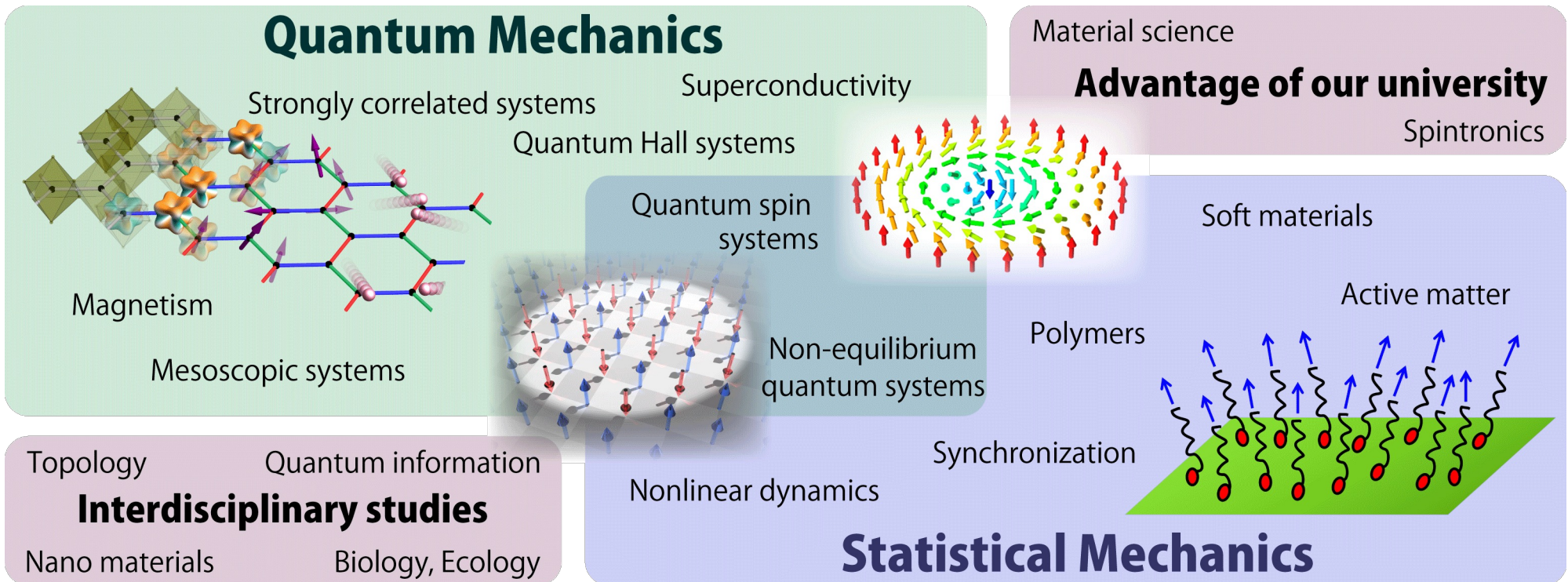
- Exame
- Contínua: entrega da resolução escrita de 1-3 problemas das séries seguida da resolução no quadro durante as TPs (20%) e exame final (80%)

# AREAS OF PHYSICS BY DIFFICULTY

HARDER →



# 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 ?

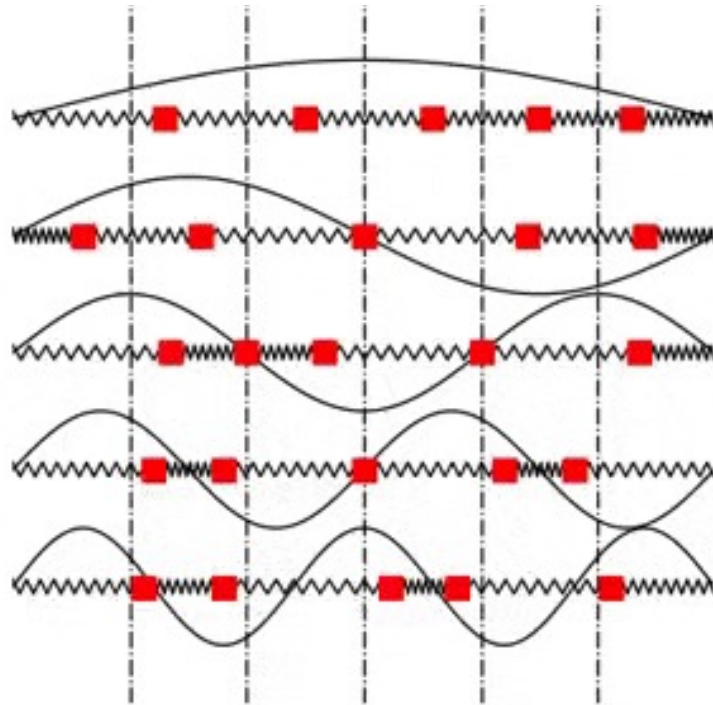
Properties of materials in terms of the interacting building blocks:

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

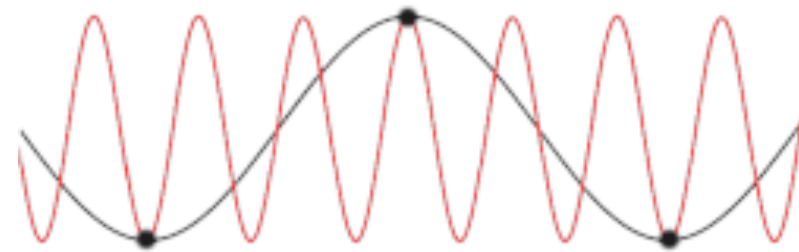
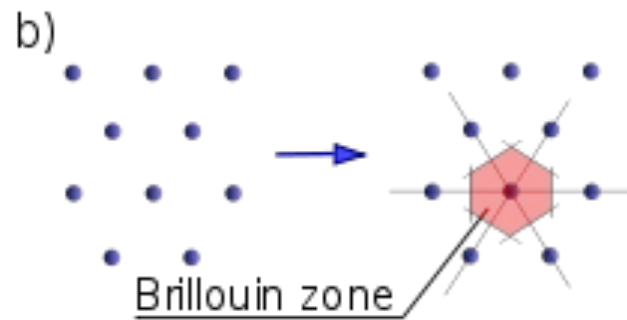
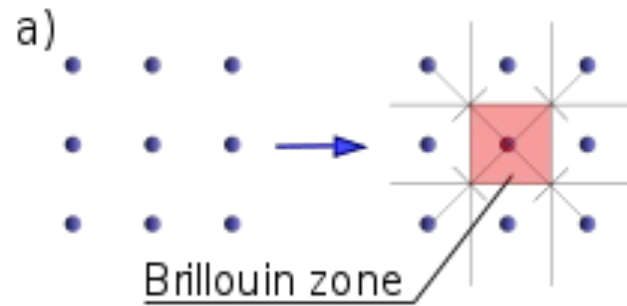
Response to external fields:

- Linear
- Non-linear

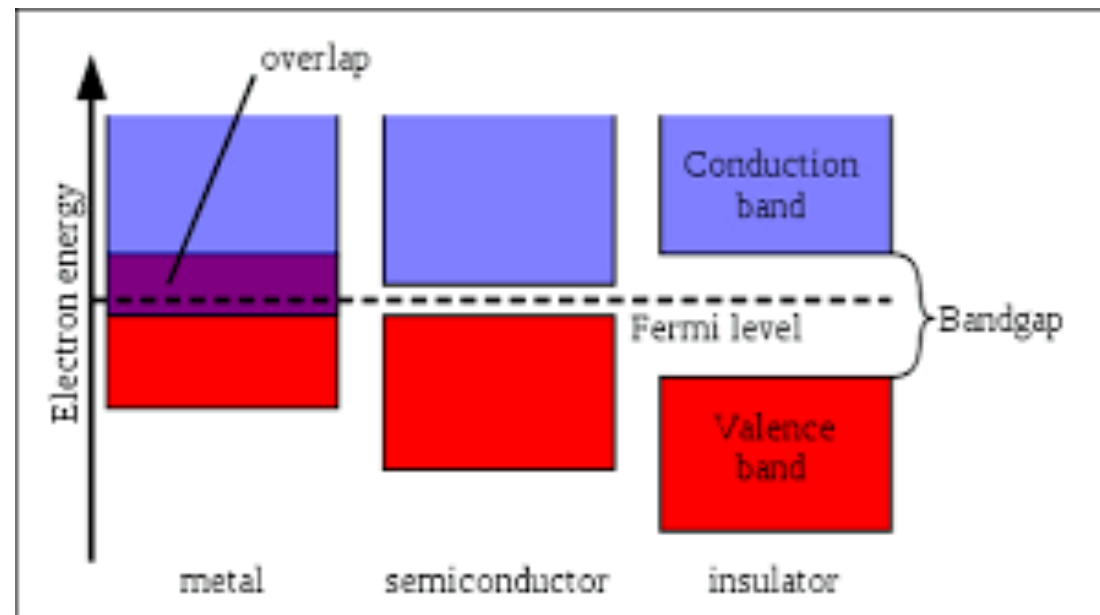
## 6. Vibrações atômicas



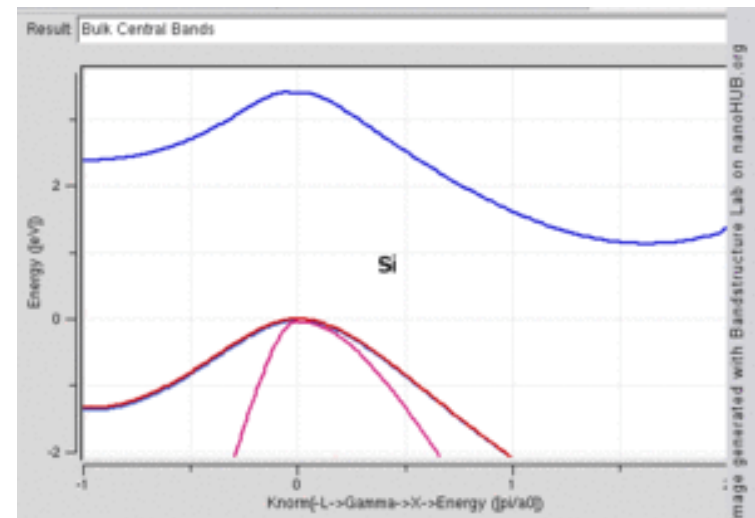
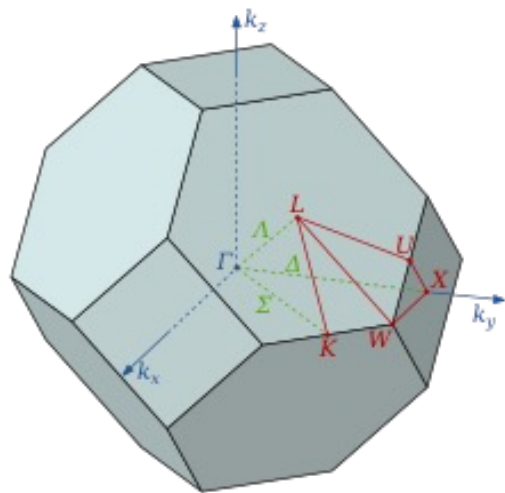
# 7. Termodinâmica de fonões



## 8. Estados electrónicos



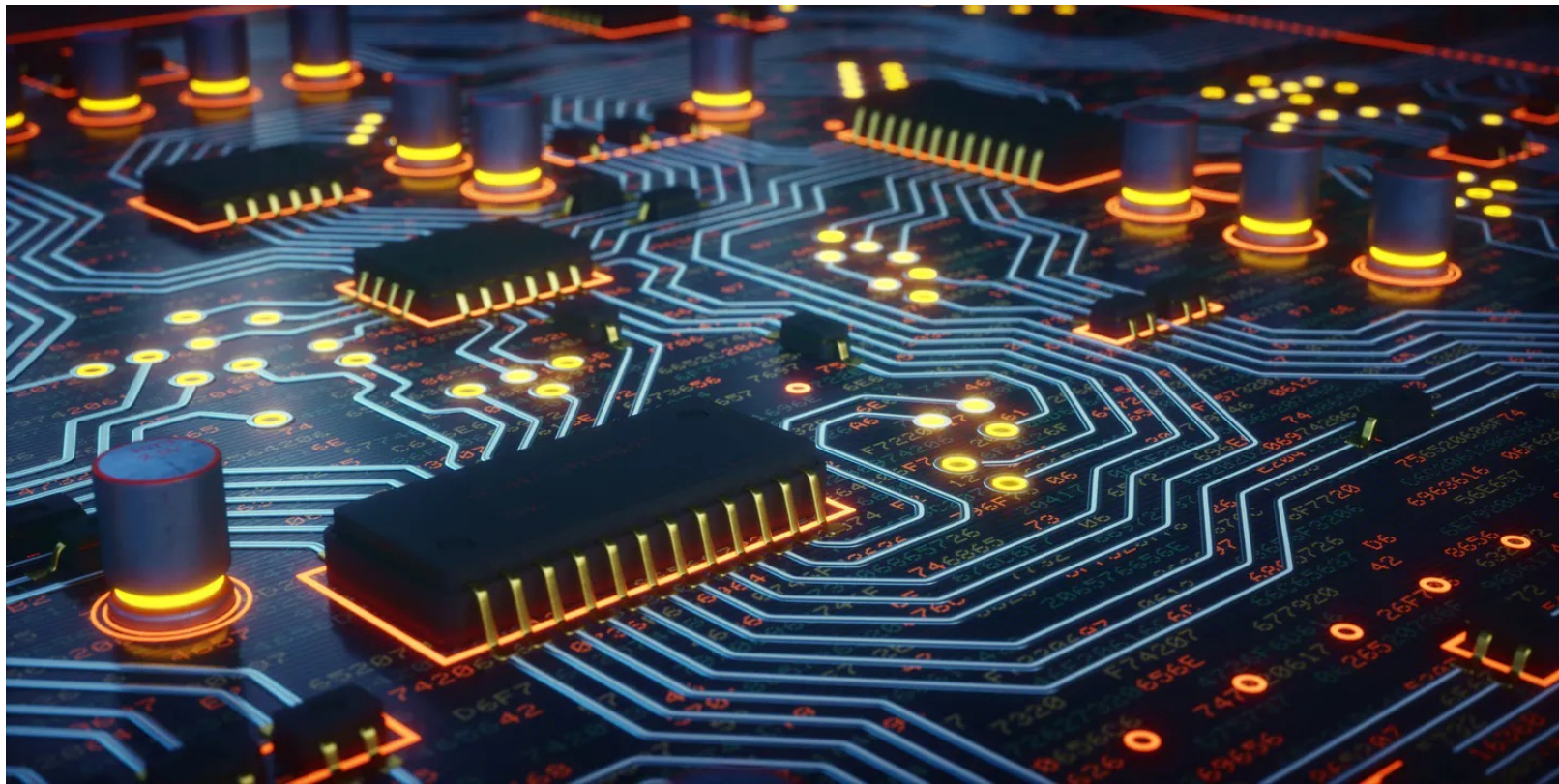
# 9. Termodinâmica de elétrons



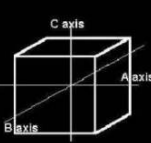
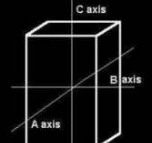
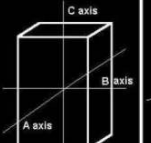
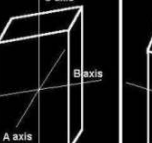
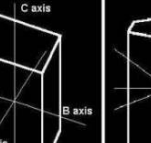
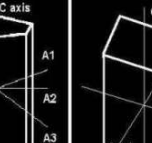
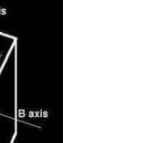



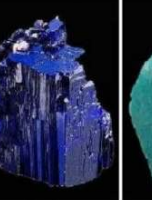



## 10. Condutividade elétrica e térmica



# 11. Electrões em semi-condutores



# 1. Crystal structure: Lattices

Crystal Systems						
Isometric	Tetragonal	Orthorhombic	Monoclinic	Triclinic	Hexagonal	Trigonal
						
						
Fluorite	Wulfenite	Tanzanite	Azurite	Amazonite	Emerald	Rhodochrosite



$$\log_c\left(\frac{a}{b}\right) = \log_c a - \log_c b$$

$$\sum_{k=1}^n k = \frac{1}{2}n(n+1)$$

$$\log_a 1 = 0$$



$$100 = c^2$$
$$\sqrt{100} = \sqrt{c^2}$$
$$\pm 10 = c$$

B.14

$$f(-x) = a(-x) + b = -(ax - b)$$

$$(x+y)^n = \sum_{k=0}^n {}^n C_k x^{n-k} y^k$$



$$3^0 = 1$$

$$a^b a^c = a^{b+c}$$



$$\frac{x}{x+2} - \frac{8}{x+6} =$$
$$= \frac{16}{x^2 + 8x + 6}$$

# Geometry of crystals

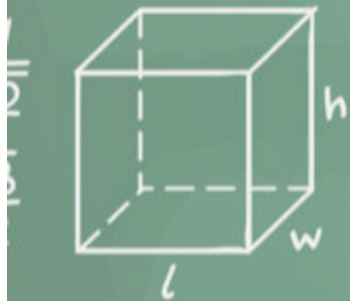
$$\sin^2 y + \cos^2 y = 1$$

$$y = \frac{k}{x}$$

$$\sqrt[n]{x} = x^{1/n}$$

$$c^2 = a^2 + b^2$$

$$\tan 60^\circ = \sqrt{3}$$



$$+2lh + 2wh$$

$$(a-b-c)^2 = a^2 + b^2 + c^2 - 2ab + 2bc - 2ca$$

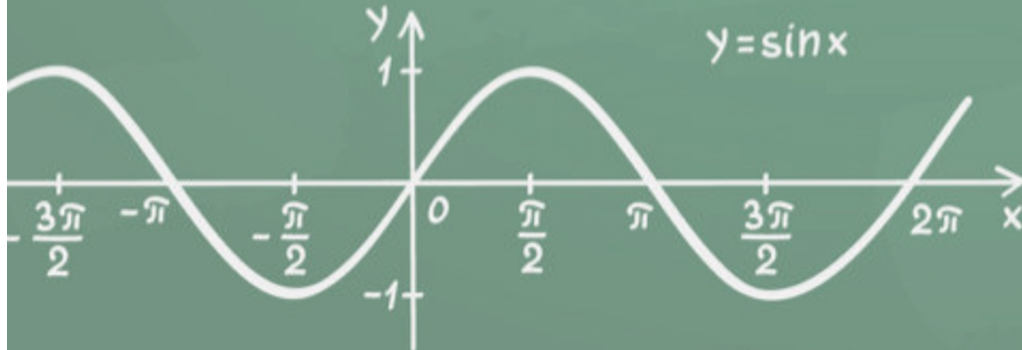
$$y = \sin x$$

$$y = ax^2 + bx + c$$

$$A = \frac{1}{2}ar + \frac{1}{2}br + \frac{1}{2}cr$$



$$C = 2\pi r$$



$$\left(\frac{2}{3}\right)^{-3} = \left(\frac{3}{2}\right)^3$$

$$s = \frac{a+b+c}{2}$$

$$A = sr$$

$$r = \frac{A}{c}$$

$$\tan 30^\circ = \frac{1}{\sqrt{3}}$$

$$(8^2)^3 = 8^{2 \times 3} = 8^6$$

# Ideal solid

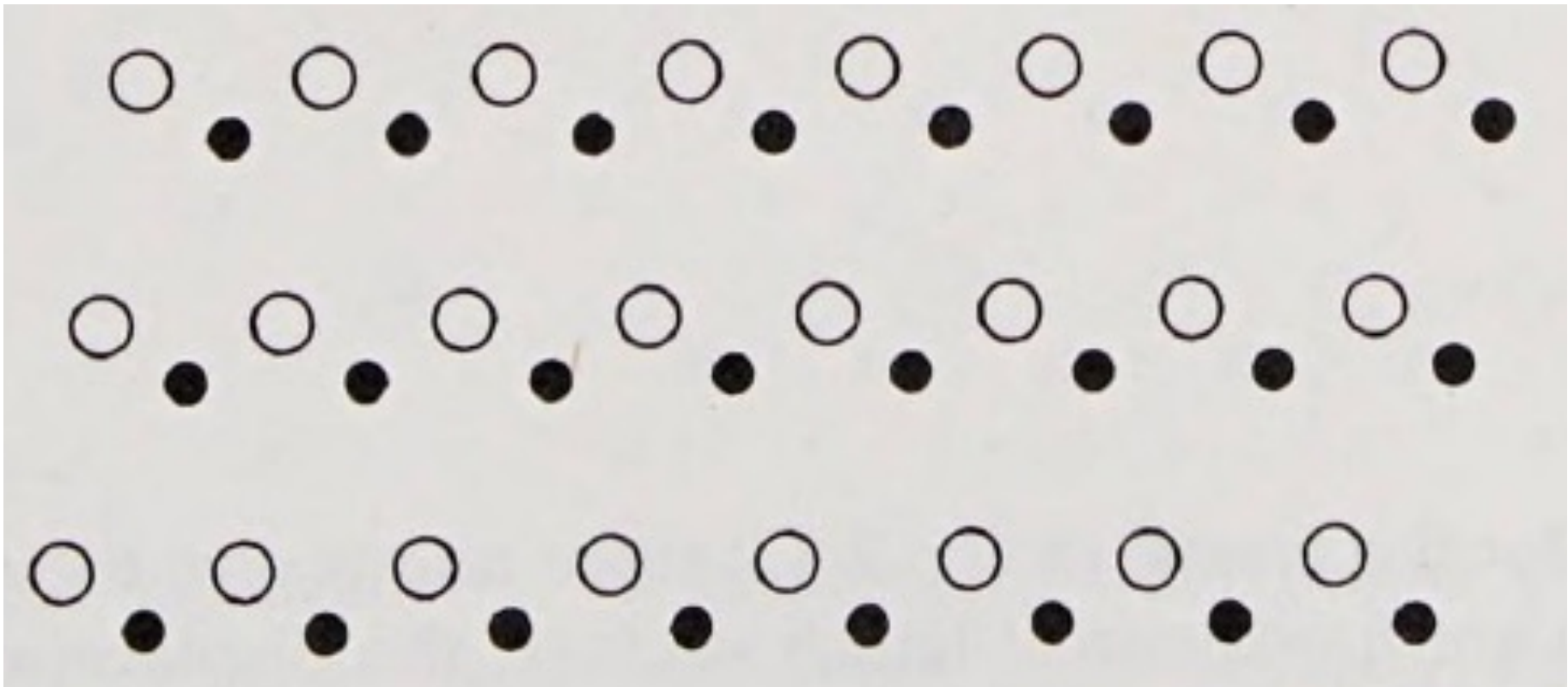
Periodic structure where the atoms are placed regularly with the medium exhibiting symmetry of translation.

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

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

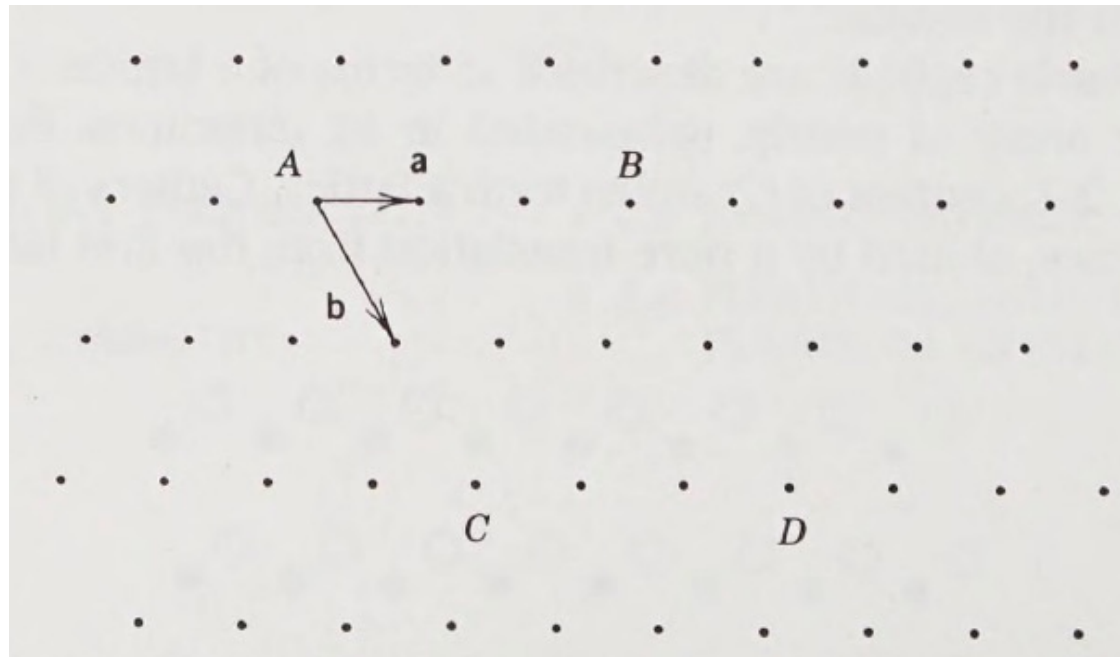
for all integers  $n_i$

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

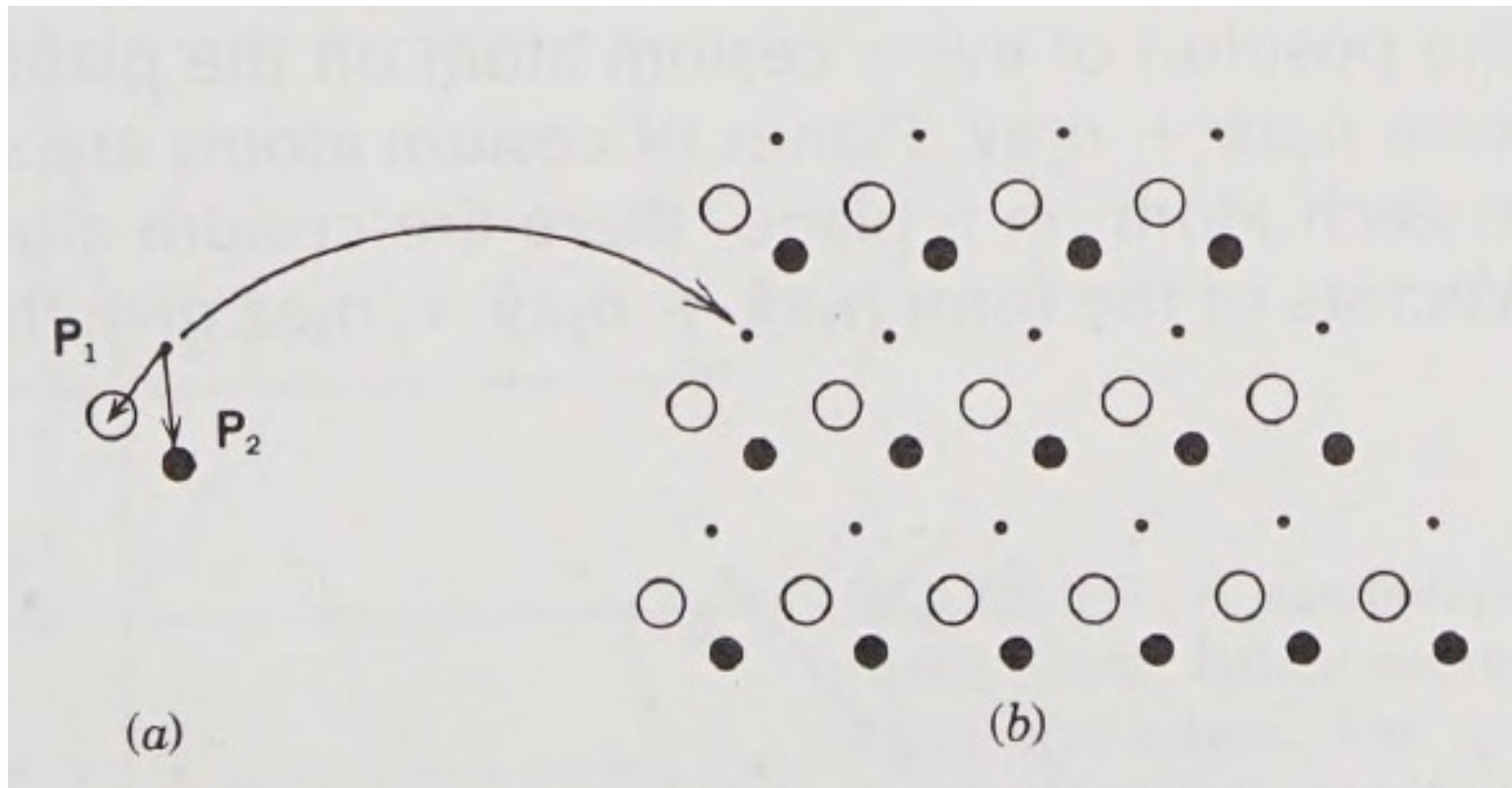


Lattice points give the positions of the basis  
**a** and **b** are fundamental lattice vectors

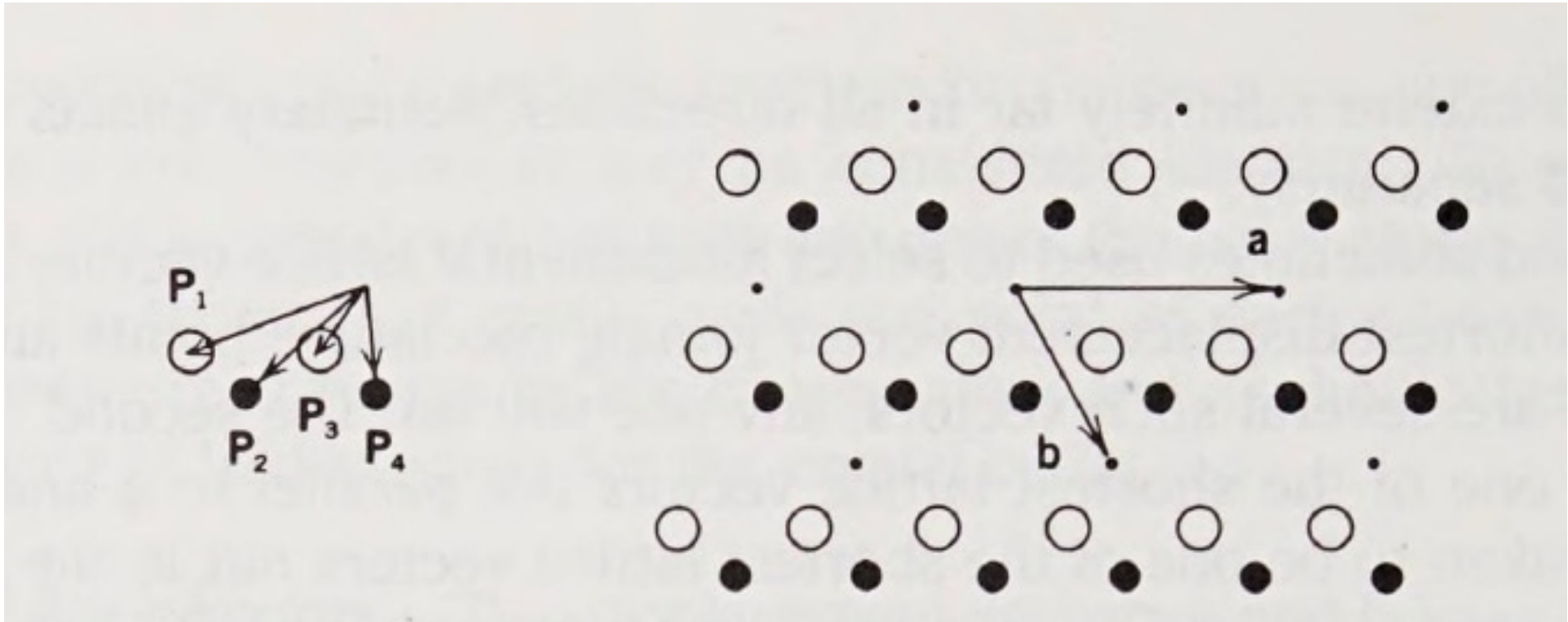
Displacement of any lattice point is  $n_1\mathbf{a}+n_2\mathbf{b}$



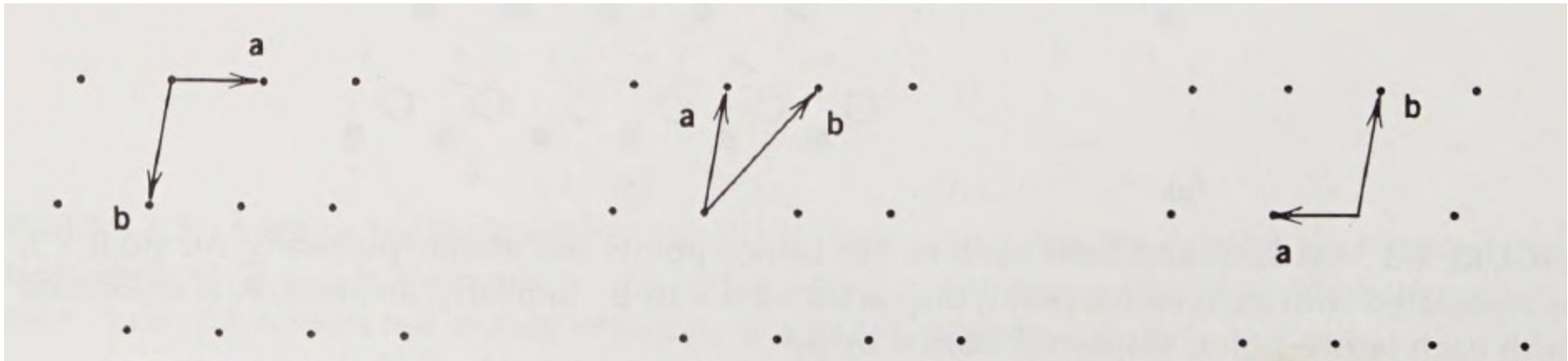
Basis and basis vectors (a) lattice points and atomic positions (b)



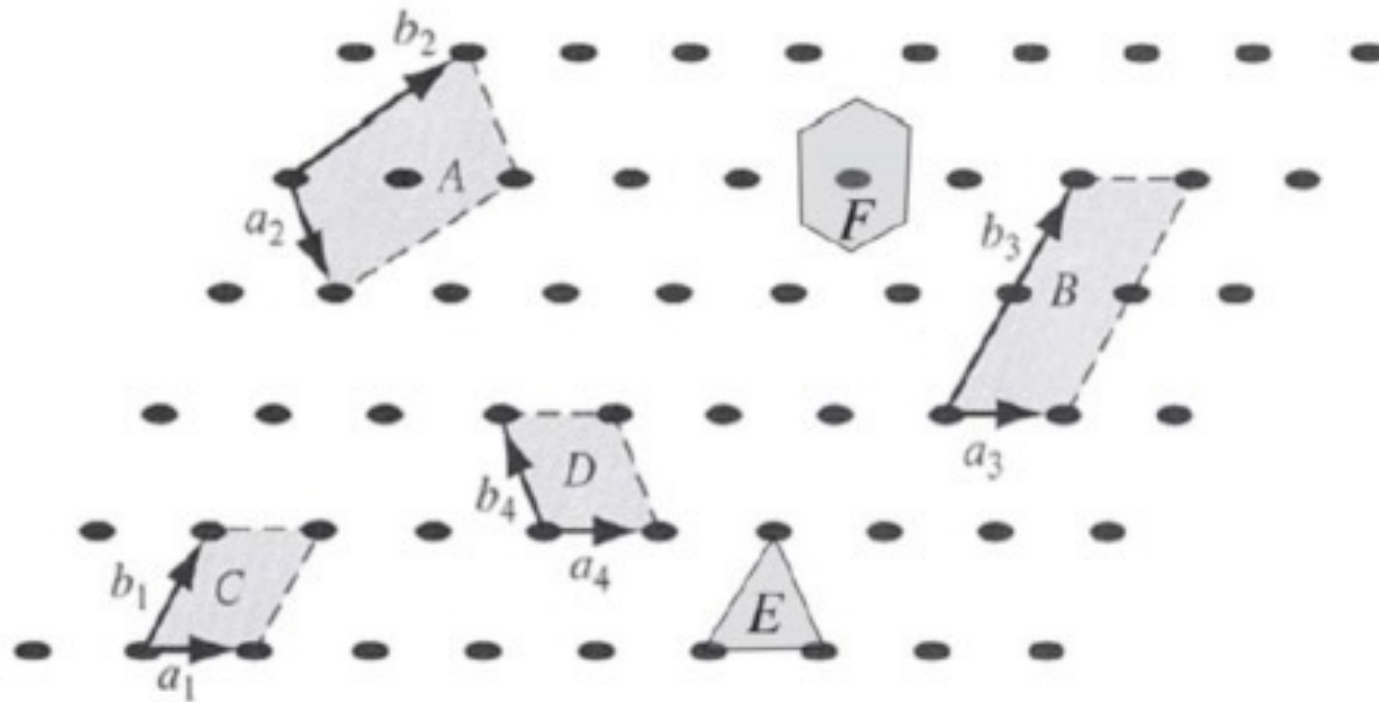
Another basis and the same lattice



Primitive lattice vectors correspond to the smallest possible basis

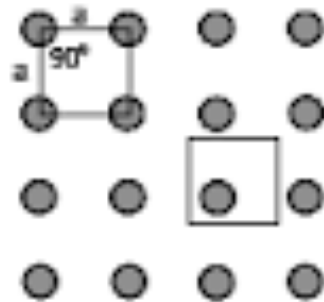


# Lattice vectors and unit cells

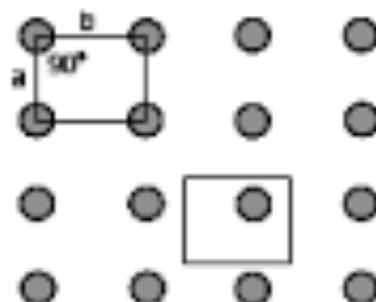




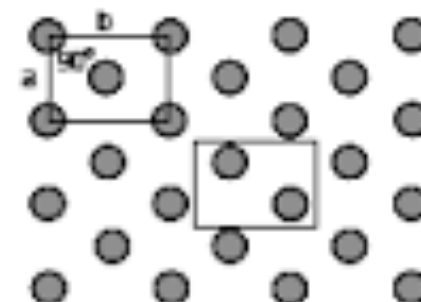
# Unit cells



square lattice  
square unit cell

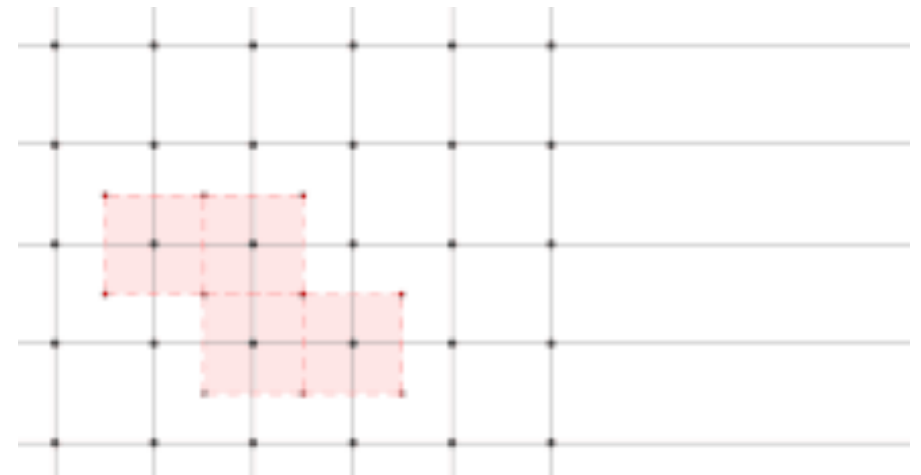
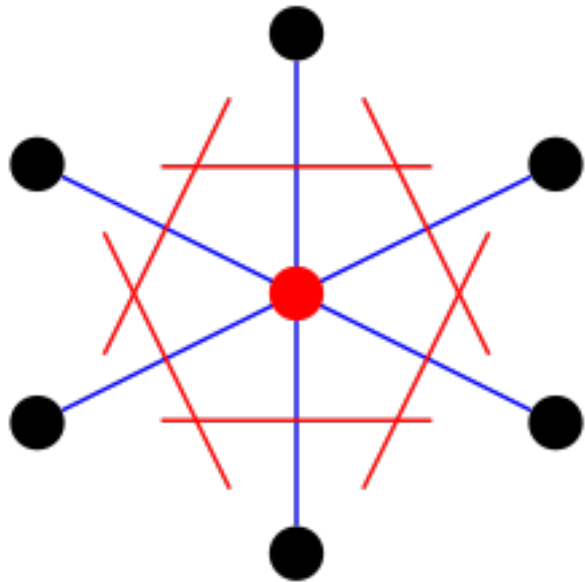


rectangular lattice  
rectangular unit cell

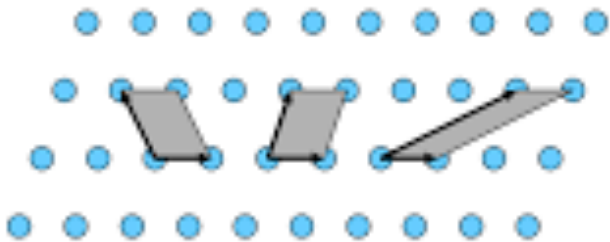


rectangular lattice  
centered rectangular unit cell

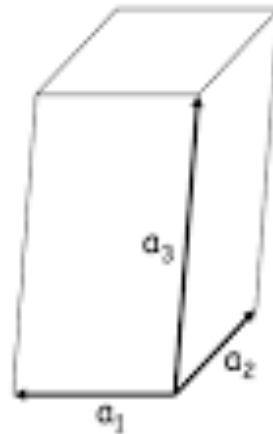
# Wigner-Seitz cell



# Volume of a unit cell



There is more than one choice for a primitive unit cell



Primitive unit cell

Volume of a unit cell  
 $|\mathbf{c} \cdot \mathbf{a} \times \mathbf{b}|$

# Rigid symmetry operations: Point & spatial



Reflection



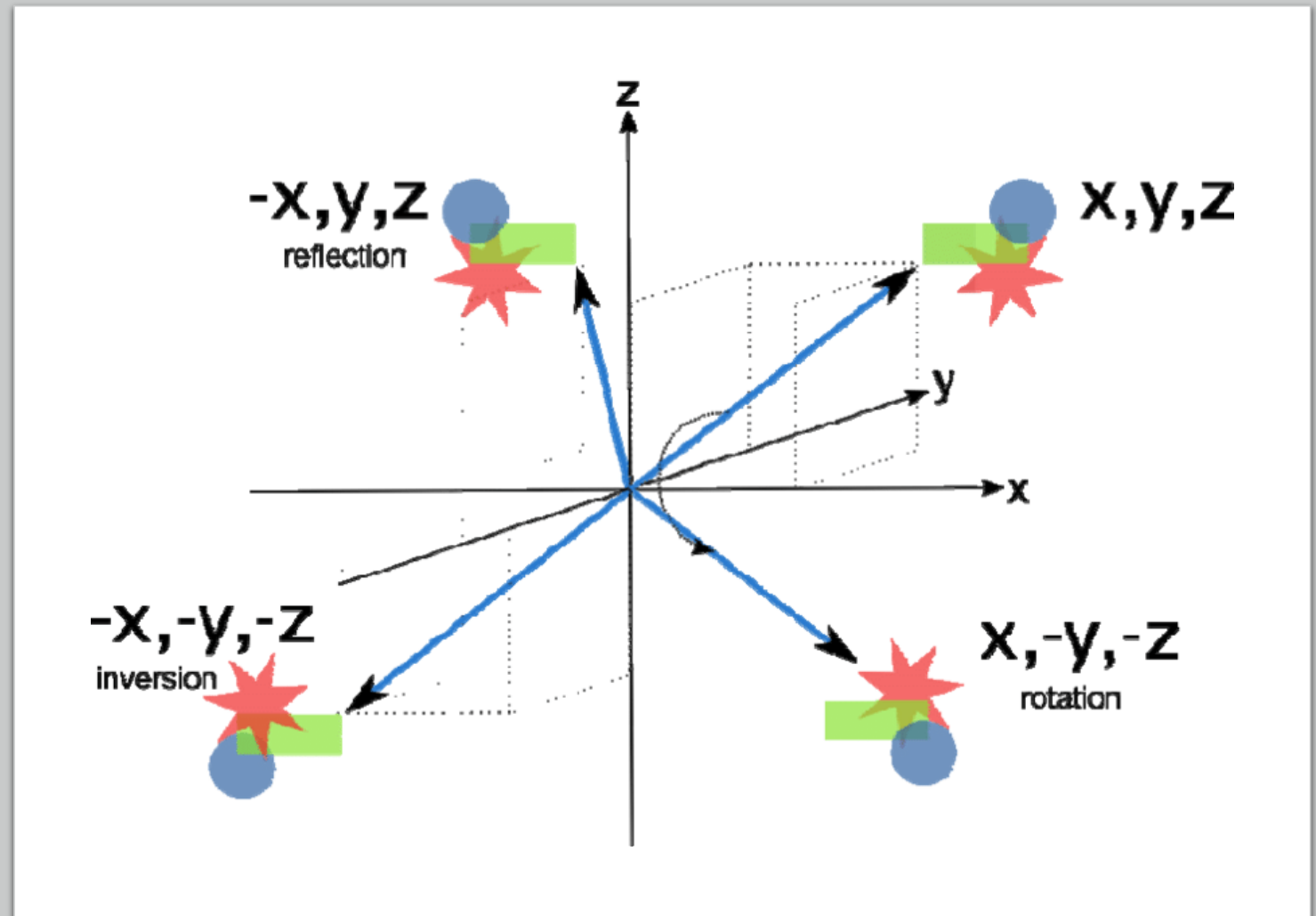
Rotation



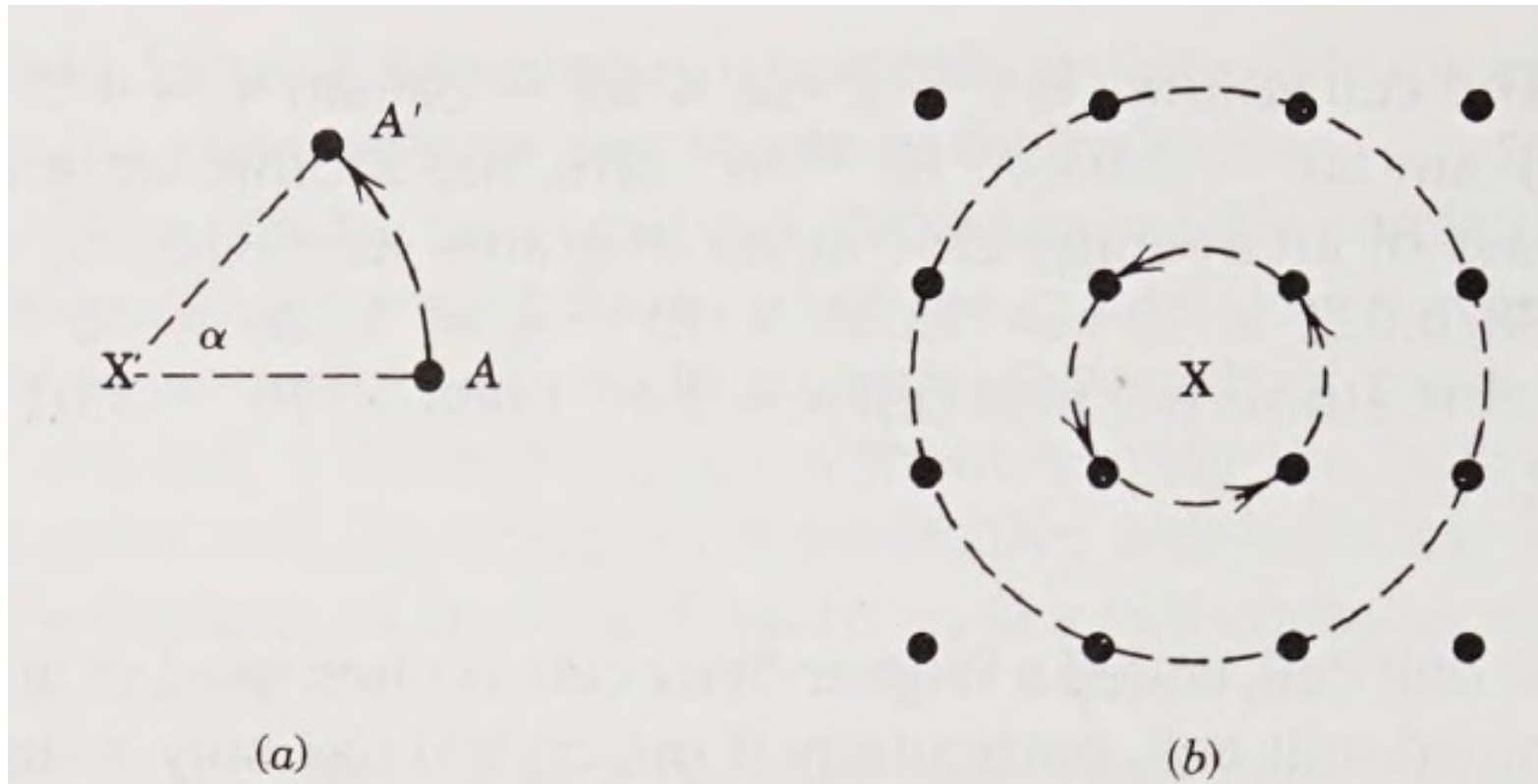
Translation

# Point symmetries

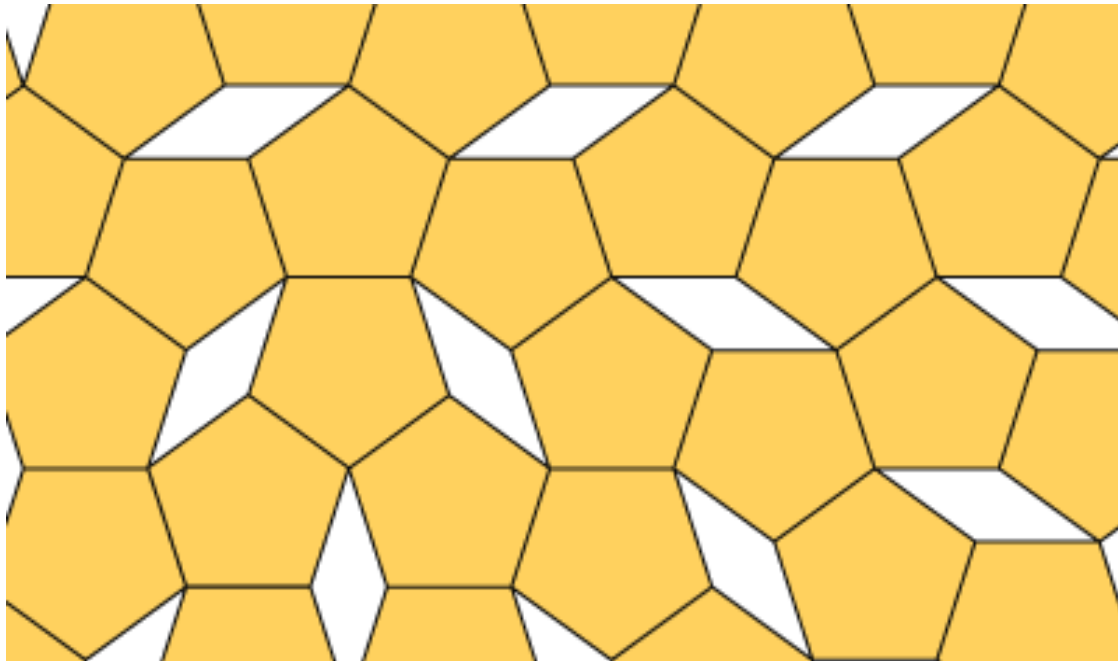
Mirror, rotation and inversion

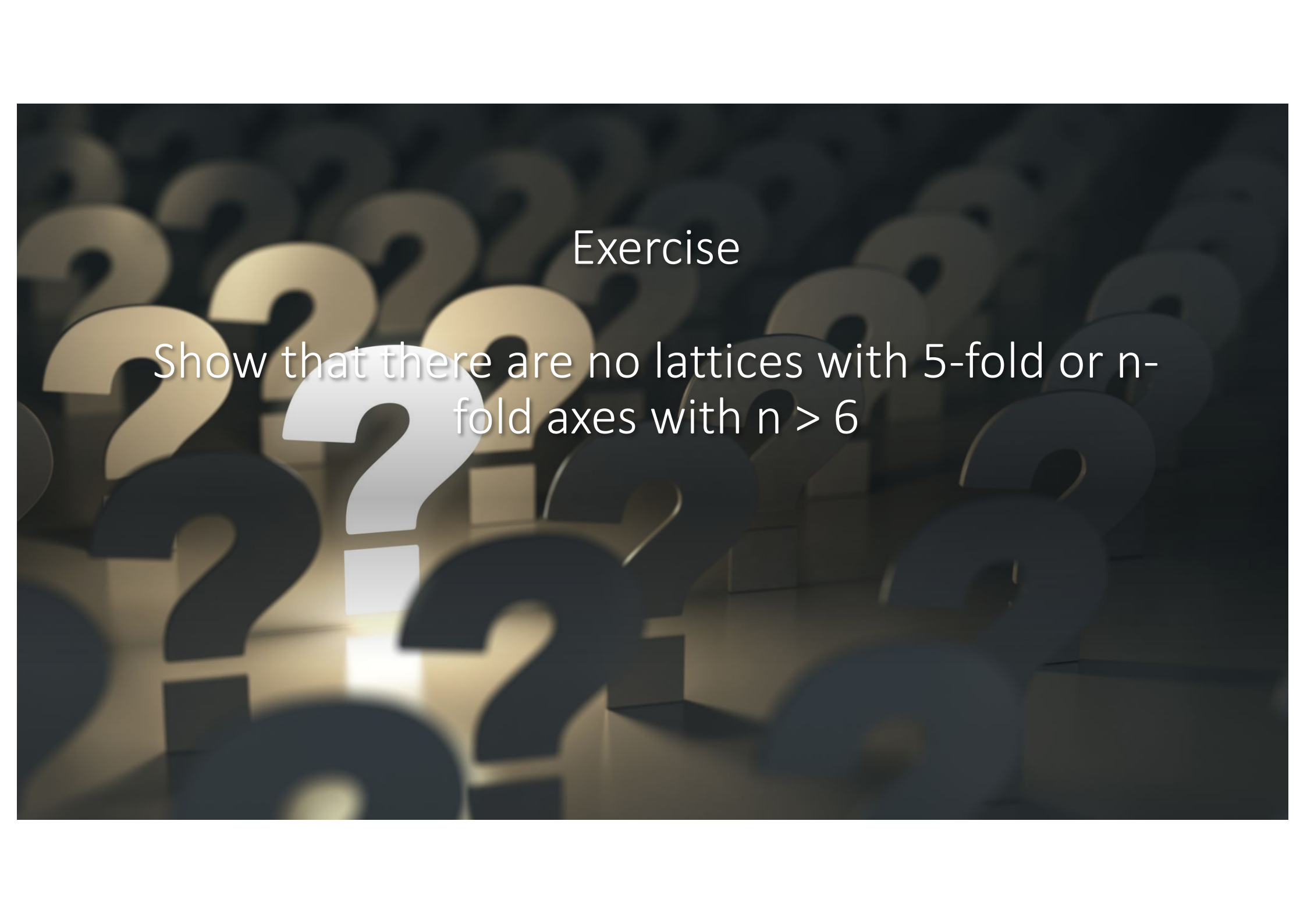


# Rotational symmetry



Crystals do not have 5-fold rotational axes



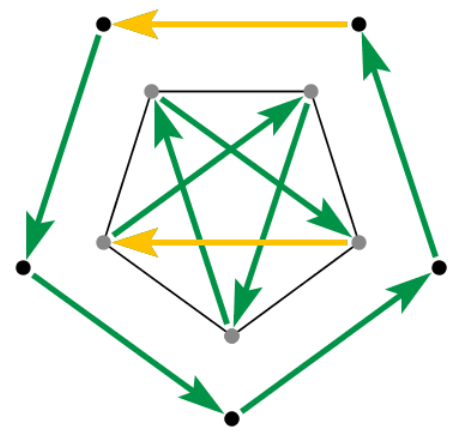
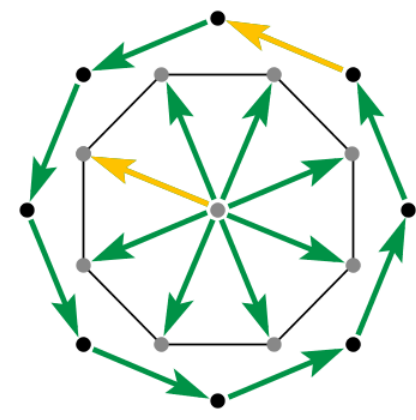
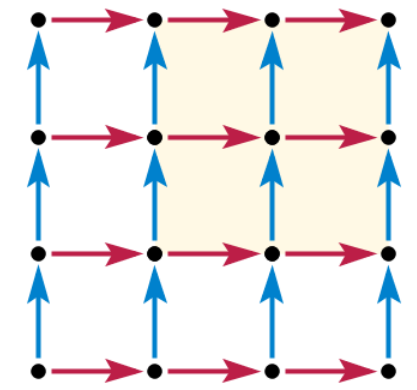
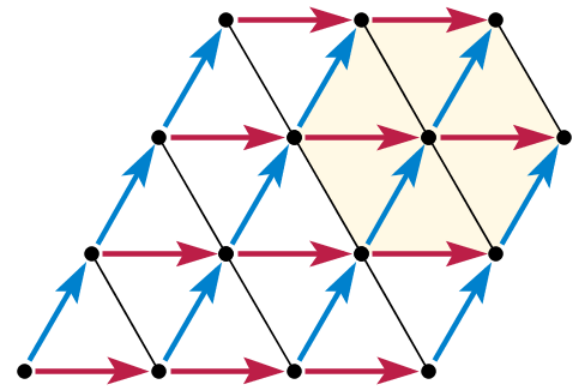
The background of the slide is a dark, textured surface covered with numerous question marks. Some question marks are in shades of gold and yellow, while others are dark grey or black. The lighting is dramatic, with a bright spot in the lower-left quadrant that creates a strong glow and highlights the question marks in that area. The overall effect is one of mystery and inquiry.

## Exercise

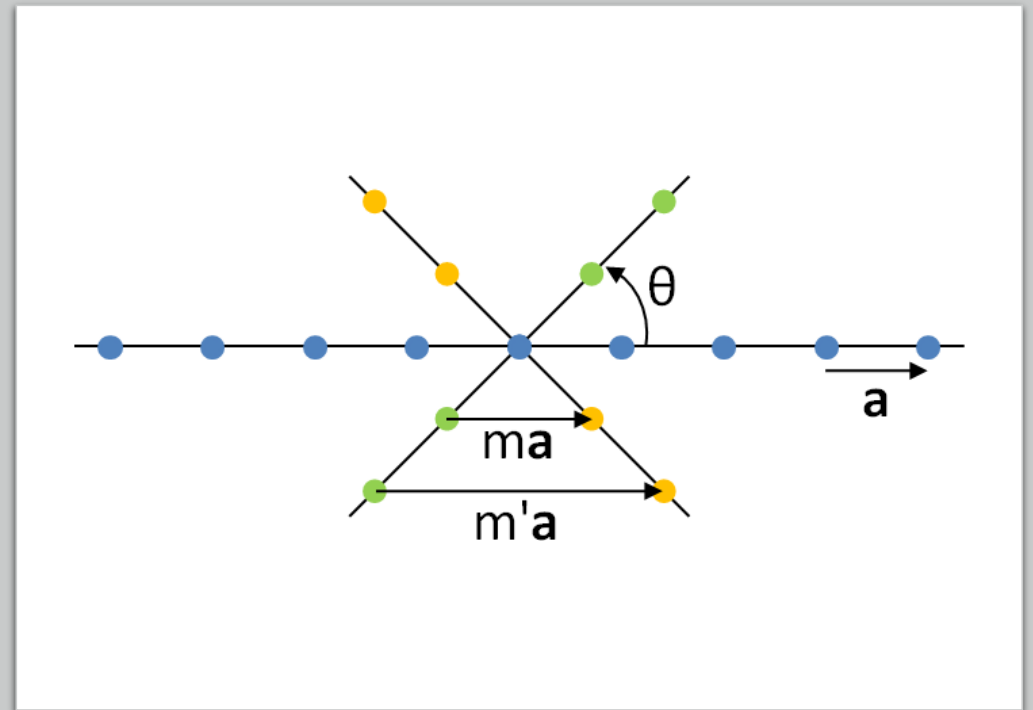
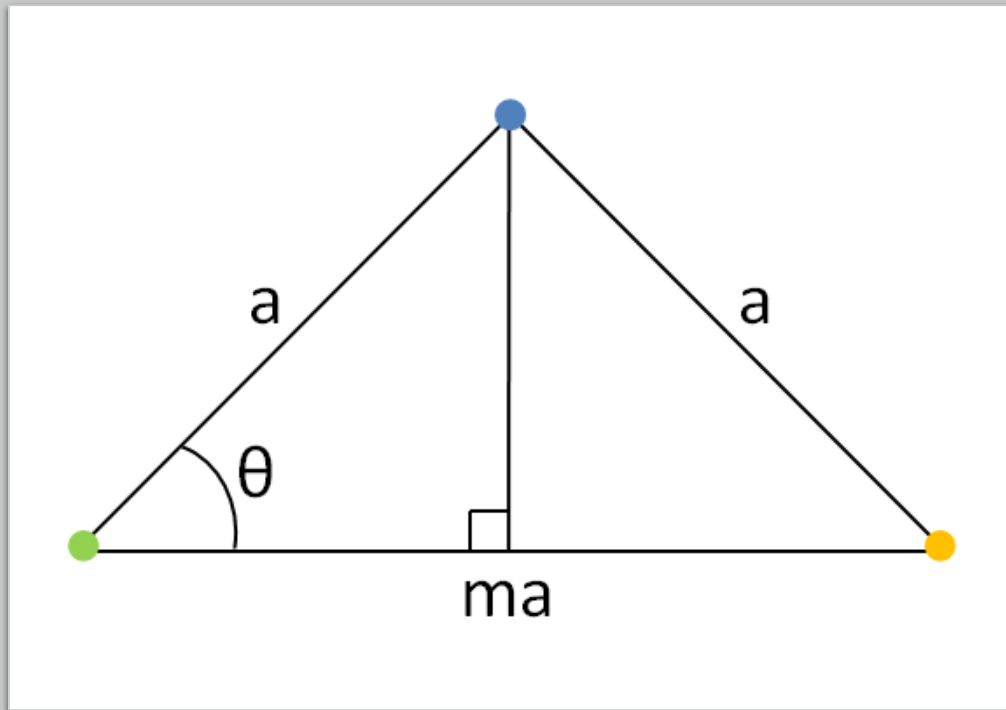
Show that there are no lattices with 5-fold or  $n$ -fold axes with  $n > 6$



# Lattice proof



# Geometric proof



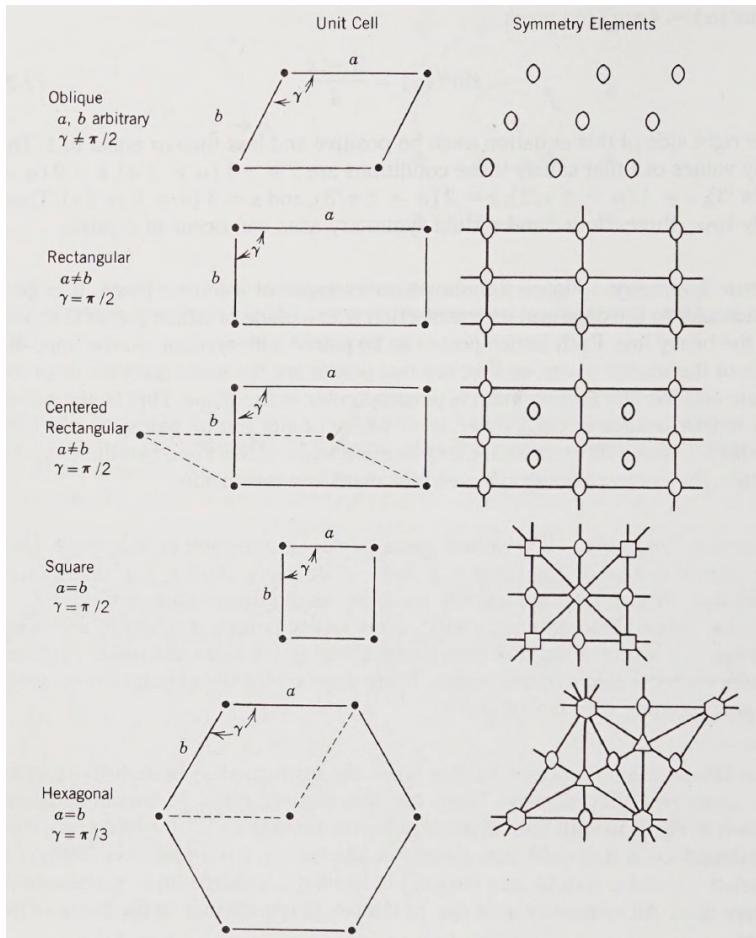
# Rigid symmetries are not independent

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

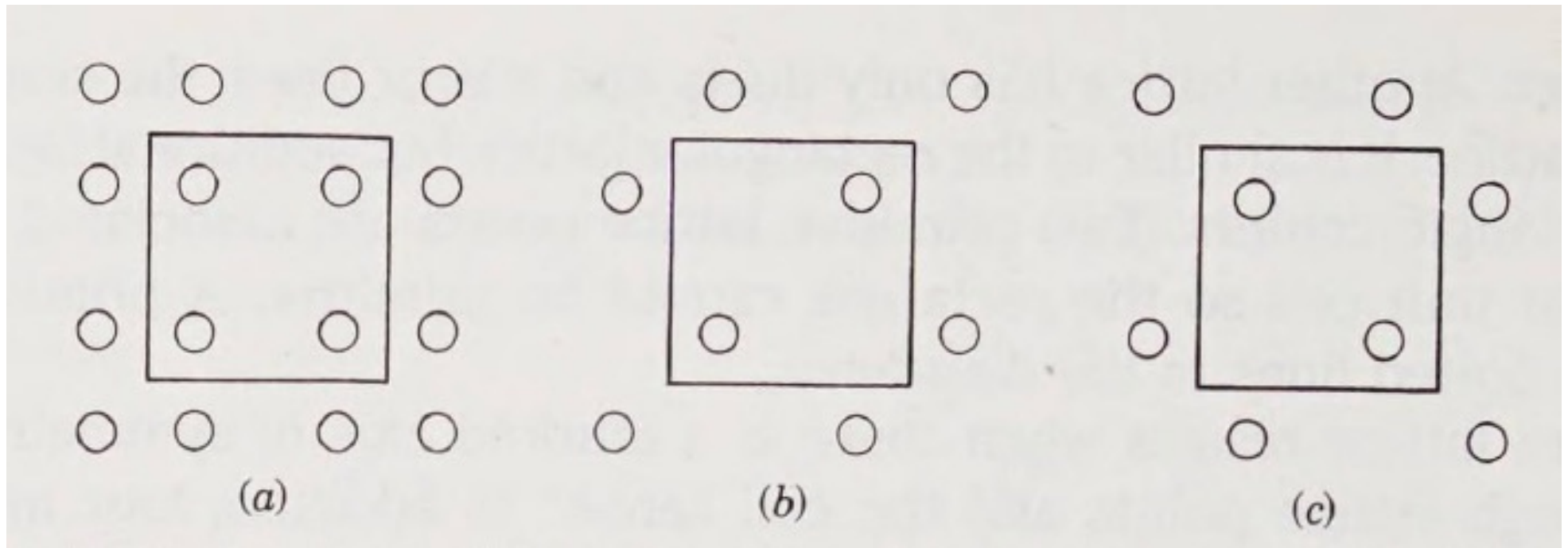


2D

Unit cells and symmetry groups

5 Bravais lattices

4 crystallographic systems

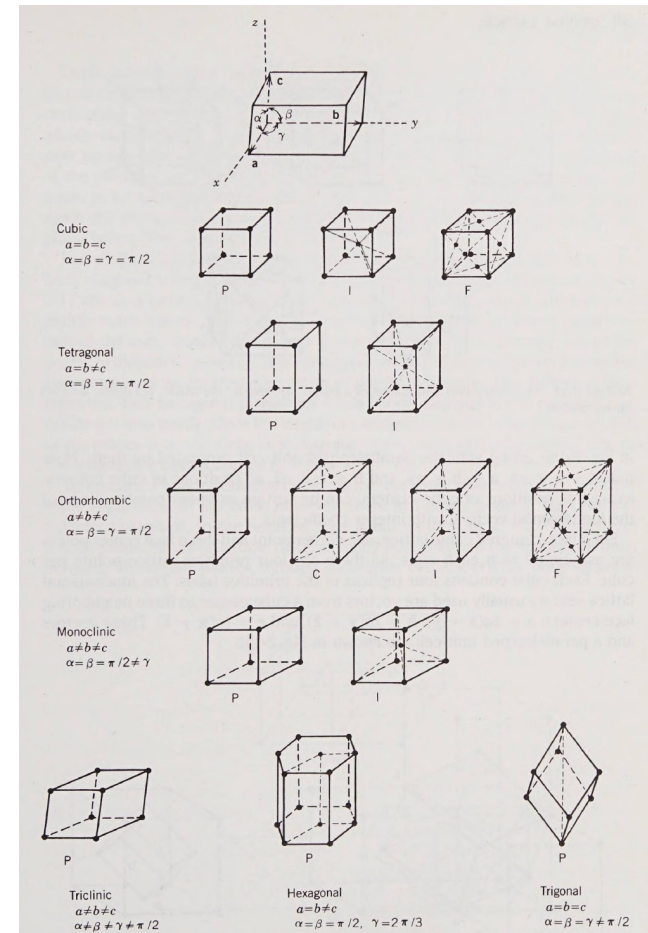


3D

# Unit cells and symmetry groups

14 Bravais lattices

7 crystallographic systems

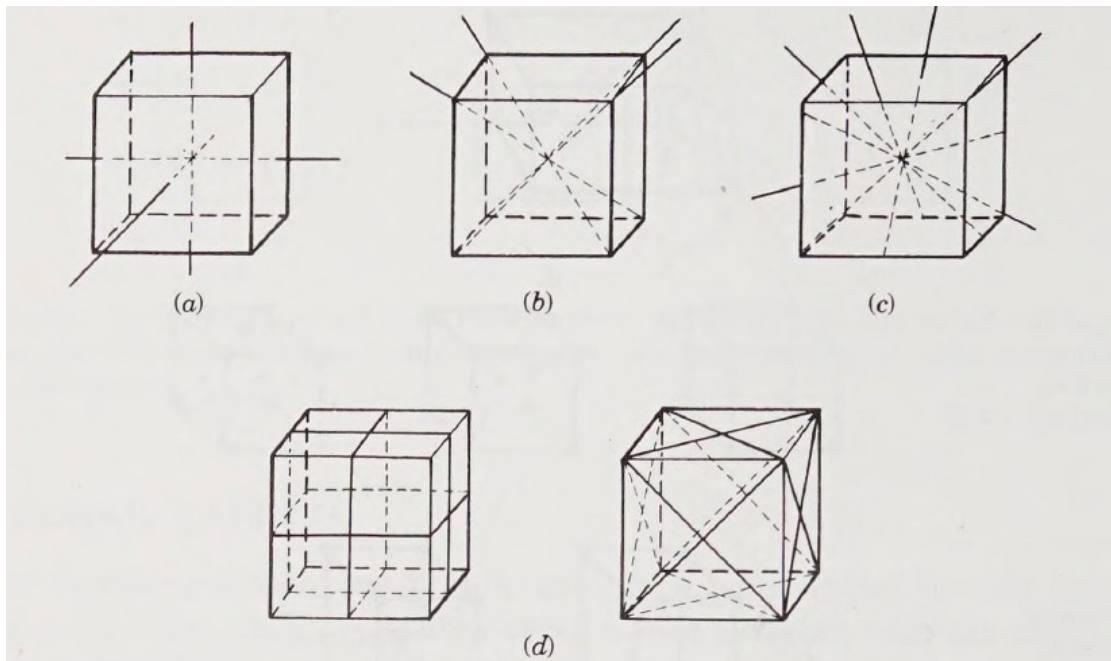




## Questions

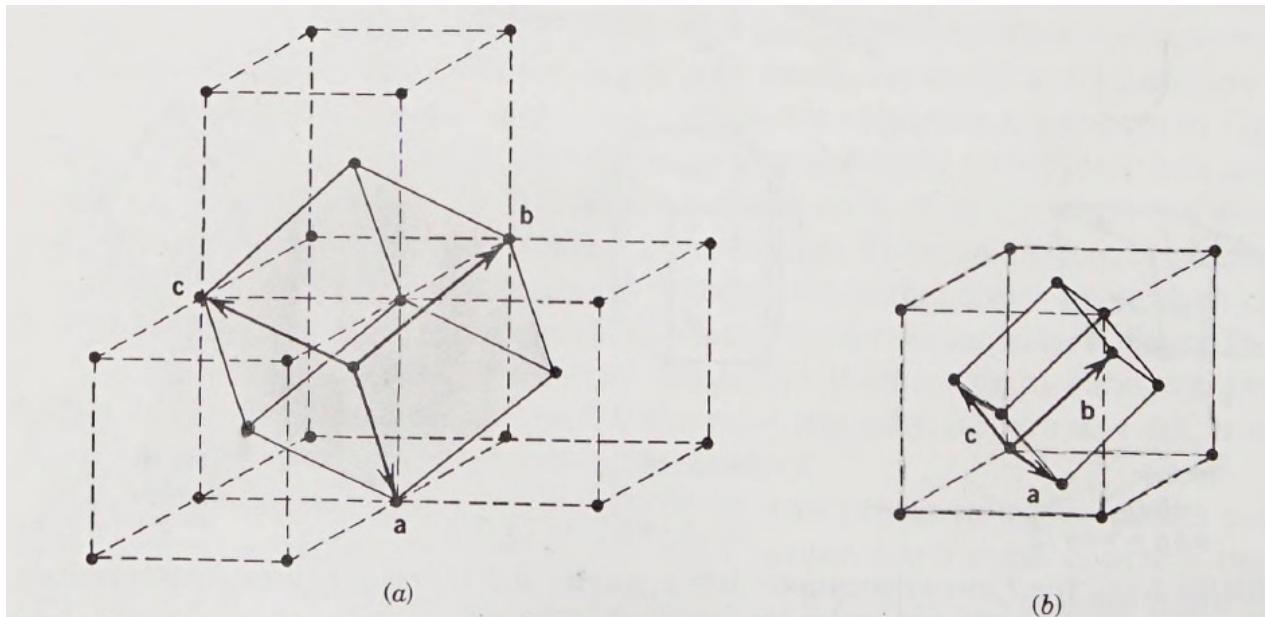
Why is there no cubic lattice of type C ?  
And tetragonal of type F ?

# Symmetry axes and planes of a cube

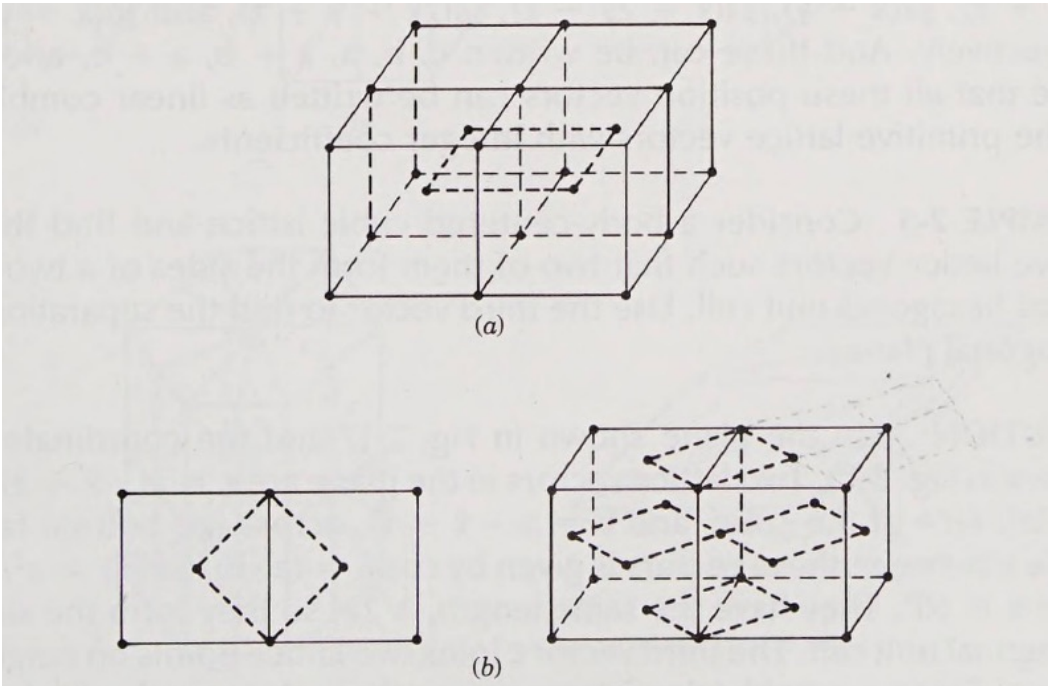




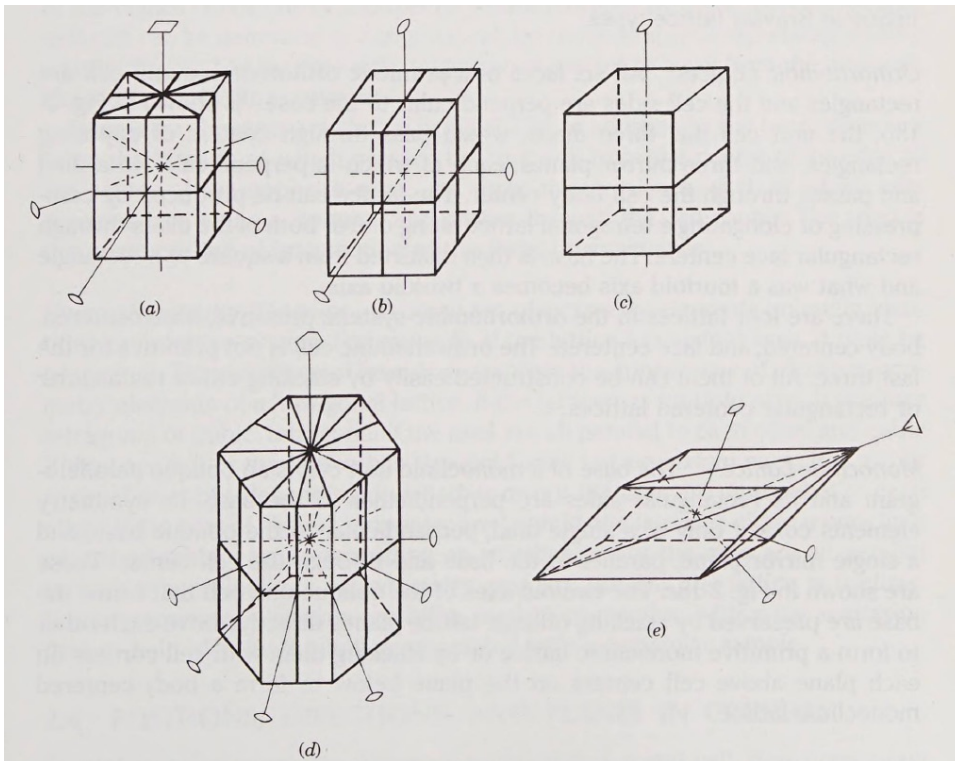
# Primitive translation vectors and primitive cells for bcc and fcc



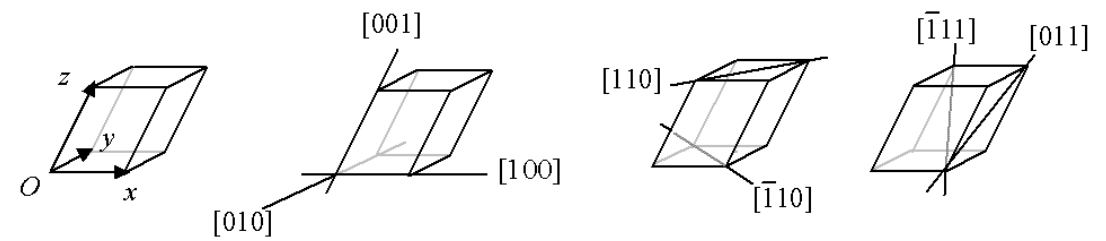
# Stacking of square lattices to form bcc and fcc



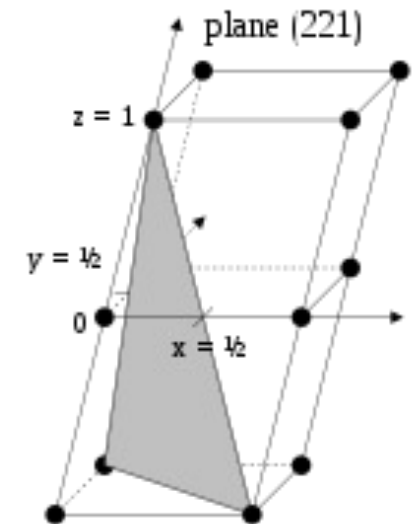
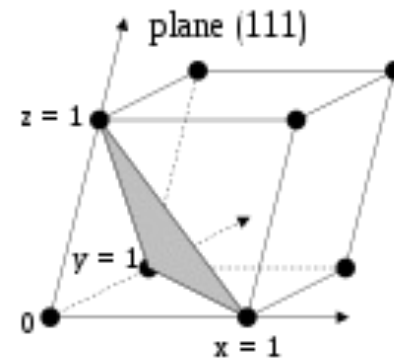
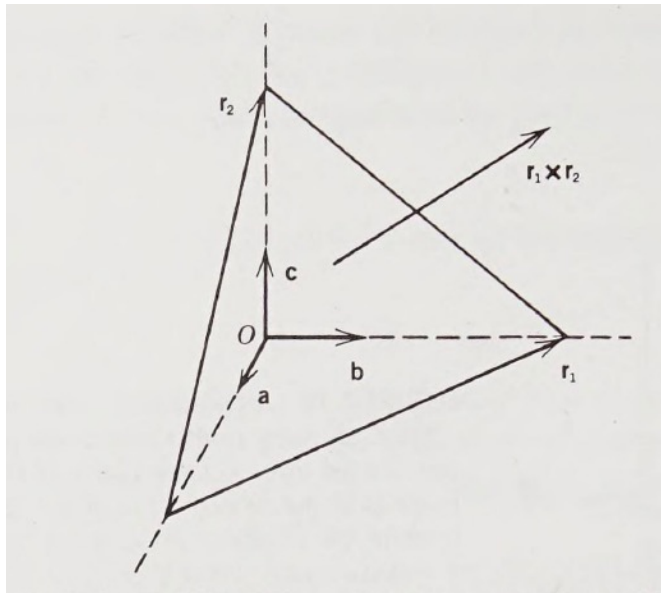
# Symmetry elements of unit cells



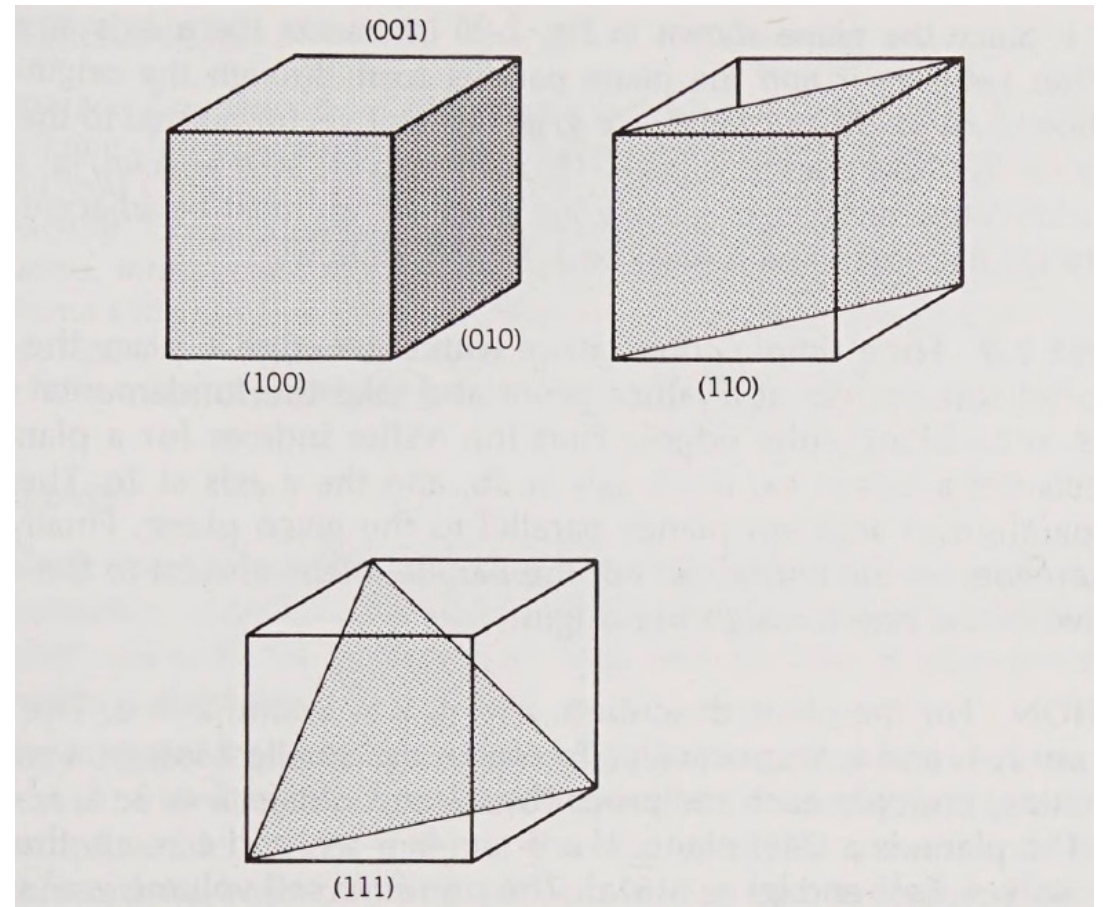
# Directions



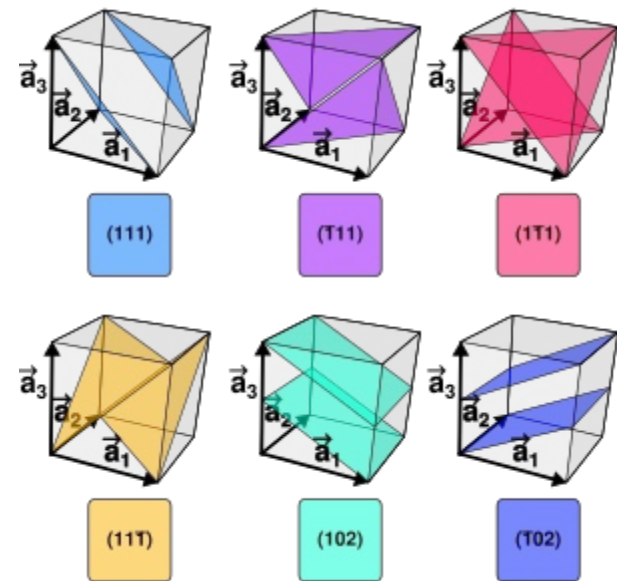
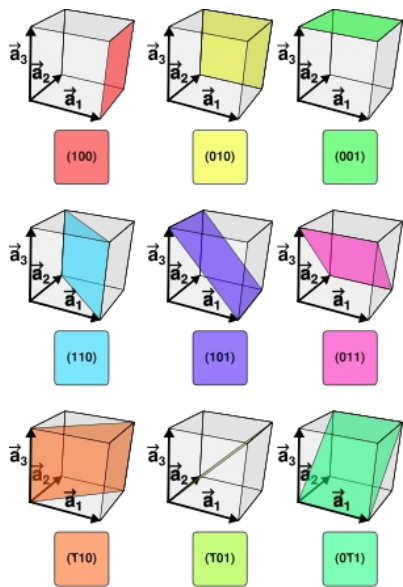
# Crystallographic planes: Miller indices



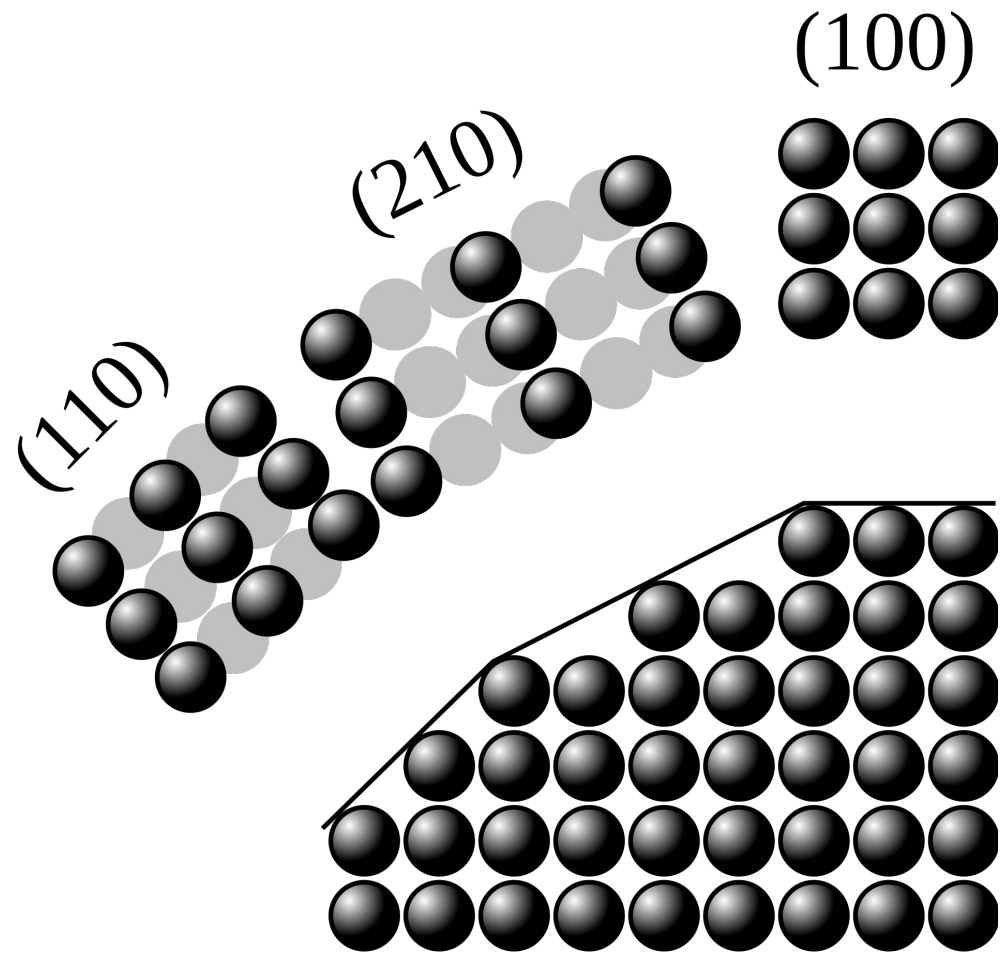
# Planes of cubic lattices



# Planes of cubic lattices

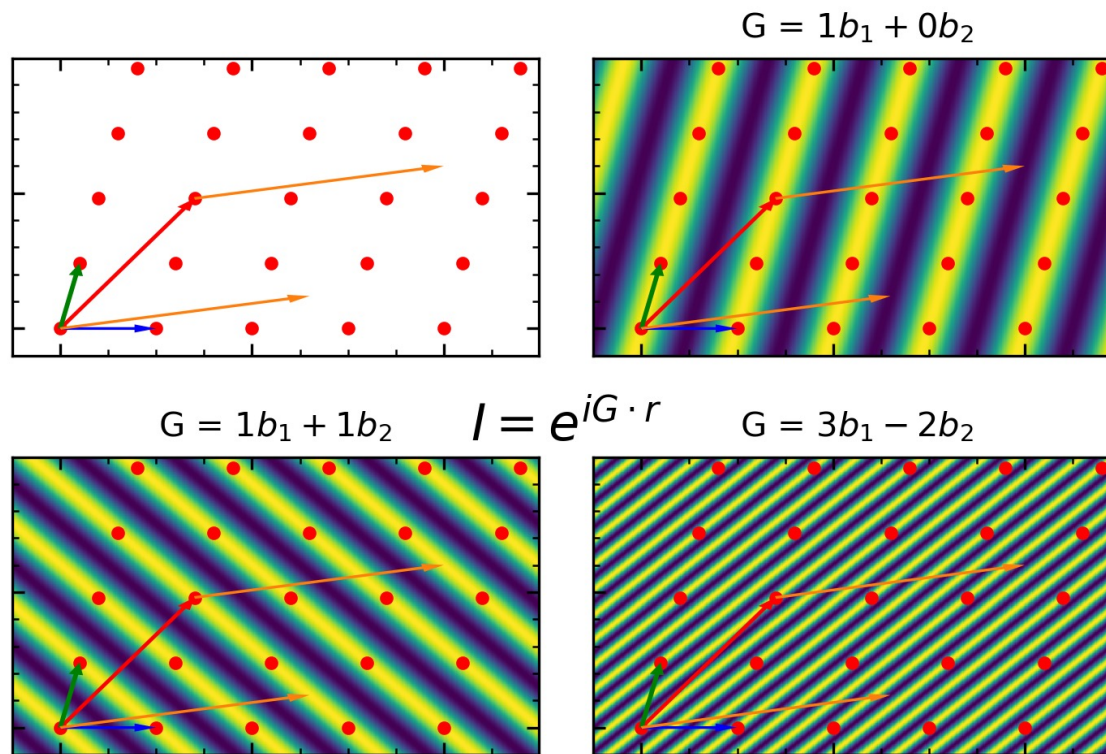


Dense  
crystallographic  
planes





# Reciprocal lattice



# Reciprocal lattice vectors

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

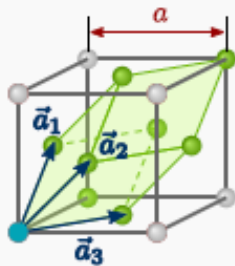
$$\vec{b}_2 = 2\pi \cdot \frac{\vec{a}_3 \times \vec{a}_1}{V}$$

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

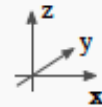
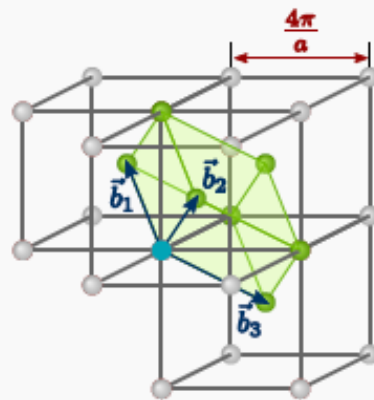
- As we have seen above, the reciprocal lattice of a Bravais lattice is again a Bravais lattice.
- The reciprocal lattice of a reciprocal lattice is the (original) direct lattice.
- The length of the reciprocal lattice vectors is proportional to the reciprocal of the length of the direct lattice vectors.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

# Reciprocal lattice of an fcc lattice

direct lattice:  
fcc with edge length  $a$



reciprocal lattice:  
bcc with edge length  $4\pi/a$



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

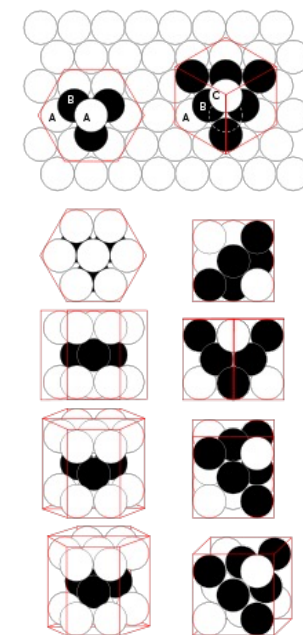
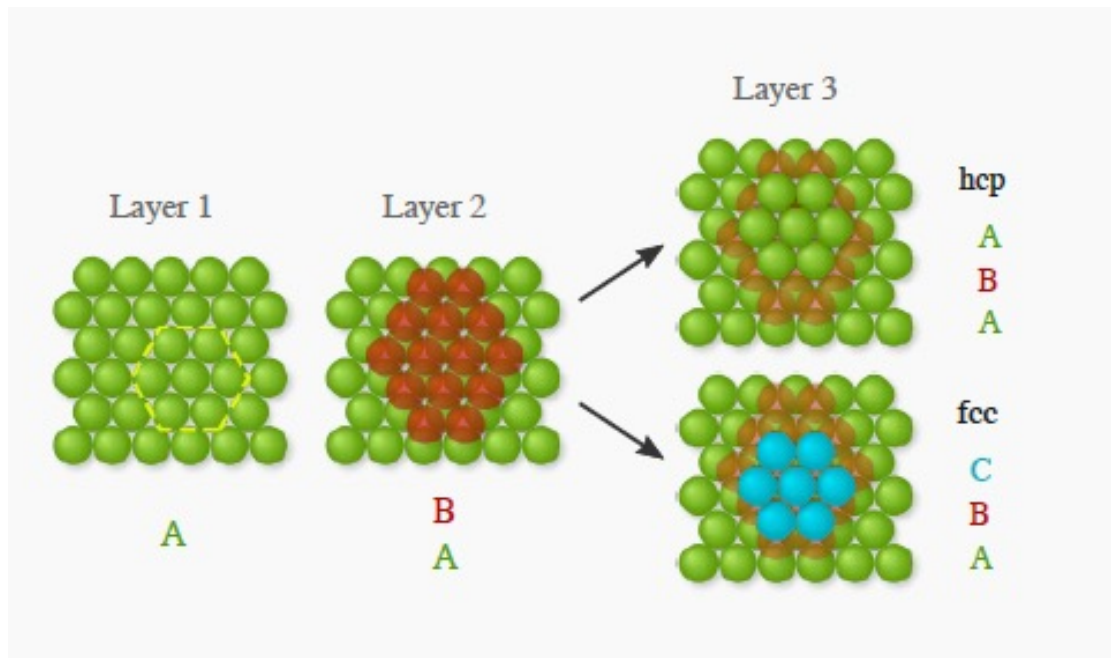
$$\vec{b}_2 = \frac{8\pi}{a^3} \cdot \vec{a}_3 \times \vec{a}_1 = \frac{4\pi}{a} \cdot \left( \frac{\hat{x}}{2} - \frac{\hat{y}}{2} + \frac{\hat{z}}{2} \right)$$

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

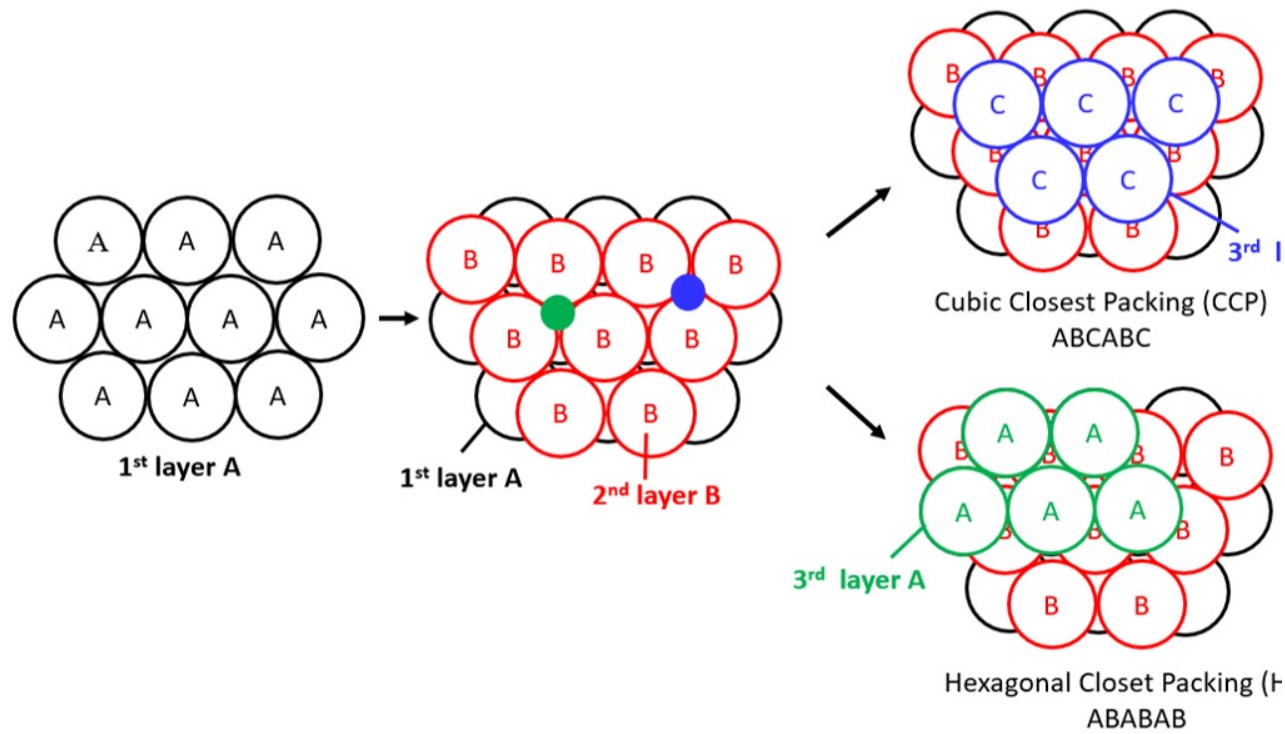
### 3. Structures of solids



# Close packed structures



# Close packed structures

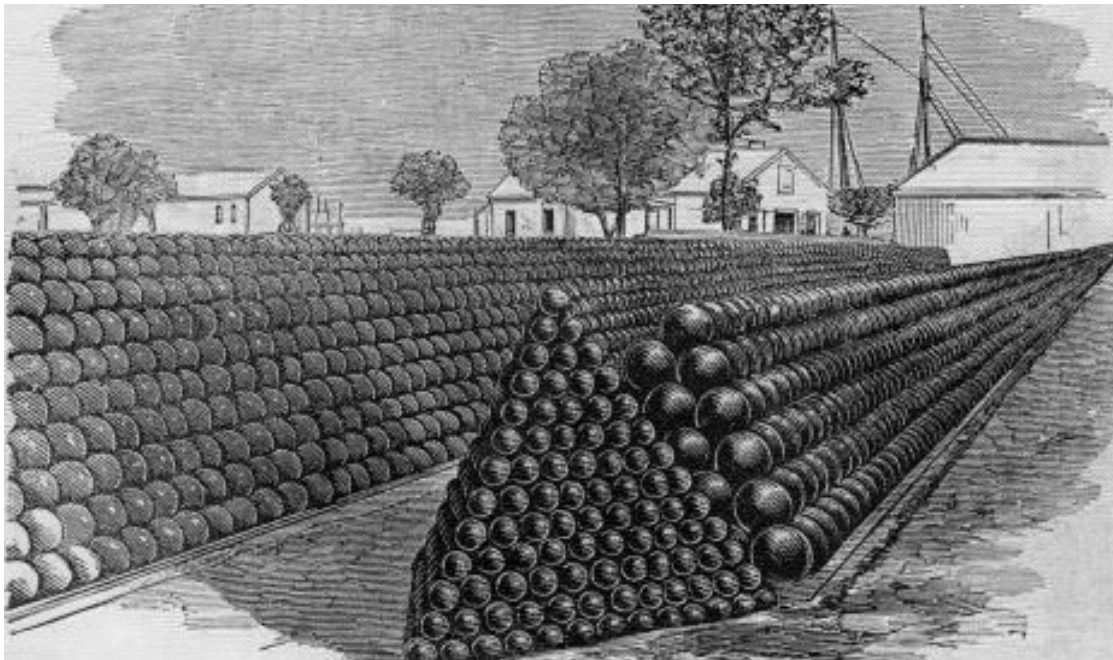


# Close packed structures



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

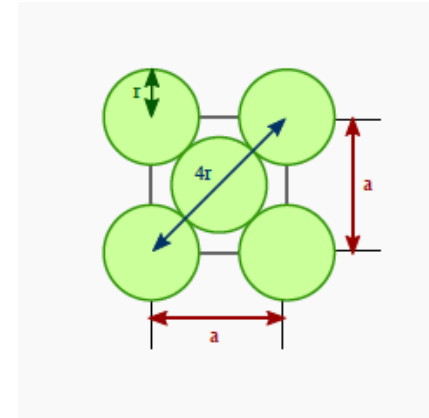
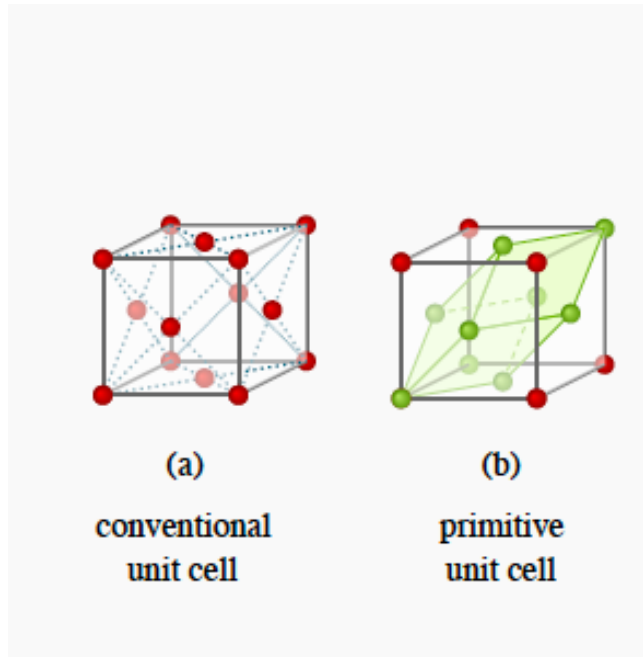
# The cannon ball mathematical problem (1587)



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

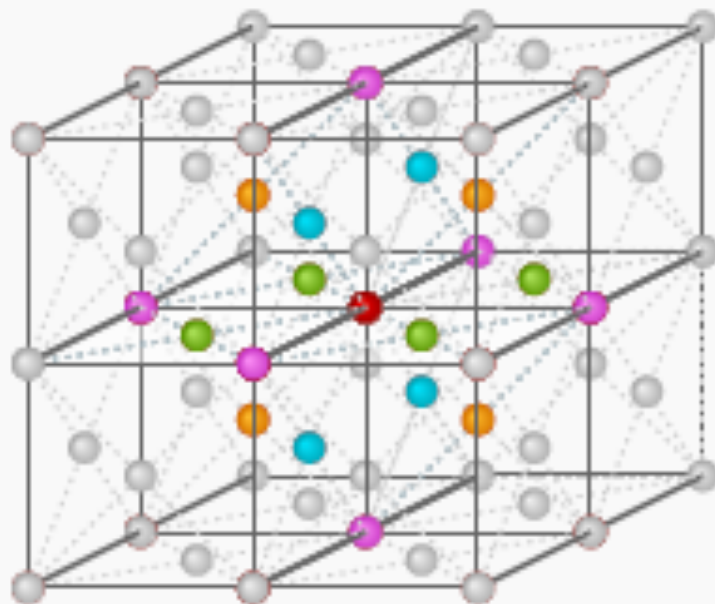


# Close packed density: fcc lattice



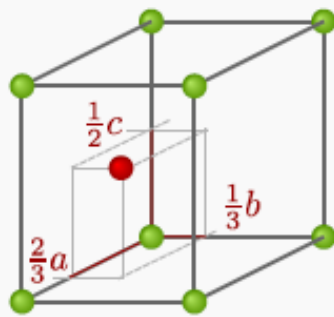
$$\rho = \frac{n \cdot V_{\text{sph}}}{V_{\text{uc}}} = \frac{4 \cdot \frac{4}{3} \pi \cdot \left(\frac{\sqrt{2}}{4}\right)^3 a^3}{a^3}$$
$$= \frac{\sqrt{2} \pi}{6} \approx 74\%$$

# Nearest-neighbours

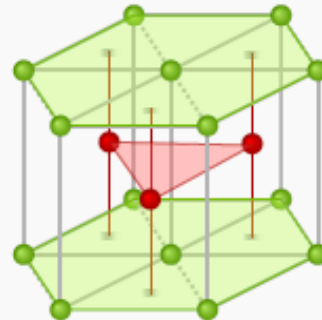


- reference point
- ● ● 12 nearest neighbours
- 6 next-nearest neighbours

# Second periodic close packed density: hcp structure

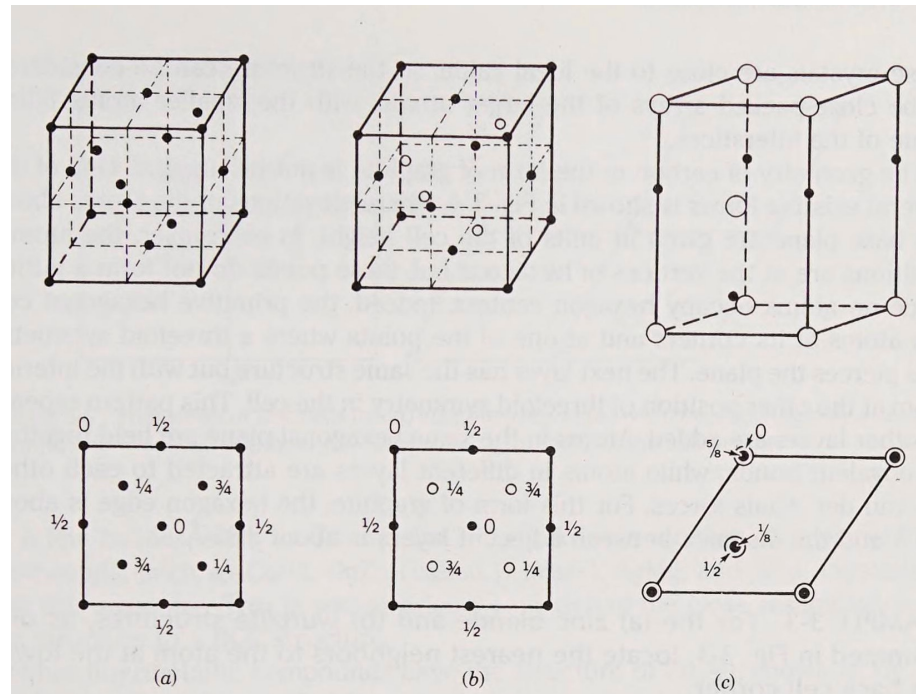


(a)

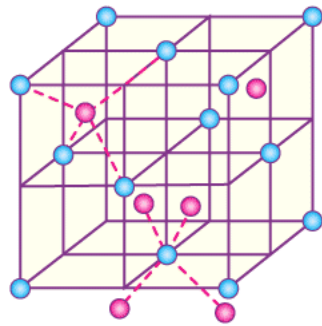
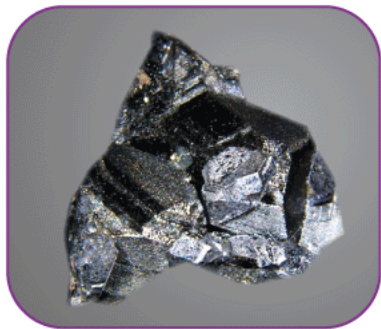


(b)

# Other crystal structures: diamond, zinc blende and wurzite

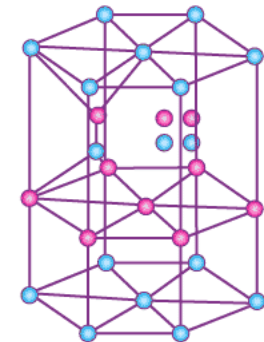
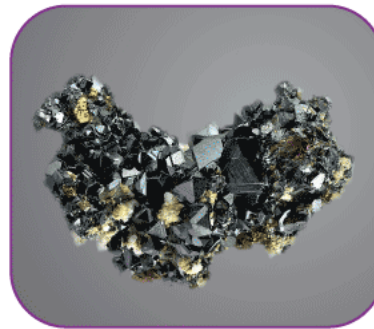


## ZINC BLENDE STRUCTURE



● S<sup>2-</sup> ● Zn<sup>2+</sup>

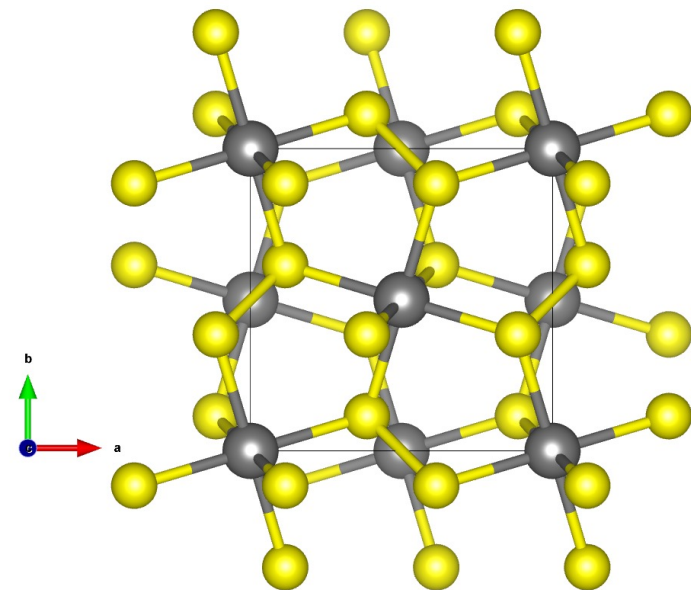
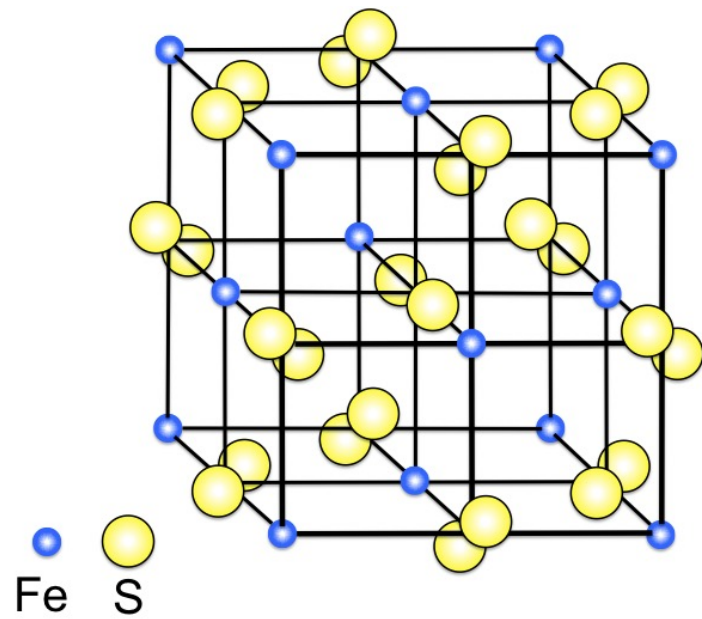
## WURTZITE STRUCTURE OF ZINC SULFIDE



● S<sup>2-</sup> ● Zn<sup>2+</sup>

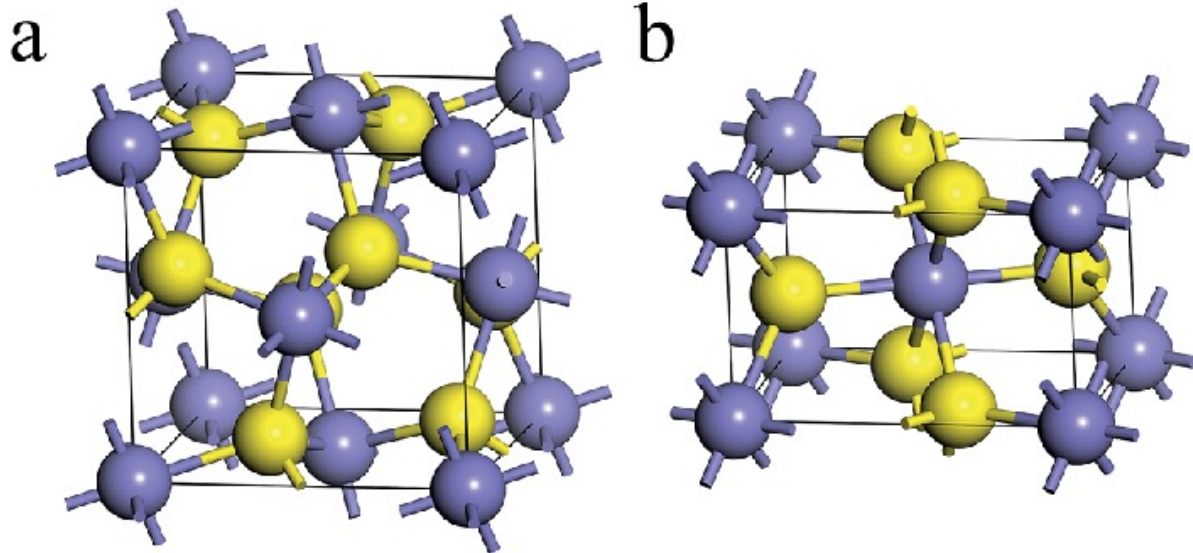
Zinc blende and wurzite  
(Zinc sulfide)

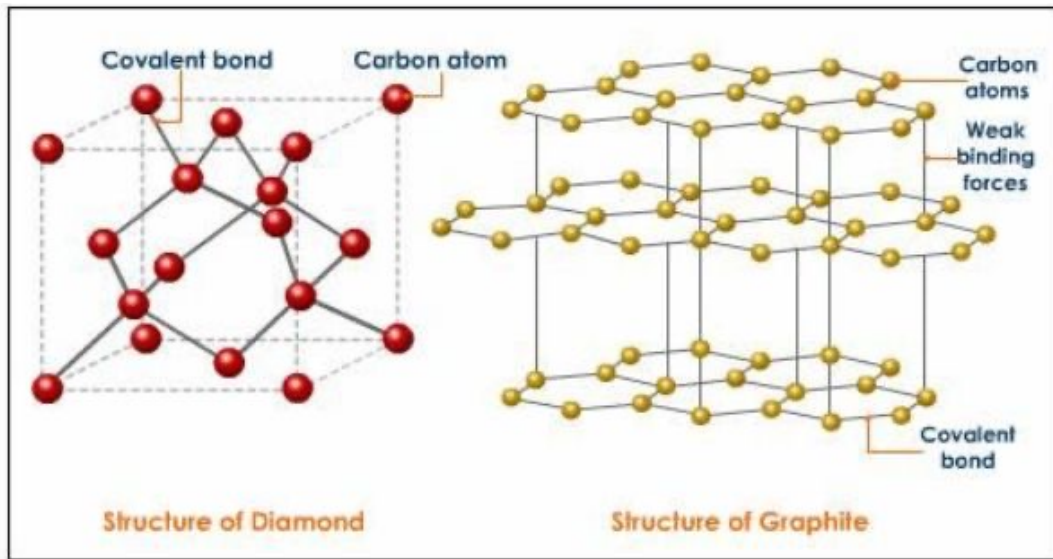
# Pyrite (Fools Gold)





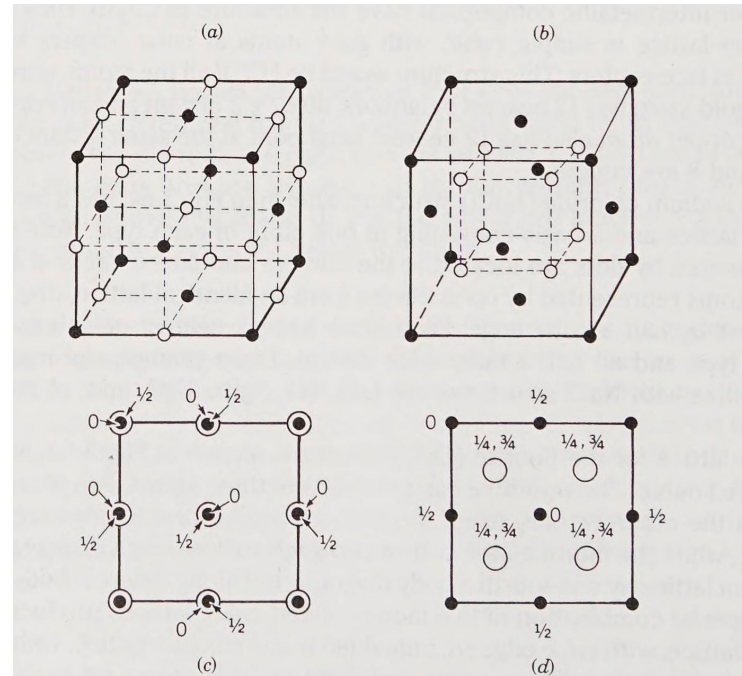
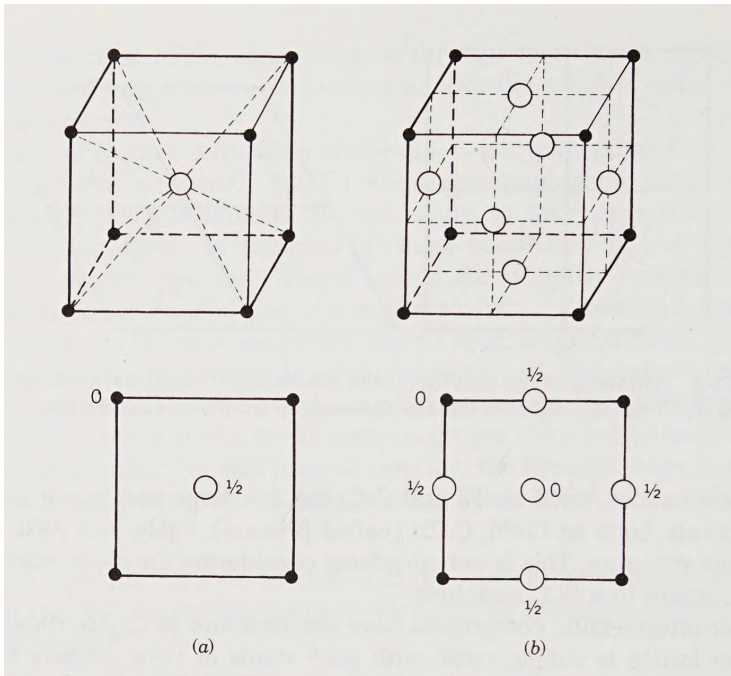
Pyrite and marcasite  
(Iron sulfide)





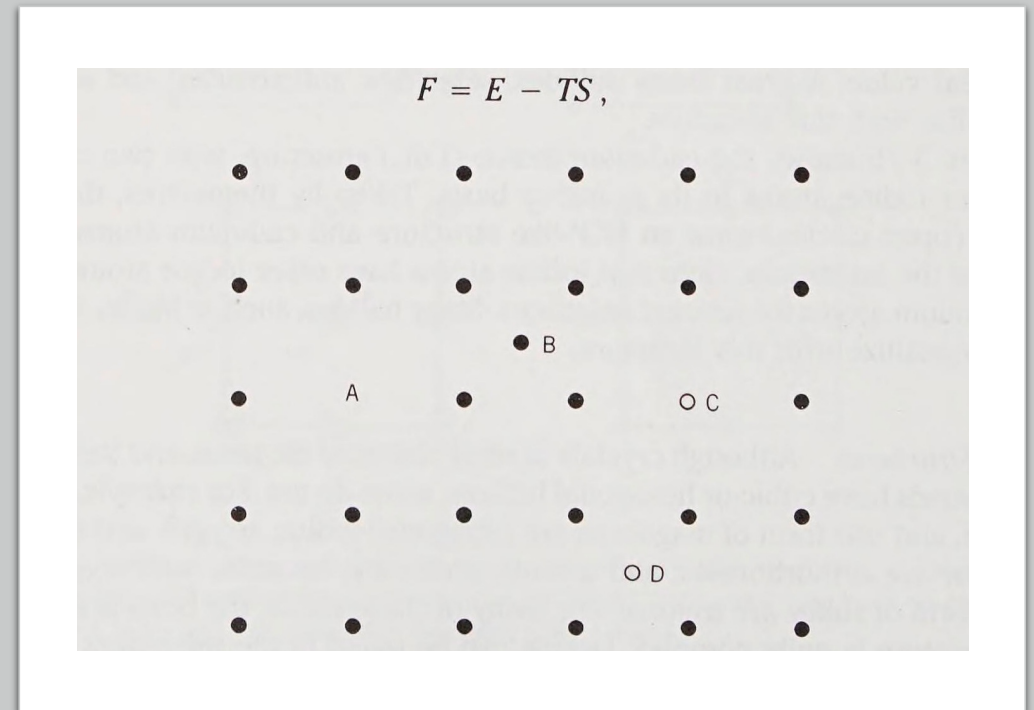
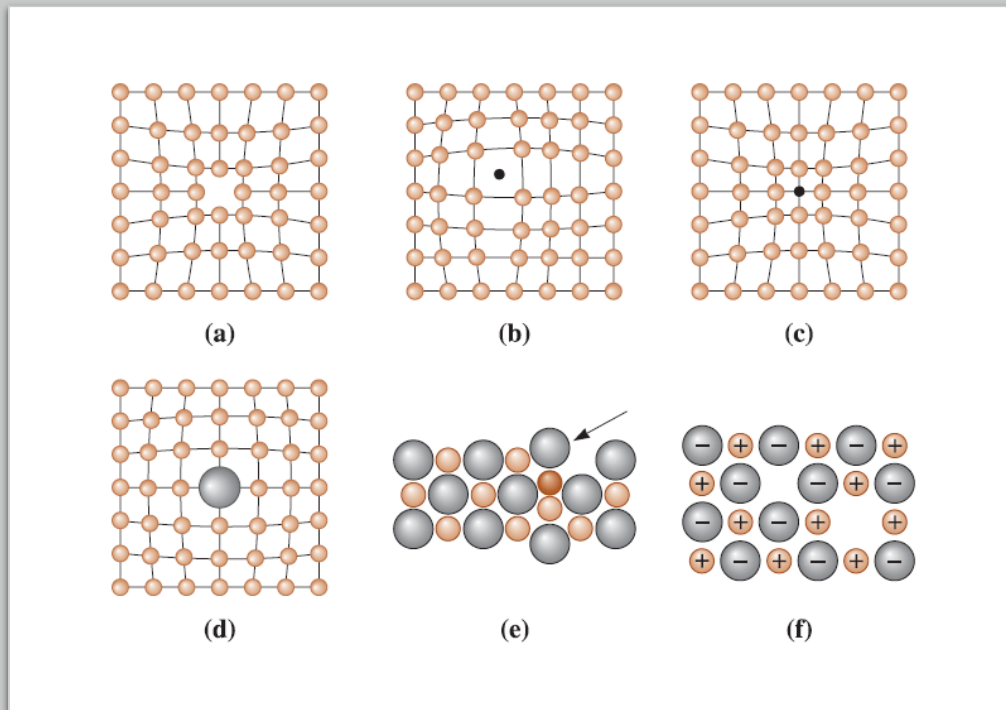
# Diamond and graphite

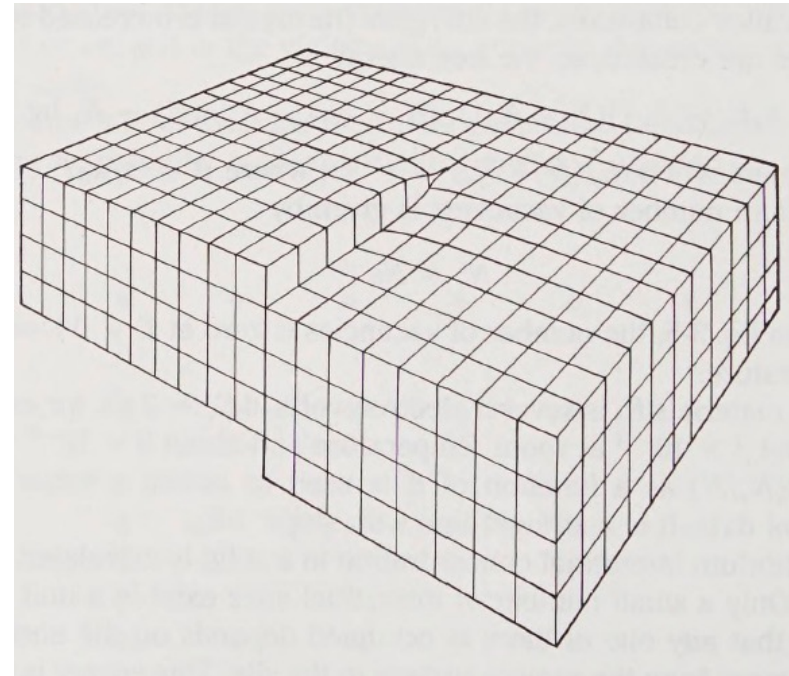
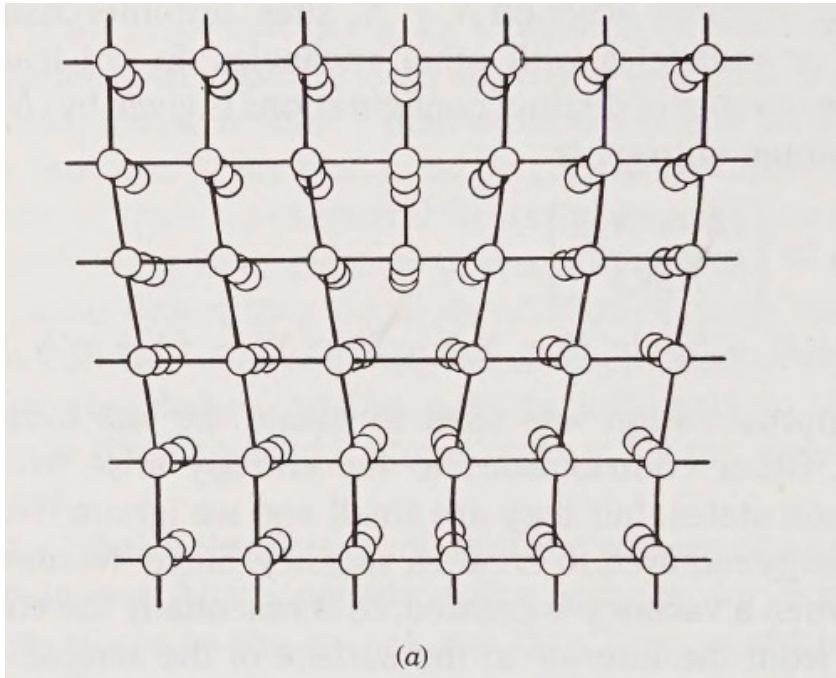




Other cubic structures: CsCl, Cu<sub>3</sub>Au, NaCl, CuFe<sub>2</sub>

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

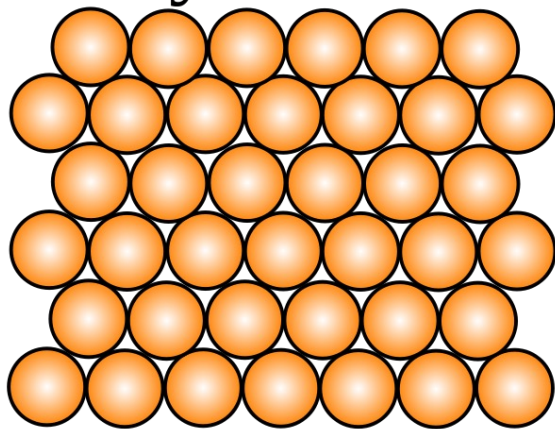




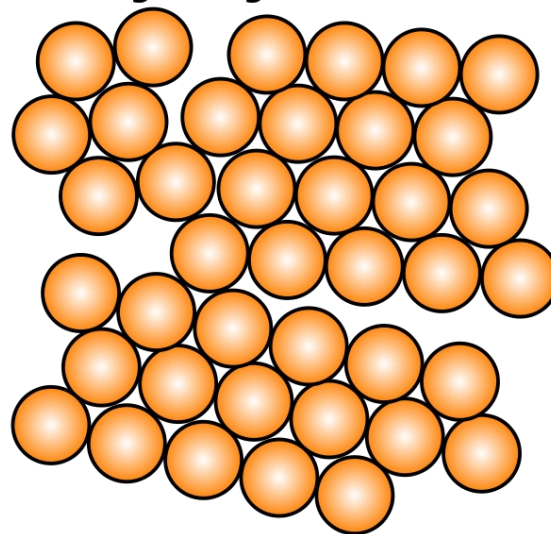
Dislocations: Edge (a) and screw (b)

# Amorphous structures

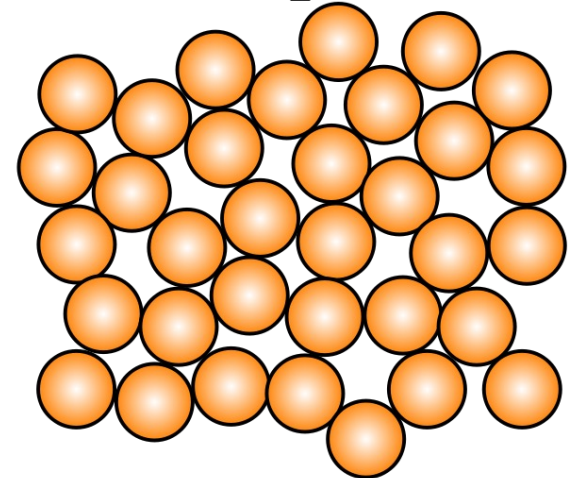
Crystalline



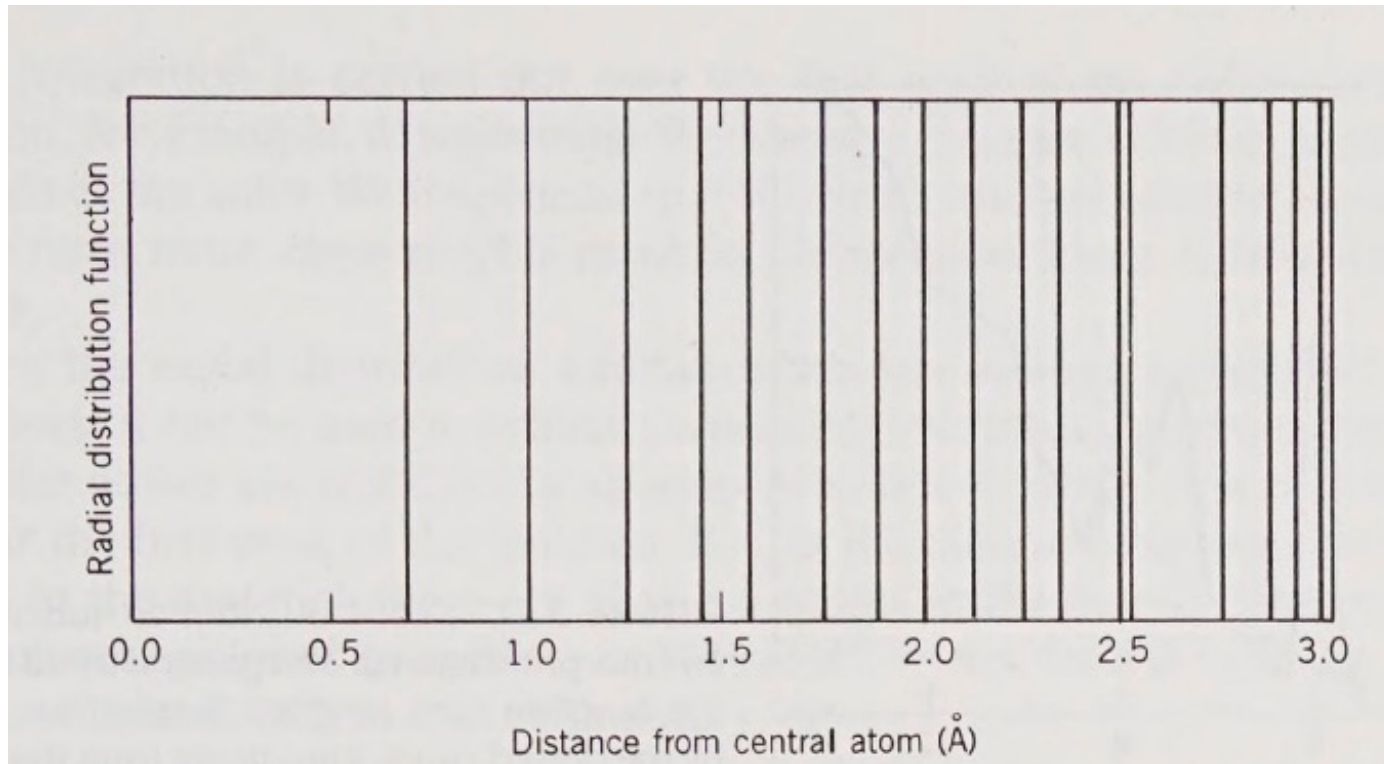
Polycrystalline



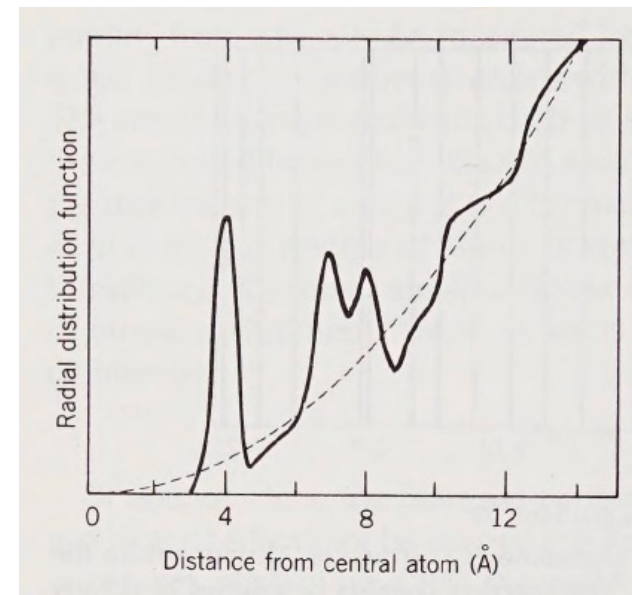
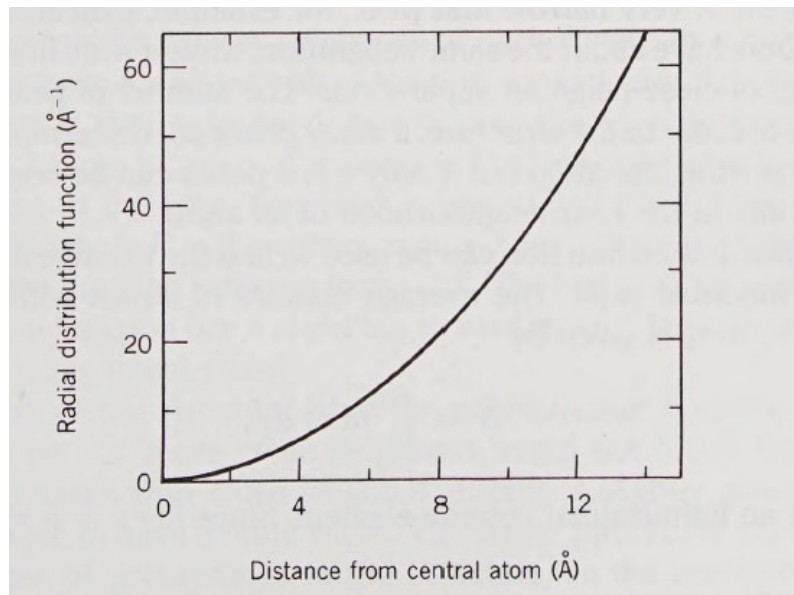
Amorphous



# Radial distribution function of crystalline fcc structure



# Radial distribution function of amorphous structures



# Liquid crystalline order

