

# Modeling a crystal

## Computational Material Science Lecture 2



# Presentation topics

Possible topics for the presentations

Modeling of:

- Biomaterials
  - Composite materials
  - Self-healing materials
  - Graphene
  - Carbon nanotubes
  - Metamaterials
  - Polymers
  - Your choice
- 
- Journals: Modeling in Materials Science and Engineering, Computational Material Science, Journal of the Mechanics and Physics of Solids, Acta Materialia, Mechanics of Materials.

The first presentations will be on March 27.

15 minutes each

# Last time

- There are different simulation techniques to address different length scales
- The smaller the scale the more accurate the description of the material, but the more computationally expensive the simulation
- In this course we will tackle the nano, the micro and the macro-scale.
- Diffusion can be modeled as the random walk of vacancies

# Today

- Averaging and Binning
- Modeling atomic crystals
- Sums of interacting pairs of objects
- The simplest interatomic potential: Lennard-Jones

## Learning objectives:

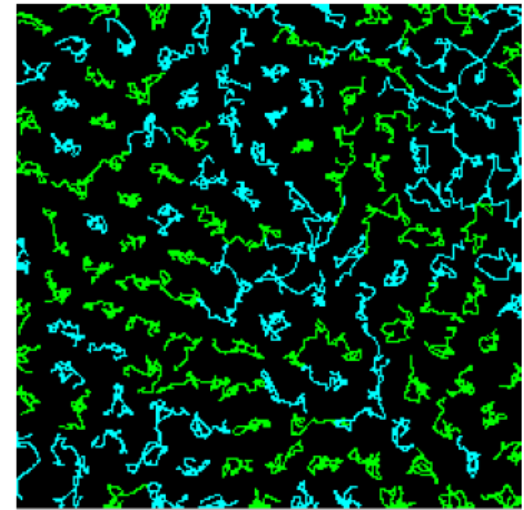
- Modeling a crystal and its cohesive energy by using the Lennard-Jones potential

# Averaging

Important point:

Very often when modeling materials it is essential to average over various simulations.

The behavior of a single particle, vacancy, atom, dislocation...is unlikely representative of the behavior of the entire system



Trajectories

The smaller is the system one considers the more important is averaging. This is true also in experiments.

# The end-to-end probability distribution

We have generated many equivalent trajectories.

After  $n$  jumps where is most likely the vacancy?

Random walk in one dimension starting from zero, reaches a certain position  $x_n$

If we average over enough trajectories we will end up with the probability of finding the atoms at a given position  $x_n$ .

How can I tell if the trajectories I am taking are 'enough'?

# Probability of $x_n$ for a random walk

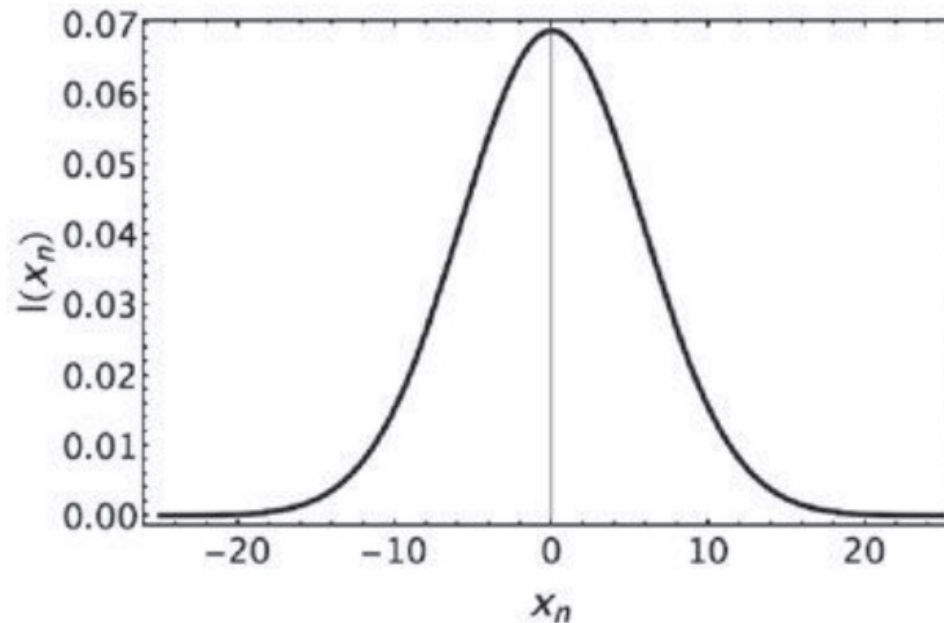
What is the probability that a walker is at  $x_n$ ? For a random walk it is a gaussian distribution:

$$I(x_n) = \left( \frac{3}{2\pi na^2} \right)^{1/2} \exp \left\{ - \frac{3x_n^2}{2na^2} \right\}$$

$n$ =number of jumps  
 $a$ =step size

**Q1:** What is the probability of a straight walk?

**Q2:** do you notice something odd/unphysical?



$n=100$   
 $a=1$

# End-to-end probability distribution

The probability distribution in 3D takes the form:

$$\mathcal{P}(\mathbf{R}_n) = I(x_n)I(y_n)I(z_n)$$

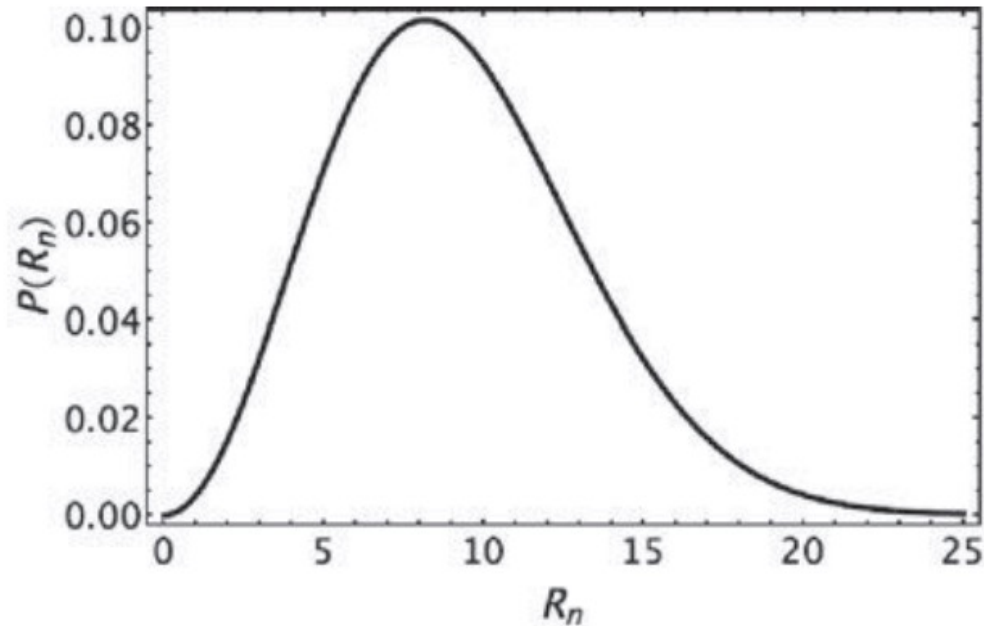
$\mathcal{P}(\mathbf{R}_n)$  gives the probability that the vector  $\mathbf{R}_n$  is at a position  $(x_n, y_n, z_n)$ .

Changing  $x, y, z$  to polar coordinates and integrating over the angles leads to the end-to-end probability distribution of  $R_n$ , a measure of how far the atom has diffused in  $n$  steps (without info on the orientation)

$$\mathcal{P}(R_n) = \left( \frac{3}{2\pi na^2} \right)^{3/2} 4\pi R_n^2 \exp \left\{ - \frac{3R_n^2}{2na^2} \right\}$$



# End-to-end probability distribution

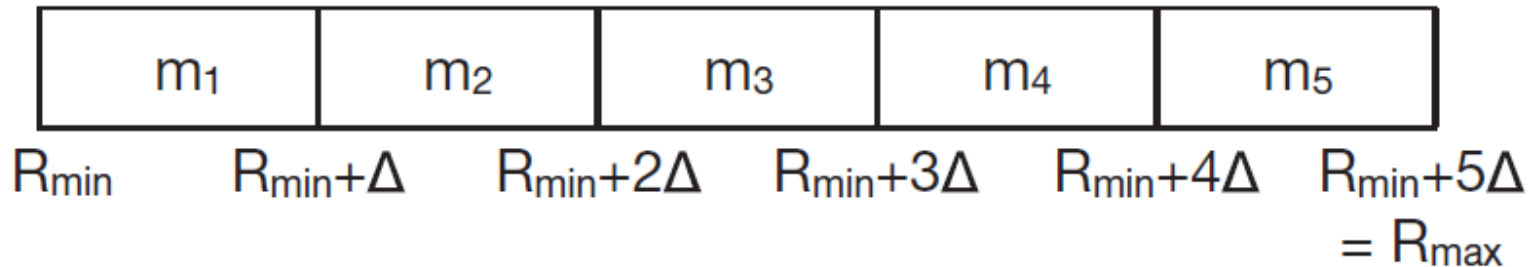


$$\mathcal{P}(R_n) = \left( \frac{3}{2\pi n a^2} \right)^{3/2} 4\pi R_n^2 \exp \left\{ - \frac{3R_n^2}{2na^2} \right\}$$

# Binning

To create the discrete representation of  $\mathcal{P}(R_n)$   
m runs = m trajectories

$$\Delta = \frac{R_n^{max} - R_n^{min}}{n_{bin}}$$



$$\mathcal{P}_i = \frac{m_i}{m}$$

# Exercise

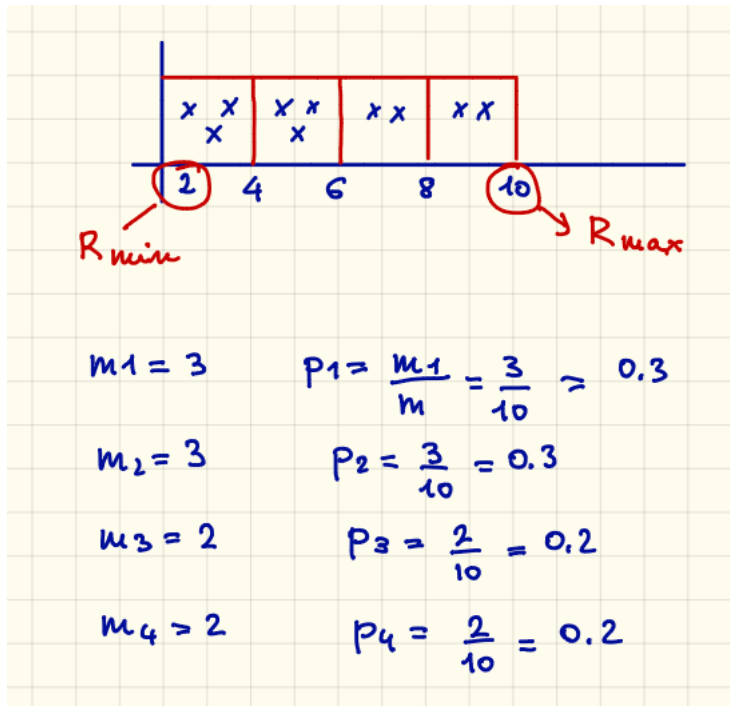
After running the code with the moving vacancy 10 times, you find the following end-to-end distances:

Values of  $R_n = 2, 4, 5, 3, 9, 7, 5, 3, 6, 10$

Calculate by hand the probability distribution of these distances, using the binning procedure.

# Solution

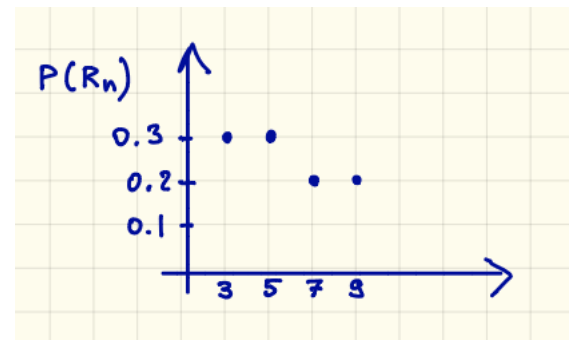
Values of  $R_n = 2, 4, 5, 3, 9, 7, 5, 3, 6, 10$   
m runs = m trajectories  $\rightarrow m = 10$



$$\Delta = \frac{R_n^{max} - R_n^{min}}{n_{bin}}$$

$$\Delta = \frac{10 - 2}{4} = 2$$

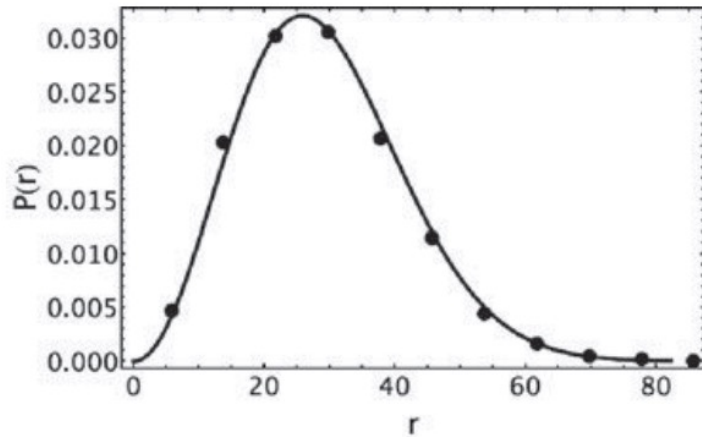
$$P_i = \frac{m_i}{m}$$



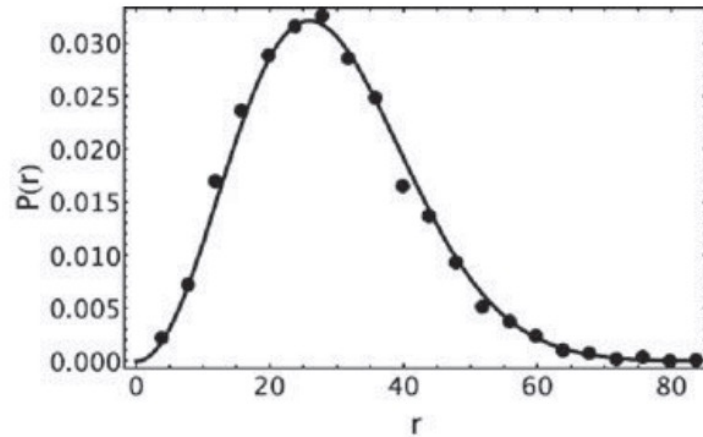
# The art of binning

Calculated end-to-end probability distribution based on  $m=2000$  trajectories at the end of a random walk for  $n=1000$  jumps on a square lattice.

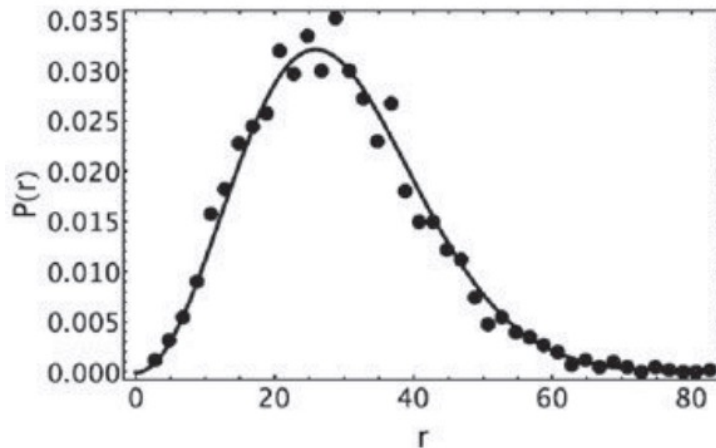
nbin=10



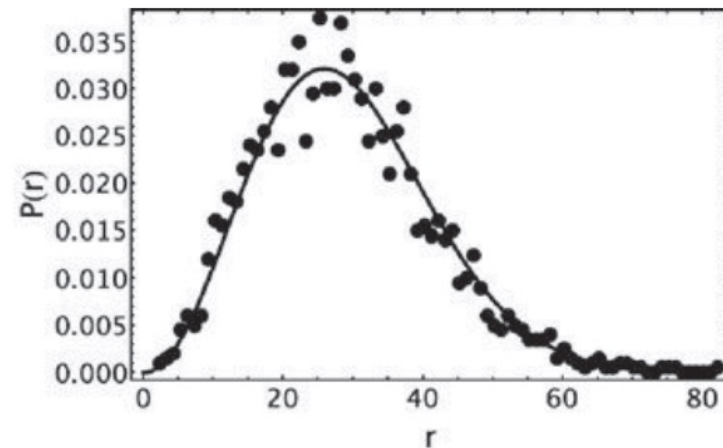
nbin=20



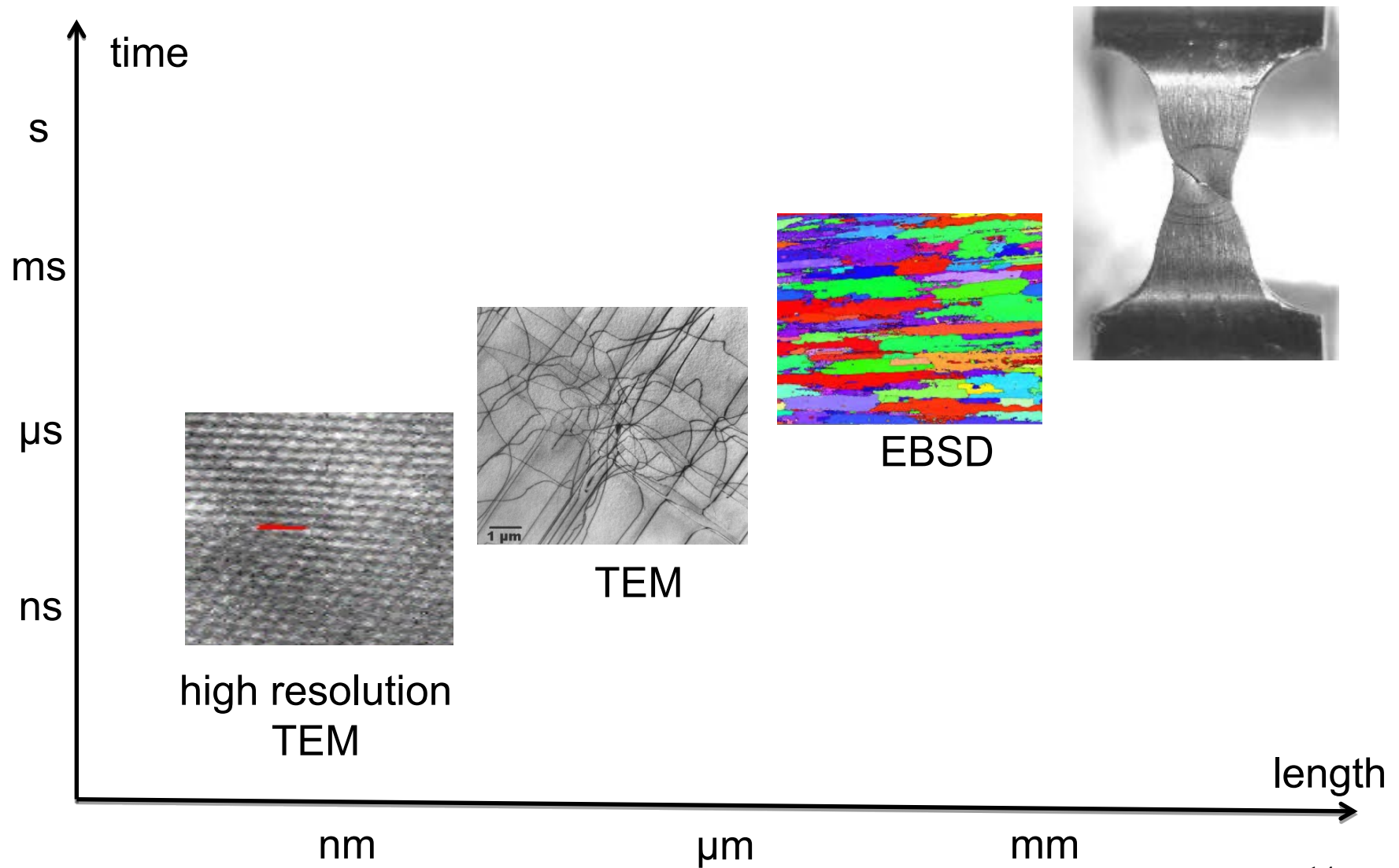
nbin=40



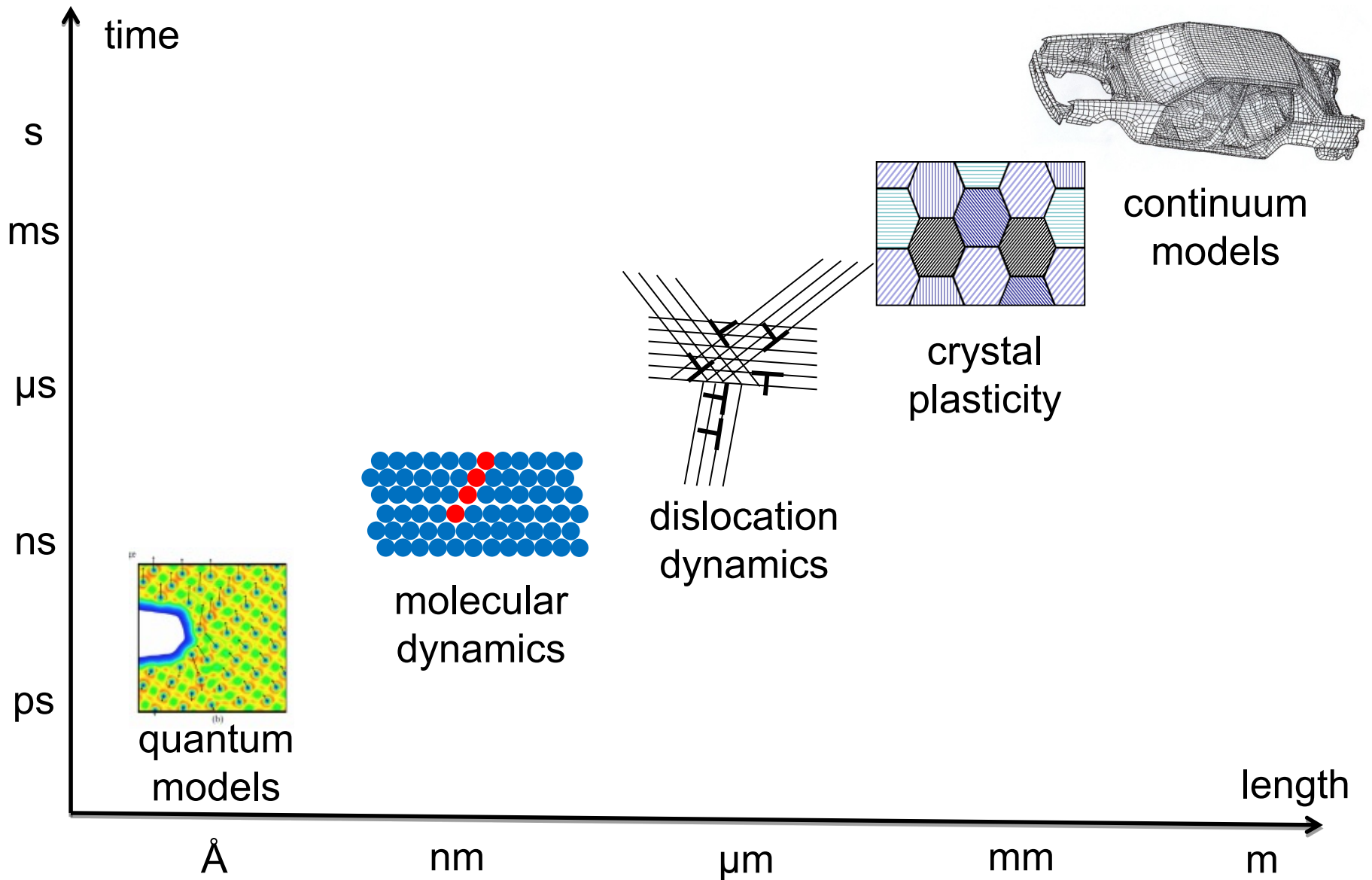
nbin=80



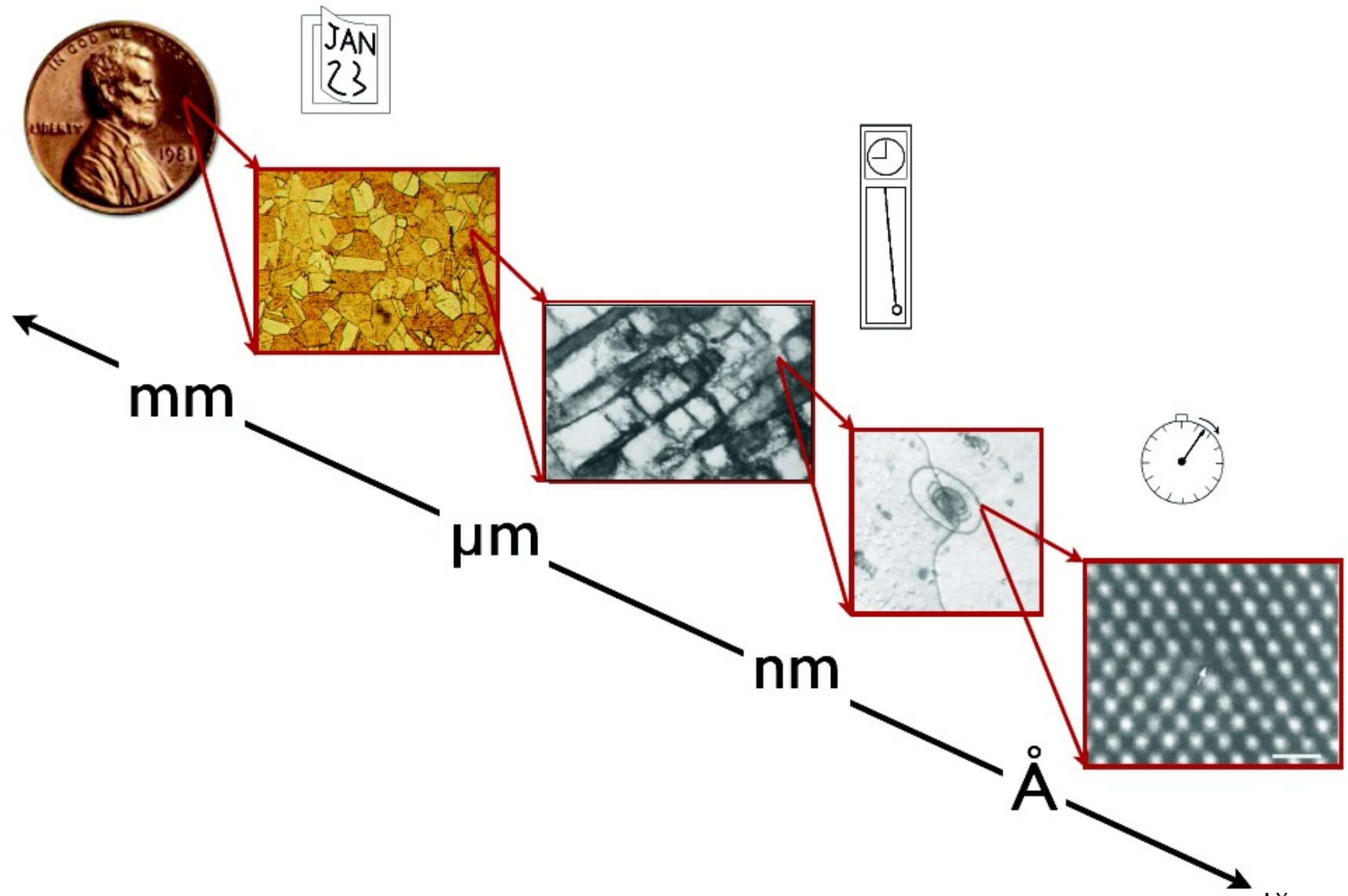
# Experimental observation at different scales



# models at different scales

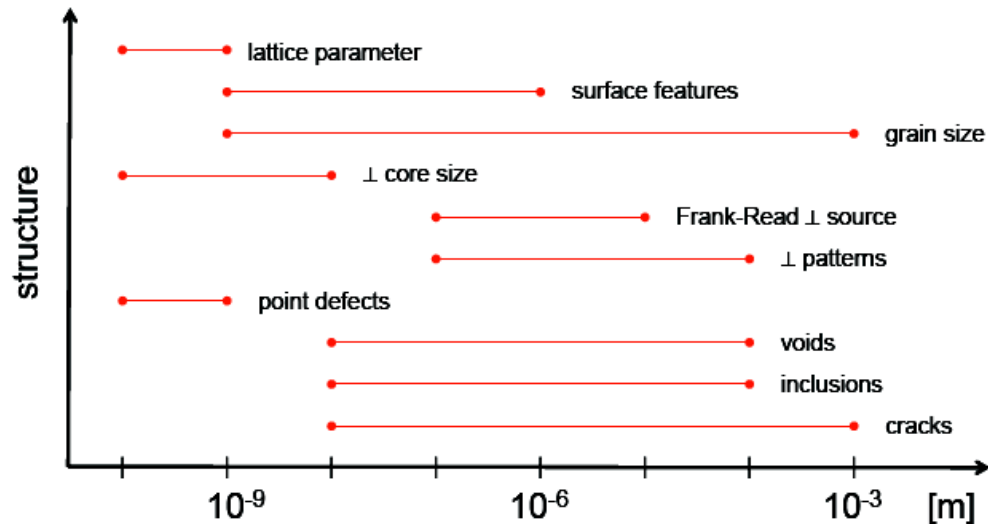


# Materials and scales





# Summary of scales

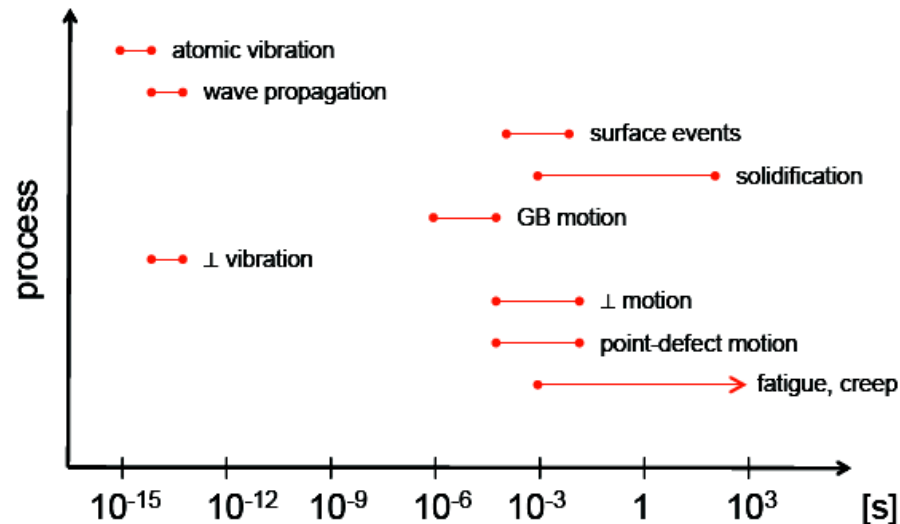


## Structural features:

- range in size from  $10^{-10}$  to  $10^{-3}$  m
- interact atomistically at short distances and over long distances via long-range elastic stress fields.

## Materials processes:

- occur over time scales ranging from  $10^{-15}$  to years.
- this broad range can sometimes be an asset when scale separation occurs.



Modeling material behavior requires methods able to span across length and time scales.

# Modelling crystalline solids

- ▶ Most engineering materials are crystalline: the atoms arrange themselves into a translationally invariant pattern of repeating unit cells. For example:

copper

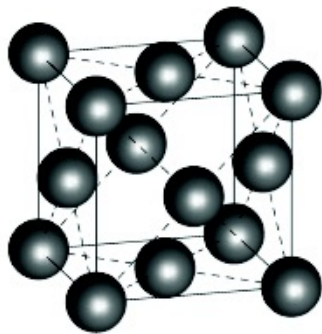


silicon

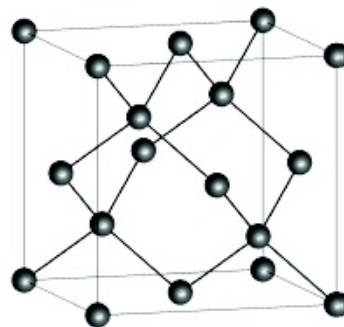


Source:Wikimedia Commons

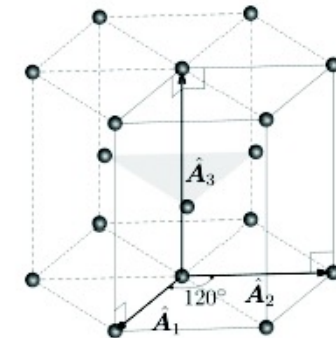
zirconium



face-centered cubic (fcc)



diamond cubic (dc)



hexagonal close packed (hcp)

# Quartz



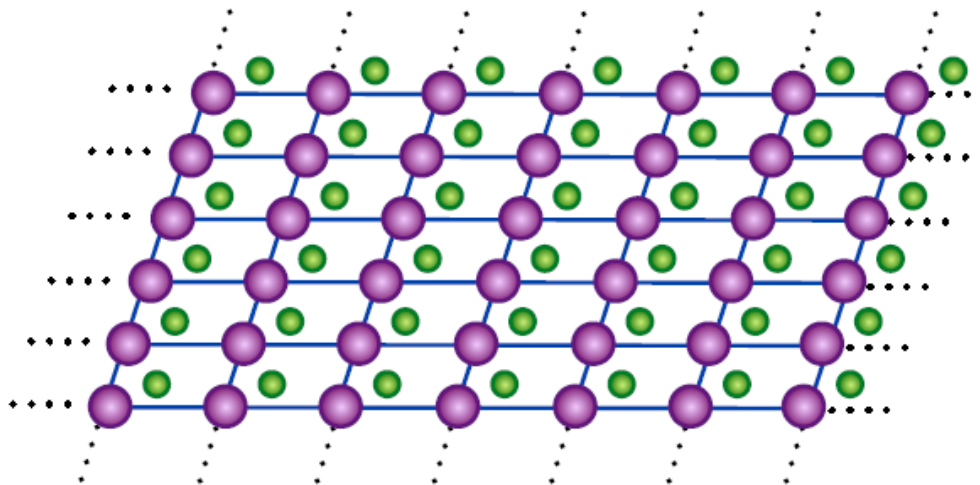
# Crystal structure

- ▶ Many engineering materials have a crystalline structure.
- ▶ An **ideal crystal** is defined by:

**lattice:** an infinite arrangement of points in a regular pattern

+

**basis:** a group of atoms positioned at each lattice site

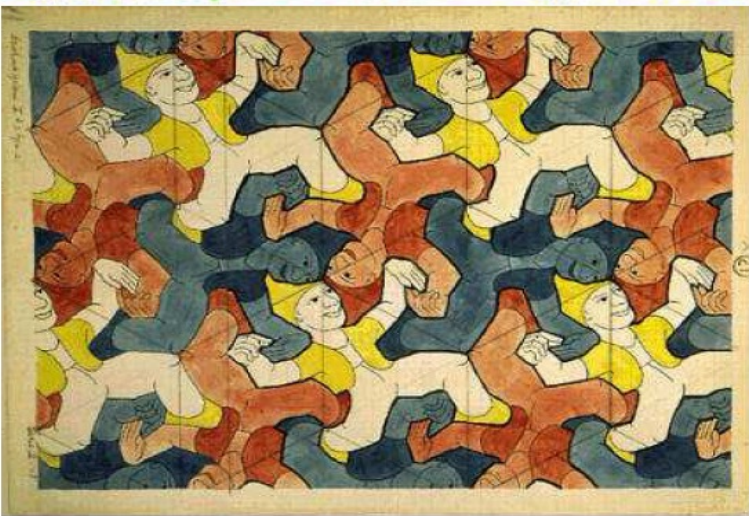
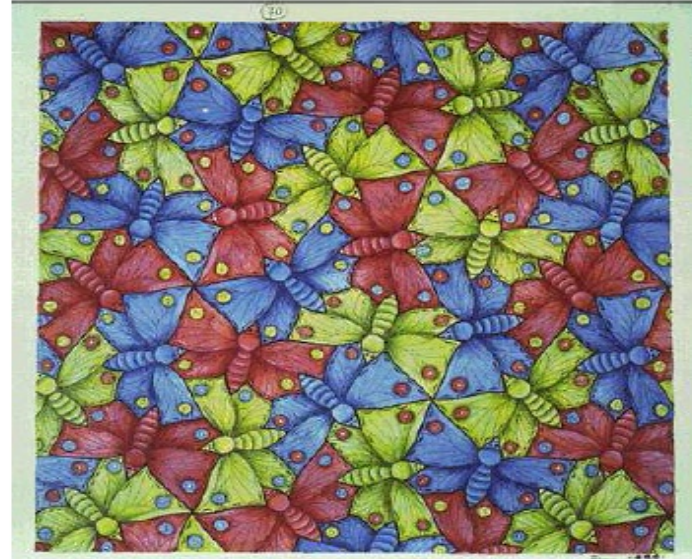
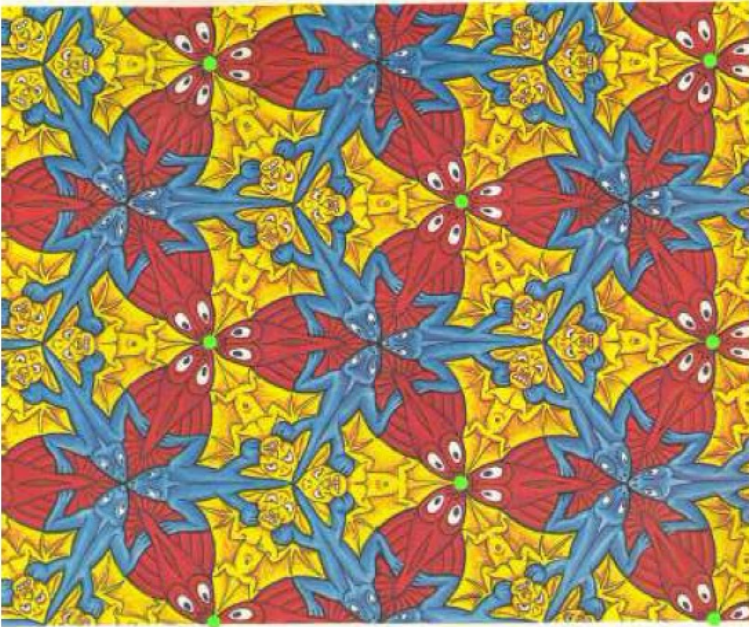


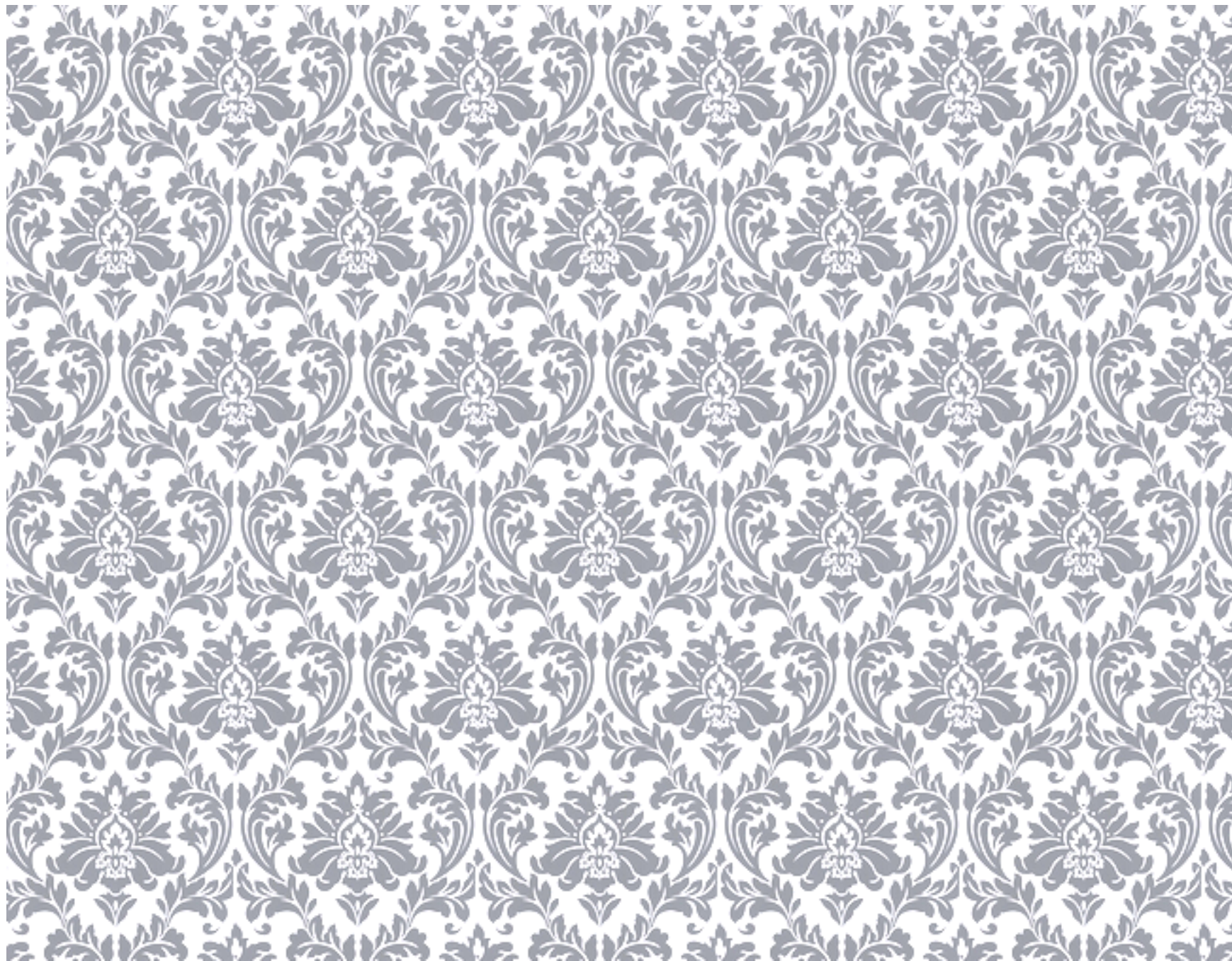
# Importance of the lattice

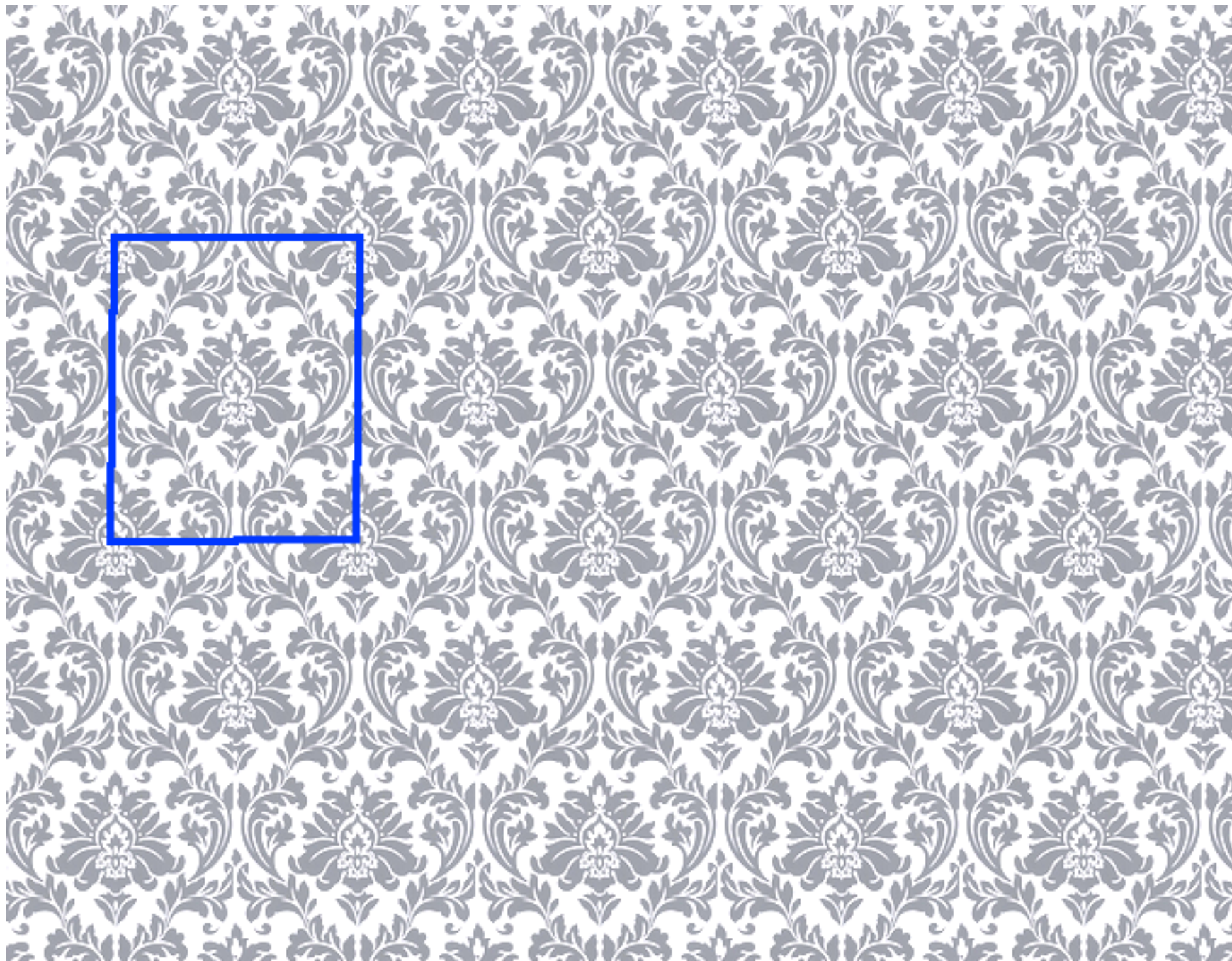
The advantage of introducing the concept of lattice and thus of exploiting symmetry and repetition is to reduce the complexity (the amount of information) of the problem

→ we are building a model

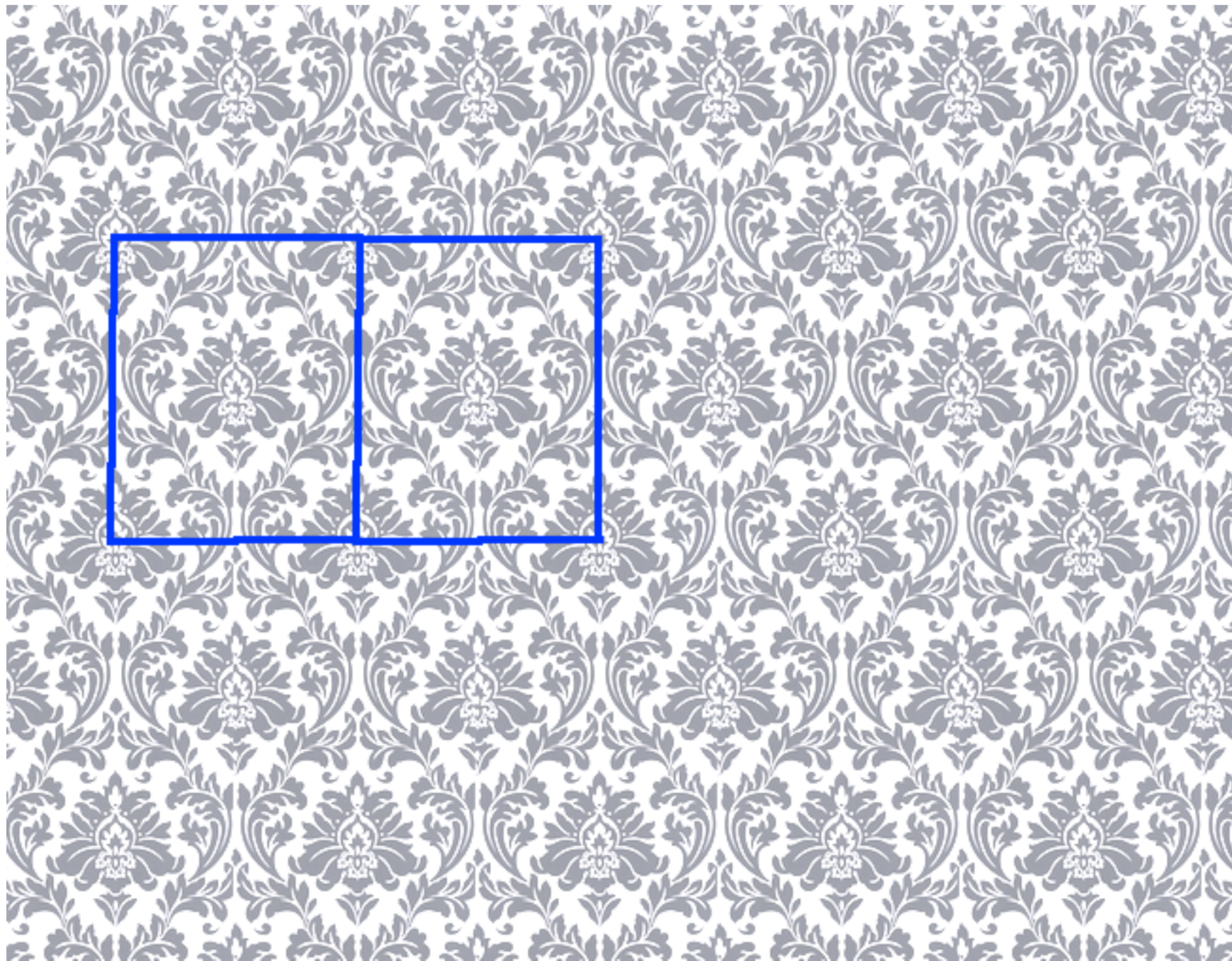
# A periodic continuum

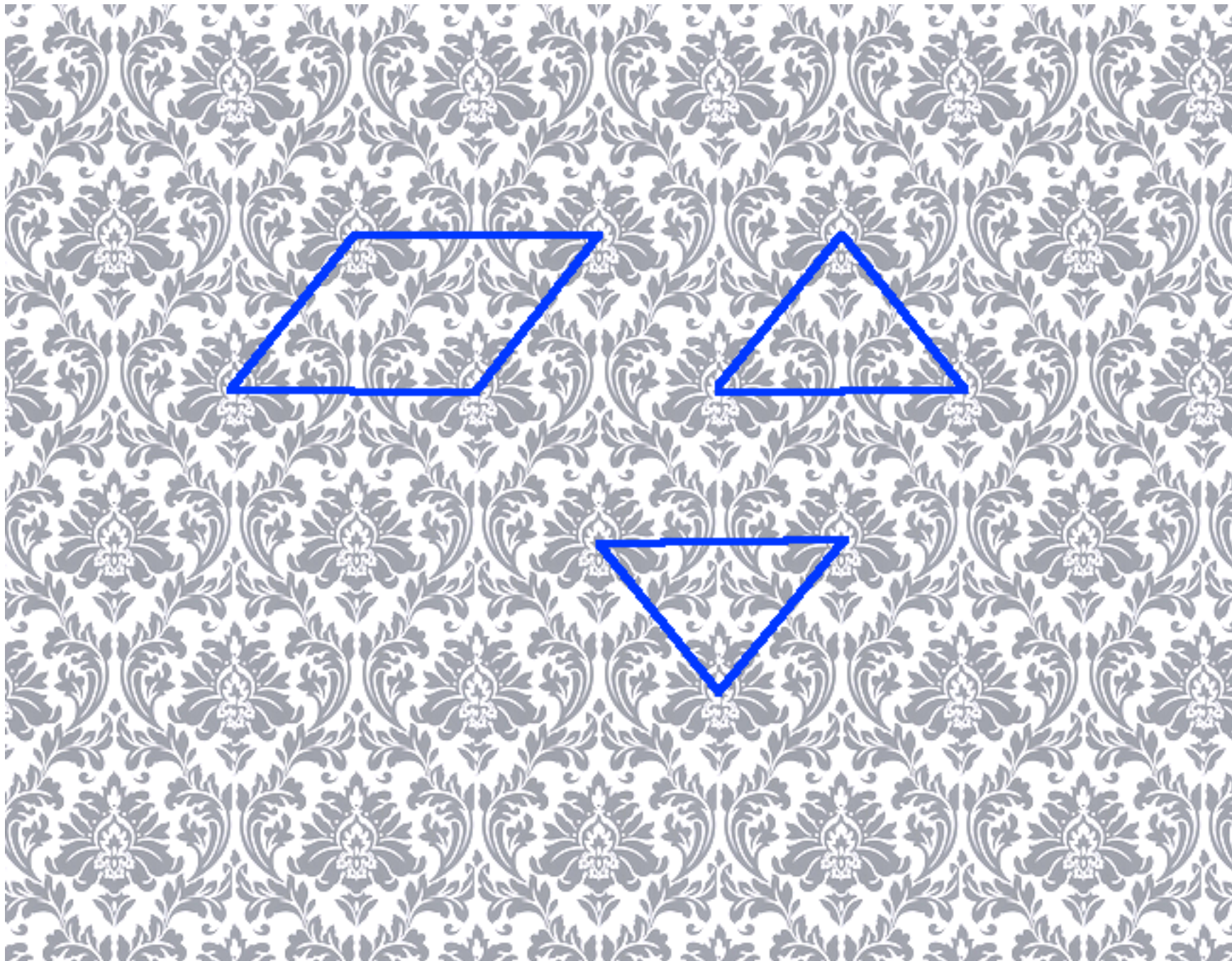






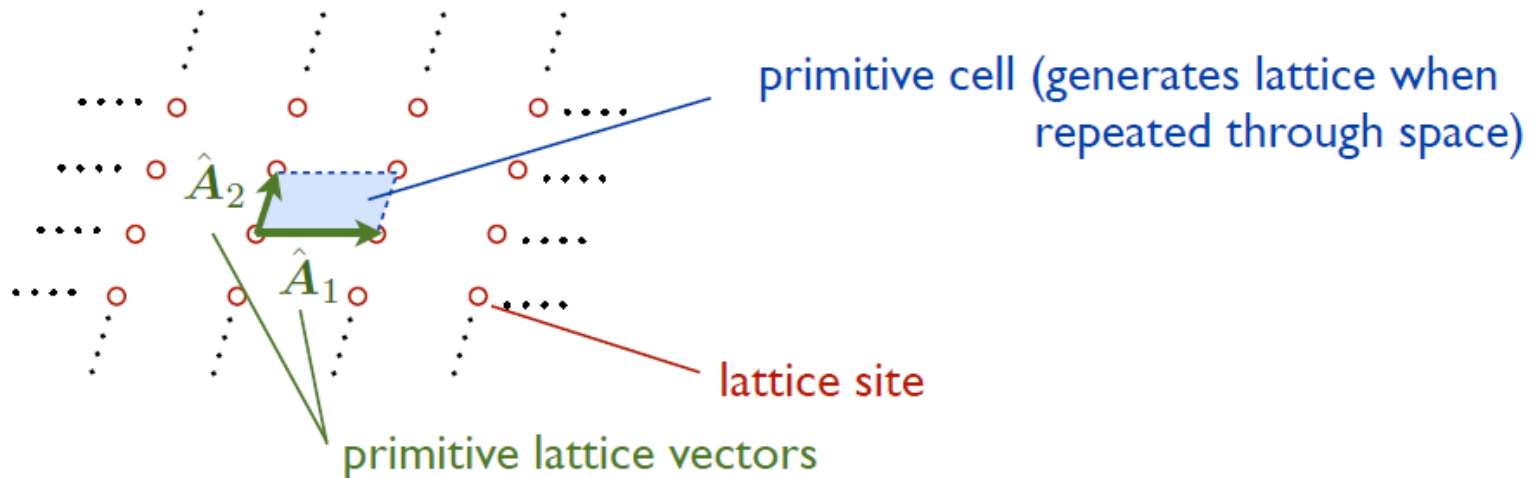






# The lattice

- ▶ A lattice is described in terms of a set of **primitive lattice vectors** (or **Bravais vectors**):



Any **lattice site** can be written as a combination of the primitive lattice vectors:

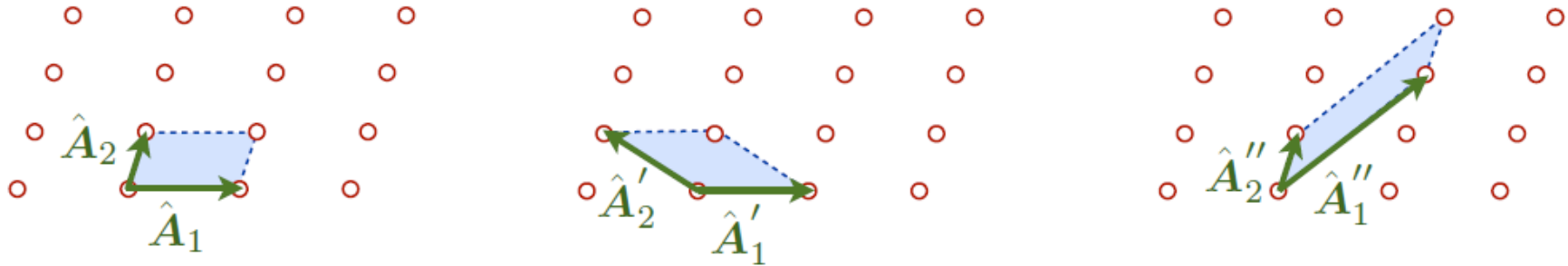
$$\mathbf{R}^{[\ell]} = \sum_{i=1}^3 l_i \hat{\mathbf{A}}_i = l_i \hat{\mathbf{A}}_i \quad (l_i \in \mathbb{Z})$$

↑  
Position of lattice site  $\ell = (l_1, l_2, l_3)$

e.g. in the above 2D lattice, the indicated lattice site is located at  $\ell = (2, -1)$

# Non uniqueness of the lattice description

- ▶ The primitive lattice vectors defining a lattice are not unique:

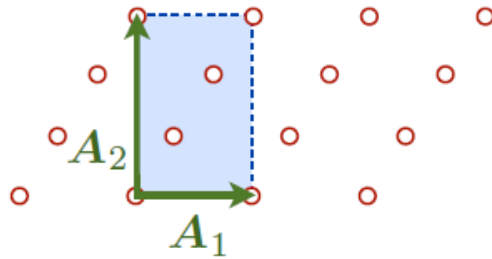


- Normal practice is to select the shortest and most orthogonal set of vectors. (“Lattice reduction” — see Arndt et al., *J. Comp. Phys.*, **228**, 4858-4880, 2009)
- The term **primitive** refers to the fact that the volume of the cell  $\hat{\Omega}_0$  is the smallest possible one (i.e. contains no internal lattice points):

$$\hat{\Omega}_0 = |\hat{\mathbf{A}}_1 \cdot \hat{\mathbf{A}}_2 \times \hat{\mathbf{A}}_3|$$

# Conventional unit cell

- ▶ It is often convenient to work with **nonprimitive lattice vectors** that more clearly reflect the symmetries of the lattice:



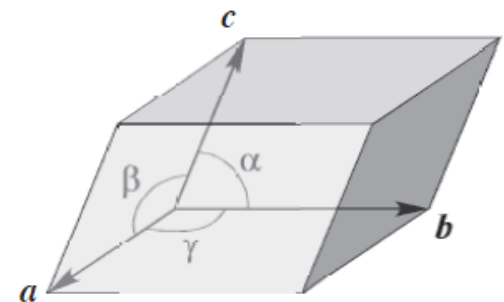
This unit cell clearly shows that the lattice is symmetric with respect to  $180^\circ$  rotation about a lattice point.

- ▶ Clearly  $\Omega_0 > \hat{\Omega}_0$

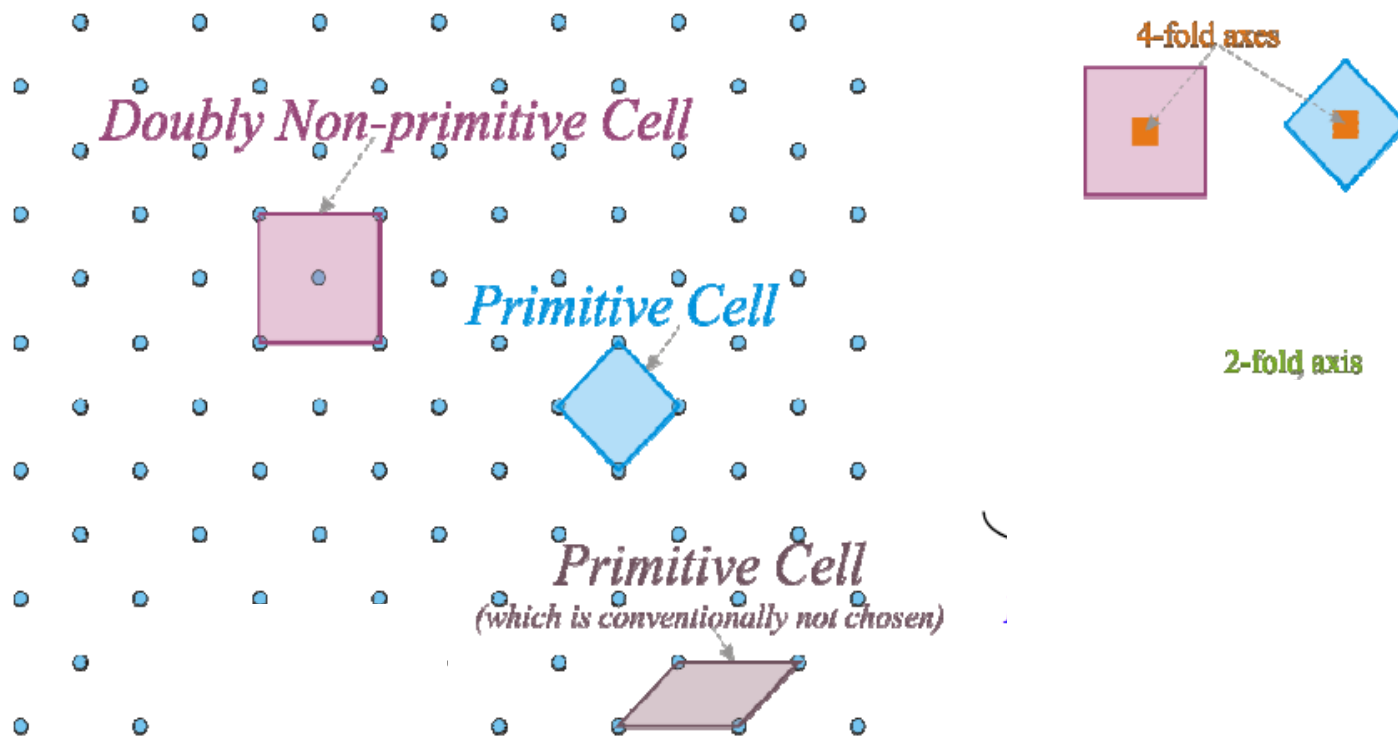
In this case, there are  $4 \times \frac{1}{4} + 2 = 3$  lattice sites per unit cell, so  $\Omega_0 = 3\hat{\Omega}_0$

corners  $\uparrow$   $\uparrow$  internal

This is called the **conventional unit cell** with axes  $a, b, c$ , lattice parameters  $a = |a|, b = |b|, c = |c|$  and angles  $\alpha, \beta, \gamma$ .

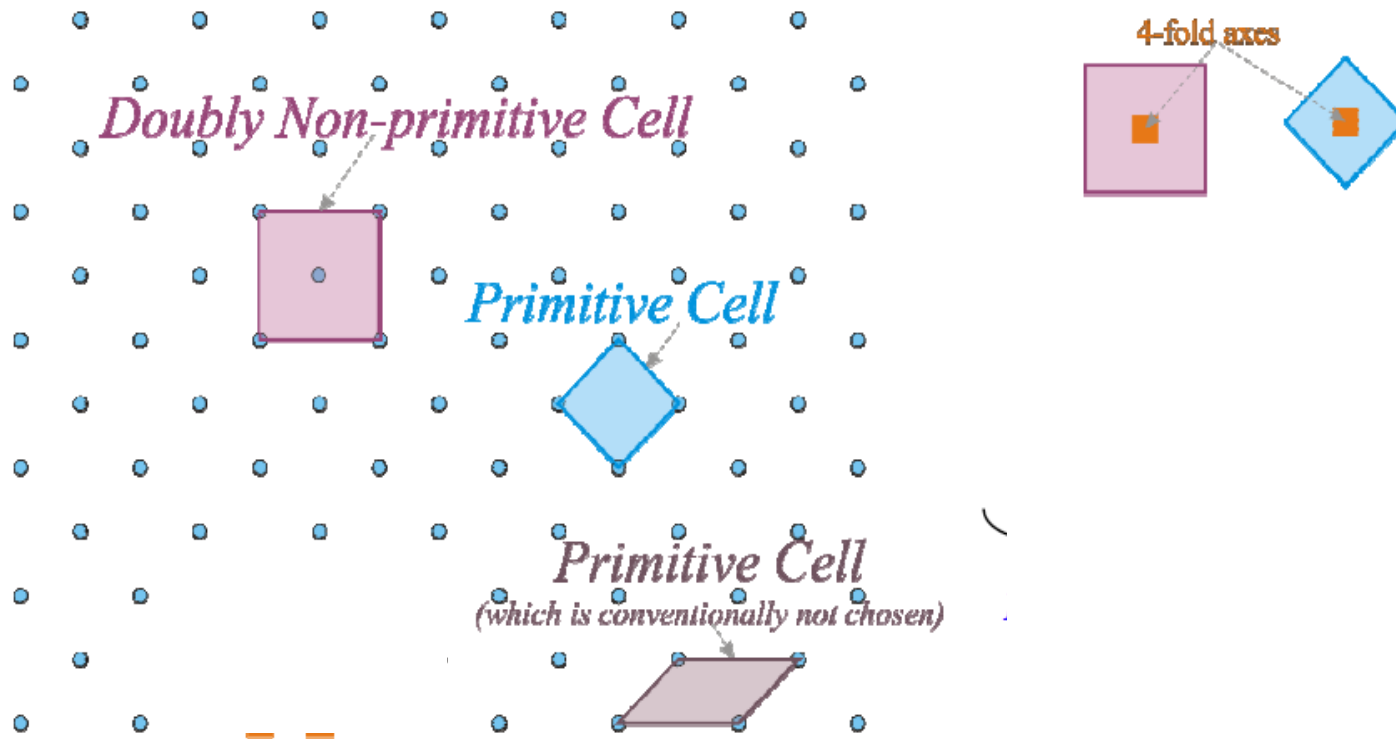


# What to choose?



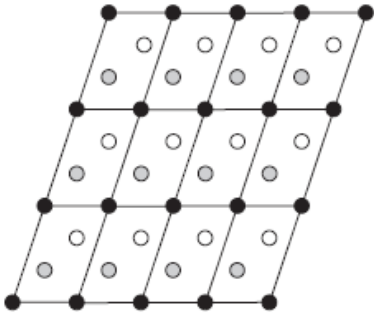
# What to choose?

The square cell because it has higher symmetry than the others

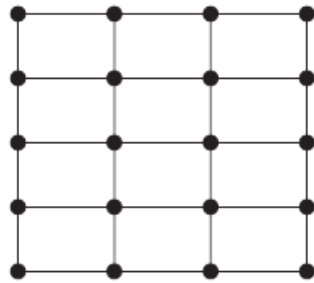


# 7 crystal systems

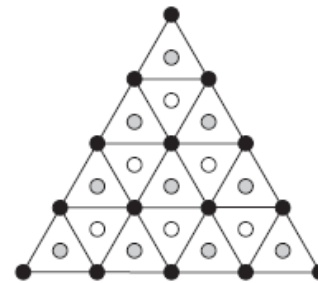
- The symmetry operations place restrictions on lattices which divides them into 7 distinct **crystal systems**:



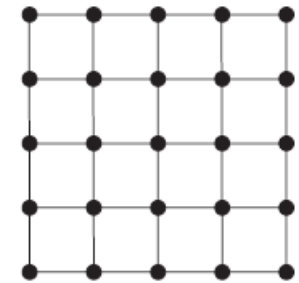
triclinic



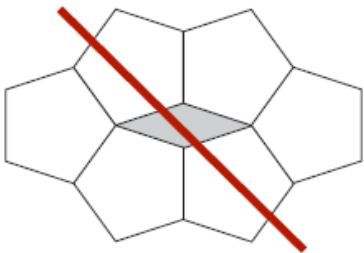
monoclinic  
and  
orthorhombic



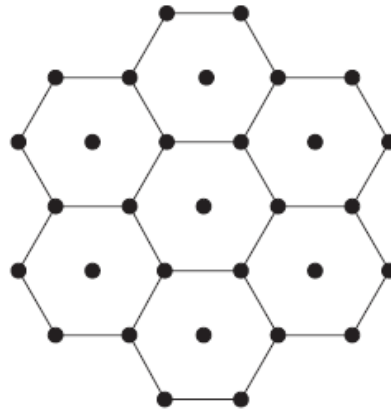
trigonal  
and cubic



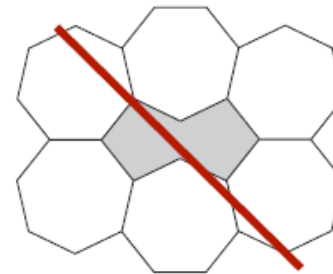
tetragonal



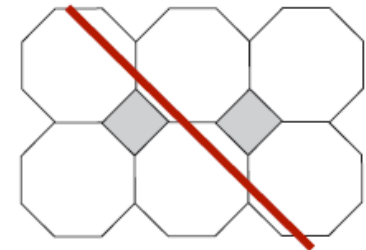
impossible



hexagonal



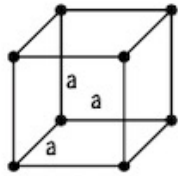
impossible



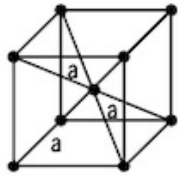
impossible



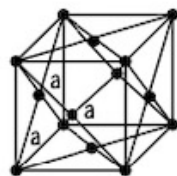
# Bravais lattices



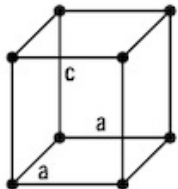
Cubico semplice (P)



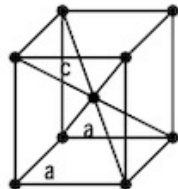
Cubico a corpo centrato (I)



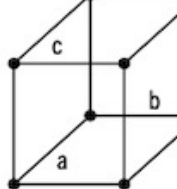
Cubico a facce centrato (I)



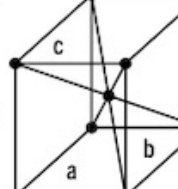
Tetragonale semplice (P)



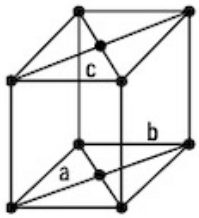
Tetragonale a corpo centrato (I)



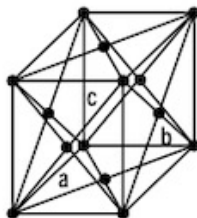
Ortorombico semplice (P)



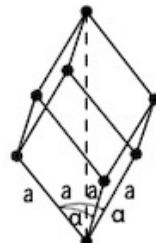
Ortorombico a corpo centrato (I)



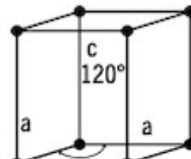
Ortorombico a basi centrate (C)



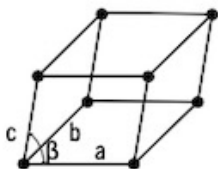
Ortorombico a facce centrate (C)



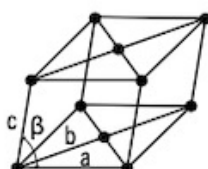
Romboedrico (R)



Esagonale (P)



Monoclino semplice (P)



Monoclino a basi centrate (C)

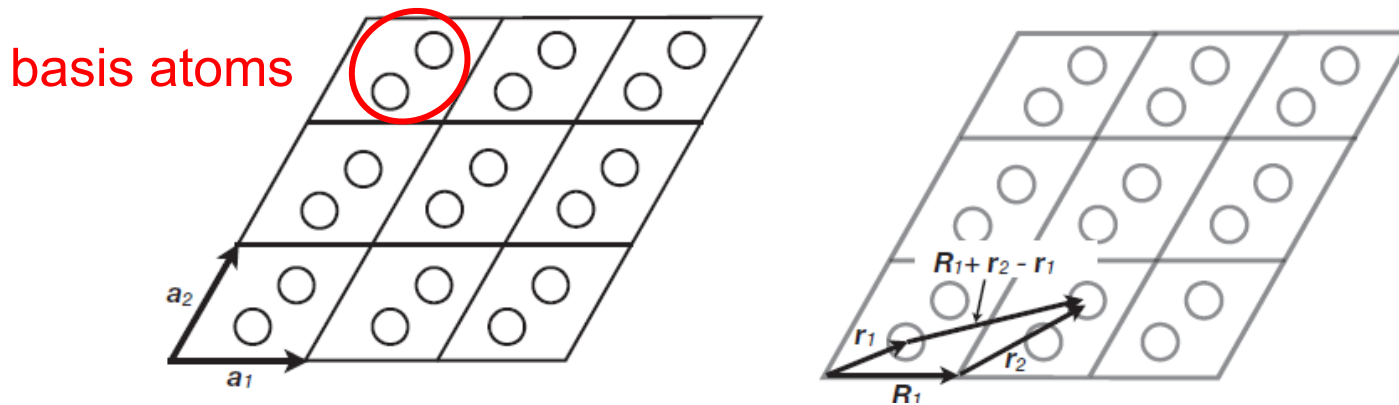


Triclino (P)

<i>Crystal System</i>	<i>Axial Relationships</i>	<i>Interaxial Angles</i>	<i>Unit Cell Geometry</i>
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

# Atomic positions

The sets of identical objects are arrayed in a periodic structure



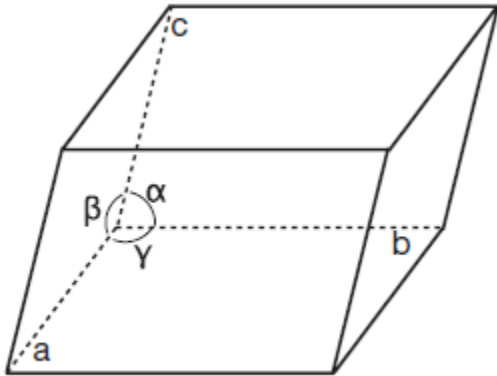
$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$  where  $n_1, n_2,$  and  $n_3$  are integers that span from  $-\infty$  to  $\infty$

The position of the  $j$ th basis atom in a cell defined by the lattice vector  $\mathbf{R}_1$  (relative to the origin) is  $\mathbf{R}_1 + \mathbf{r}_j$

The vector connecting the  $i$ th basis atom in the central cell ( $\mathbf{R} = \mathbf{0}$ ) with the  $j$ th atom in a cell located at  $\mathbf{R}_1$  is

$$\mathbf{R}_1 + \mathbf{r}_j - \mathbf{r}_i$$

# The direct lattice



It is often convenient to write the position of the basis atoms as *fractions* of the unit cell lattice vectors,

$$\mathbf{r}_i = s_{i1}\mathbf{a}_1 + s_{i2}\mathbf{a}_2 + s_{i3}\mathbf{a}_3$$

We can thus write the position of an atom ( $i$ ) within the cell as

$$\mathbf{s}_i = (s_{i1}, s_{i2}, s_{i3})$$

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

$$\mathbf{R} + \mathbf{r}_j - \mathbf{r}_i = (n_1 + s_{j1} - s_{i1})\mathbf{a}_1 + (n_2 + s_{j2} - s_{i2})\mathbf{a}_2 + (n_3 + s_{j3} - s_{i3})\mathbf{a}_3$$

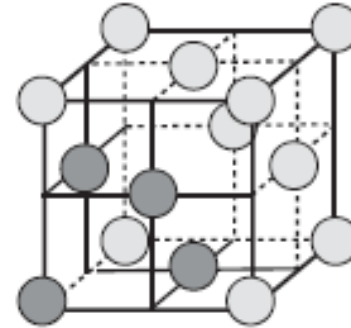
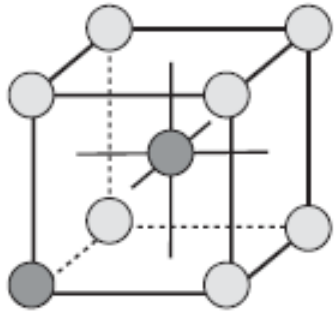
$$\mathbf{X} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3$$

$$X = \sqrt{\mathbf{X} \cdot \mathbf{X}} = |\mathbf{X}|$$

$$X^2 = x_1^2 a^2 + x_2^2 b^2 + x_3^2 c^2 + 2x_1 x_2 ab \cos \gamma + 2x_1 x_3 ac \cos \beta + 2x_2 x_3 bc \cos \alpha$$

which for cubic systems is  $X^2 = a^2(x_1^2 + x_2^2 + x_3^2)$

# BCC and FCC crystals



BCC: Fe, Cr, Mo, Cs, W

2 atoms in the unit cell:

one atom at the origin  $(0,0,0)$  + one atom in the center at  $(1/2,1/2,1/2)a$

FCC: Ag, Au, Cu, Al, Ni

4 atoms in the unit cell:

At  $(0,0,0)$ ,  $(1/2,1/2,0)a$ ;  $(1/2,0,1/2)a$ ;  $(0,1/2,1/2)a$

# Sums of interacting pairs of objects

Example: we want to compute the cohesive energy of a solid

Sum of the interactions between couples of atoms

Simplest case:

1. the interaction  $\Phi(r)$  occurs only between pairs of objects
2. It depends only on the distance  $r$  between the pairs

The vector from  $i$  to  $j$  between two objects is

$$\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$$

The distance is

$$r_{ij} = (\mathbf{r}_{ij} \cdot \mathbf{r}_{ij})^{1/2}$$

**SILLY BUT USEFUL REMARK:** An object does not interact with itself and interacts only once with the others.

# Sums of interacting pairs of objects

If the interactions are energies, which are scalars  $\phi_{ij} = \phi_{ji}$

When talking about the energy of a crystal it is customary to call the sum  $U$ , interatomic potential. The sum for four objects is:

$$U = \phi(r_{12}) + \phi(r_{13}) + \phi(r_{14}) + \phi(r_{23}) + \phi(r_{24}) + \phi(r_{34})$$

How about  $N$  objects with  $N$  very large?

Write it in a compact form, in fact you can find two compact forms, one of which is computationally less costly

# Sums of interacting pairs of objects

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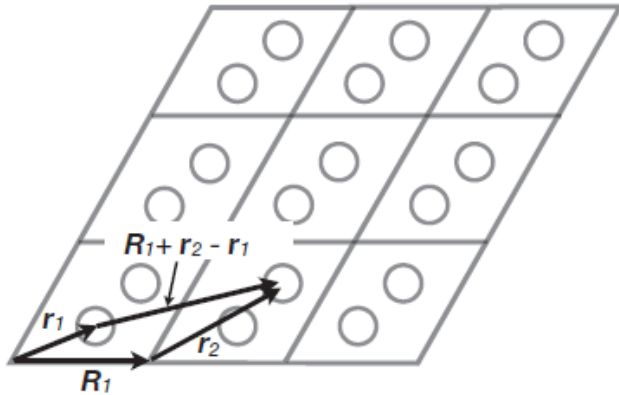
How about  $N$  objects with  $N$  very large?

Computationally expensive  $U = \frac{1}{2} \sum_{i=1} \sum_{j \neq i} \phi(r_{ij})$

Computationally efficient  $U = \sum_{i=1}^{N-1} \sum_{j=i+1}^N \phi(r_{ij})$

Check that these two are the same for  $N=4$

# Potential energy per unit cell



$$U = \frac{1}{2} \sum_{i=1} \sum_{j \neq i} \phi(r_{ij})$$

$$U_{cell} = \frac{1}{2} \sum_{\mathbf{R}} \sum_{i=1}^n \sum_{j=1}^n {}' \phi_{ij}(|\mathbf{R} + \mathbf{r}_j - \mathbf{r}_i|)$$

The ' indicates that  $i = j$  terms for  $\mathbf{R} = (0, 0, 0)$  (the central unit cell) are not included.

$U_{cell}$  is the energy *per unit cell*.

$$\text{Energy per object: } u = U_a = \frac{1}{n} U_{cell}$$



# The cohesive energy

The **potential energy of a crystal** is the sum of the energetic interactions between all atoms. At 0K the potential energy is called **cohesive energy**. The cohesive energy is the energy required to assemble a solid from its constituent atoms. For a system made of  $N$  atoms:

$$U = E(\text{all atoms}) - \sum_{i=1}^N E_i$$

where  $E_i$  is the energy of an individual atom.

GOAL: develop and use simple analytical potentials that approximate the interaction potential between individual atoms.

The details of electrons and nuclear charges are approximated, such that the analytical potentials are just an average over the electrons.

NOTE: this is a typical feature of materials modeling: using at one scale averages over properties at a lower scale.

# Terms in the cohesive energy

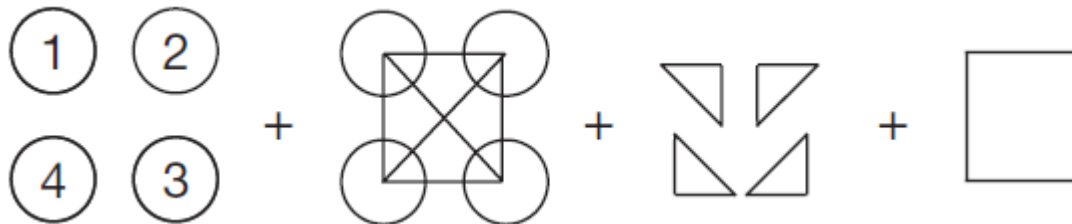
The cohesive energy can be written as a series of terms that depend on the individual atoms, pair of atoms, triplets of atom, etc.

$$U = \sum_{i=1}^N v_1(\mathbf{r}_i) + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \phi_{ij}(\mathbf{r}_i, \mathbf{r}_j) + \frac{1}{6} \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N v_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \dots$$

external field

pair potential

three-body interactions



# Interaction potentials

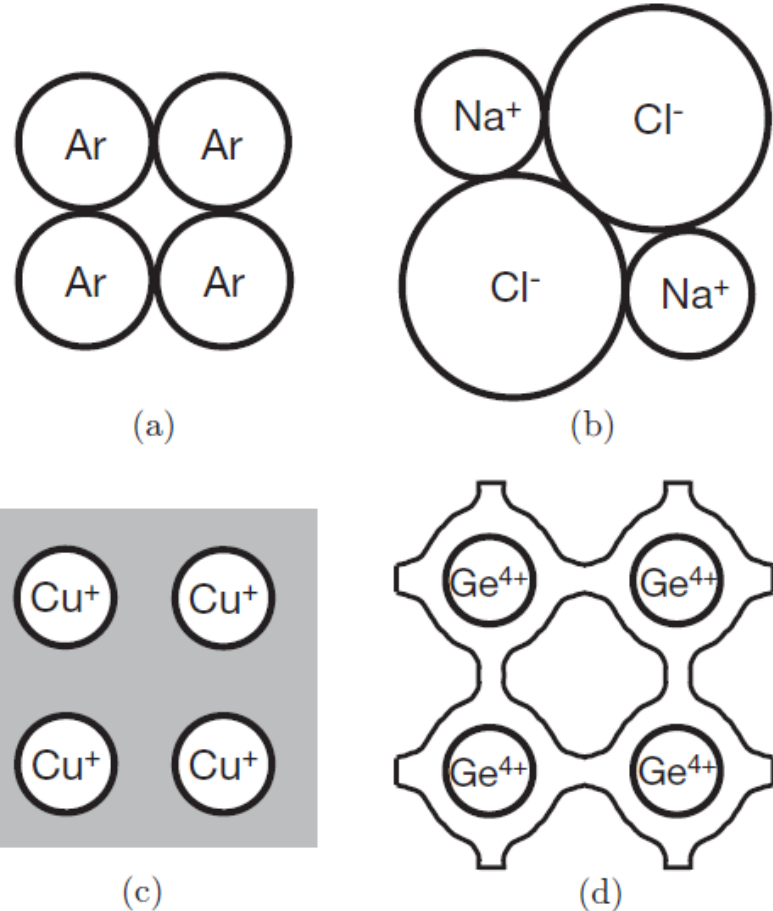
Potentials should reflect the **bonding** between the atoms.

The simplest type of bonding occurs in rare-gas solids: helium, neon, argon, chromium and xenon (a). The nucleus is surrounded by a closed shell of valence electrons. Bonding is non-directional. Potential depends only on distance.

(b) Ionic solids: also closed shell

(c) Metals: the atoms are ionized, valence electrons are distributed, non-directionally. The electron cloud needs to be accounted for.

(d) Covalent crystals with strongly directional bonds.



# Interaction energy

The **interaction energy** between two atoms is defined as:

$$\phi_{ij}(\mathbf{r}_i, \mathbf{r}_j) = E(i + j) - E(i) - E(j).$$

We know that:

- 1) At short distance atoms must repel each other or matter will collapse
- 2) At some larger distance atoms must attract each other or atoms would not form solids and fluids at normal pressure

Repulsion: atoms approach each other, electrons cannot be constrained to occupy the same small volume.

## AT SHORT RANGE

Since the density of electrons decreases **exponentially** with their distance from the atom, the short-range interactions can be modeled as:

$$\phi_{SR}(r) = Ae^{-\alpha r}$$

# Interactions at long-range

Long range means that the distance is large compared to the size of the electronic distribution.

An attractive term arises from the fluctuations of the electronic cloud. It is called **Van der Waals energy** or **dispersion energy**.

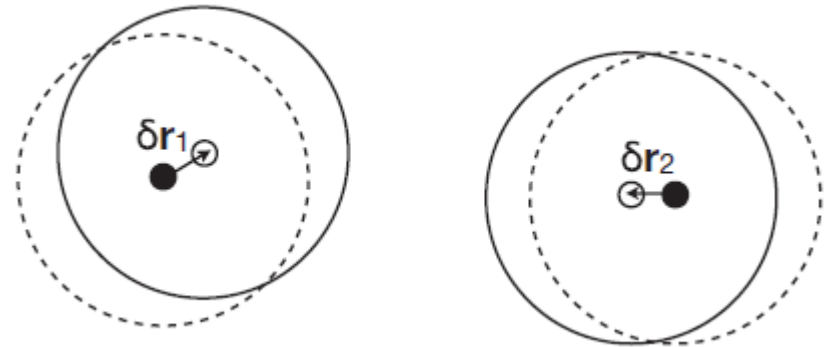
Electrons in an atom fluctuate around their nucleus destroying the spherical symmetry. The fluctuation creates an instantaneous dipole moment on the atoms. Fluctuations are small, the restoring force can be modeled as a spring

Spring energy:  $E = \frac{1}{2} k \delta r^2$

$k = N^2 / \alpha \longrightarrow$  polarizability



Number of valence electrons



Interaction between fluctuating dipoles leads to a change in the frequency of the fluctuations and therefore to the interatomic potential. For interacting, closed-shell, non-ionic systems:

$$\phi_{vdw}(r) = -\frac{A}{r^6}$$

# The Lennard-Jones potential

It was developed to model closed-shell atoms, interactions only dependent on distance

Goal: create a potential to describe the interaction energy  $\Phi(r)$  between two spherical atoms distant  $r$  which in fact can be valid for many materials



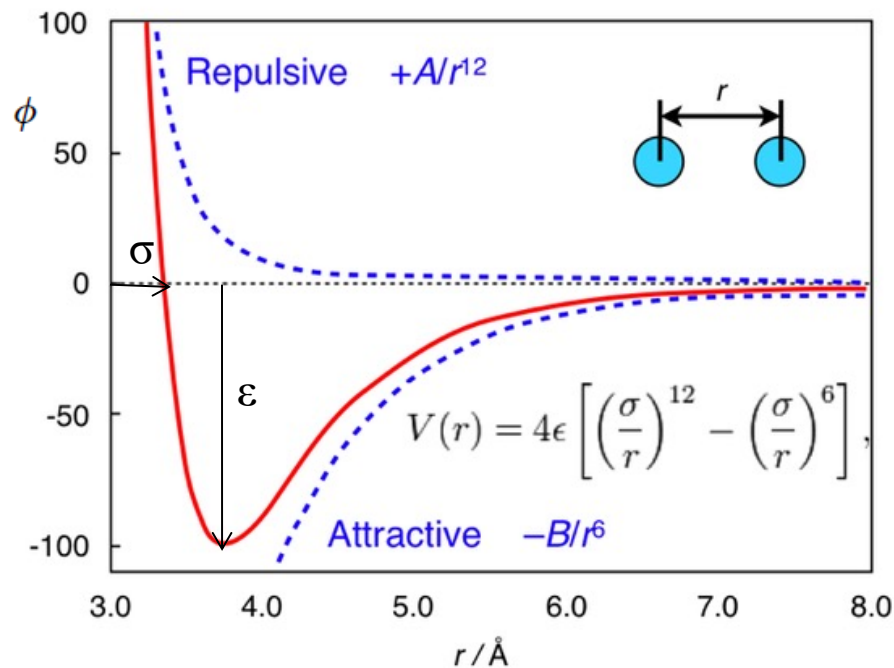
$$\phi(r) = \frac{B}{r^{12}} - \frac{A}{r^6}$$

- Jones, J. E., *Proc. Roy. Soc. A*, **106**, 441-462 (1924)
- Jones, J. E., *Proc. Roy. Soc. A*, **106**, 443-477 (1924)

# The Lennard-Jones potential

While developed to model closed-shell atoms it has been used to model almost anything....

Goal: create a potential to describe the interaction energy  $\Phi(r)$  between two spherical atoms distant  $r$  (input) which can be valid for many materials



$$\phi(r) = \frac{B}{r^{12}} - \frac{A}{r^6}$$

The potential is rewritten as:

$$\phi(r) = 4\epsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right)$$

$$\sigma = (B/A)^{1/6} \quad \phi(\sigma) = 0$$

$$\epsilon = A^2/4B$$

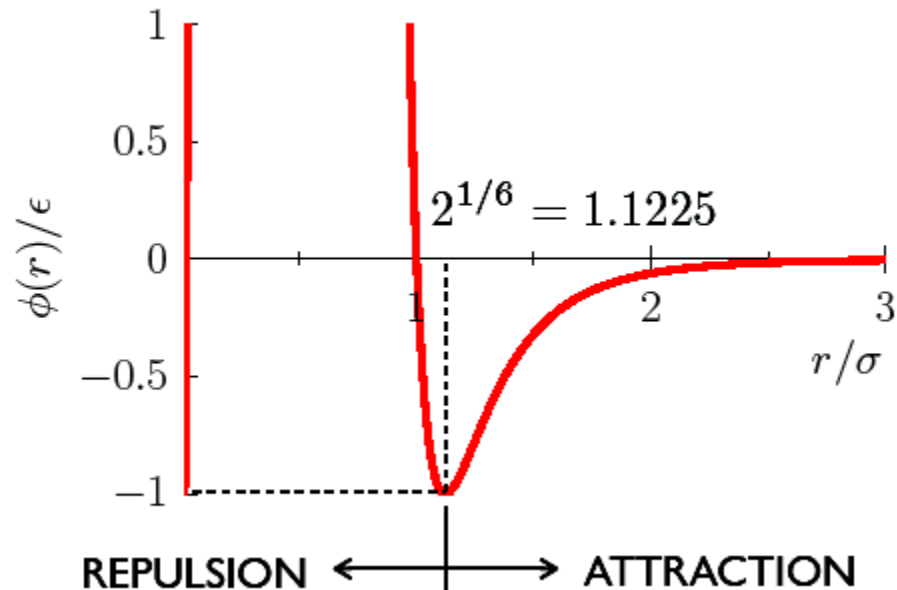
absolute value of the minimum

$\sigma$ ,  $\epsilon$  are material constants!

# Reduced units

For calculations, handy to use scaled (or reduced) units:  $\phi^* = \phi/\epsilon$  and  $r^* = r/\sigma$

$$\phi^*(r^*) = 4\left(\left(\frac{1}{r^*}\right)^{12} - \left(\frac{1}{r^*}\right)^6\right)$$





# Take home messages

- Often simulations require averaging over various cases. This is particularly true in the case of small scale simulations
- Often simulations require summing over various objects for instance to calculate the energy of the system
- The potential energy of a crystal can be described through potentials that aim at representing the interaction between atoms
- The simplest interaction potential proposed is the Lennard-Jones pair-potential

# In class assignment 1

Create a 3D lattice of atoms in an FCC crystal structure.  
Use reduced units (fractions of 1).

# FCC and BCC repeating unit

Create a 3D lattice of atoms in an FCC and in a BCC crystal structure.

Steps:

- 1) start with a single repeating unit: your unit cell
- 2) add more cells in all directions such as to create a larger crystal with cubic shape
- 3) For visualization of the atoms you can use the command **scatter3**

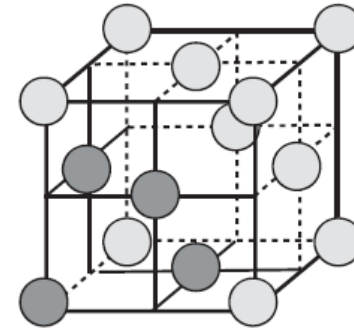
# FCC repeating unit

Call the file `fccmke.m` and write the following function:

```
function [i1,s] = fccmke (nc)
```

INPUT: nc= nr. of FCC cells in each direction

OUTPUT: i1=total nr of atoms in the cell  
s=(i1, coordinates)



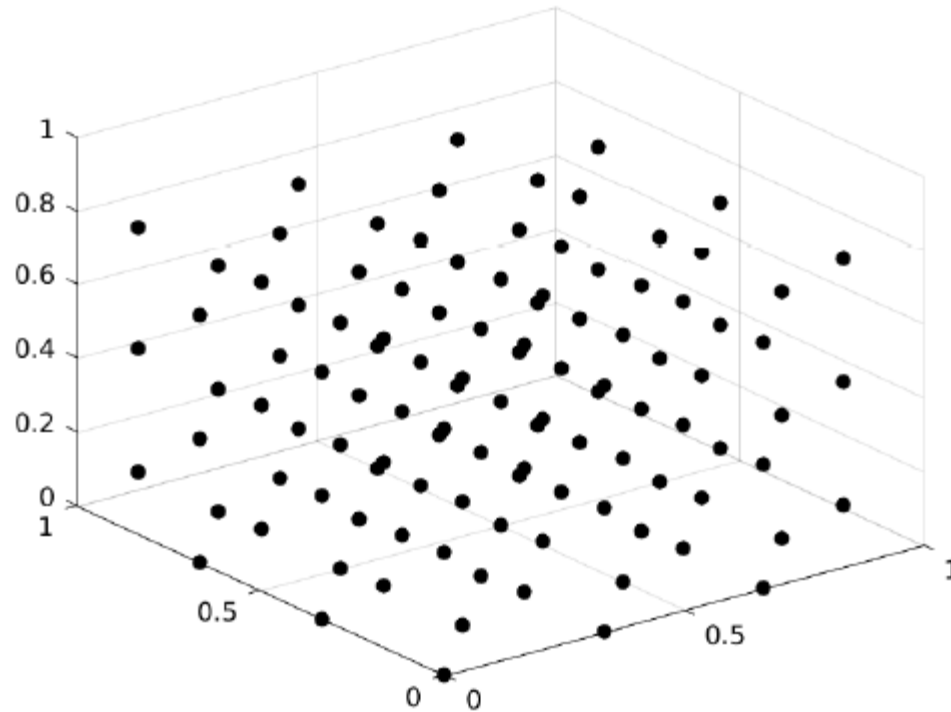
$$\vec{r}_1 = (0,0,0)$$

$$\vec{r}_2 = \left(\frac{1}{2}, \frac{1}{2}, 0\right)$$

$$\vec{r}_3 = \left(\frac{1}{2}, 0, \frac{1}{2}\right)$$

$$\vec{r}_4 = \left(0, \frac{1}{2}, \frac{1}{2}\right)$$

# FCC repeating unit



# fccmke.m

```
function[s,il]= fccmke(nc)
n=4; % number of atoms in a unit cell
%nc=2; % cells in each-direction, if fccmke is run independently of latsum
na=n*nc^3; %number of atoms in the simulation
r=[0 0 0;.5 .5 0;0 .5 .5;.5 0 .5]
il=0; % initialize the total number of atoms
s=zeros(n*nc^3,3); % s(atoms, coordinates)
for k=1:nc
    for l = 1:nc
        for m = 1:nc
            for i = 1:4
                il=il+1;
                s(il,1) = (r(i,1) + k-1)/nc;
                s(il,2) = (r(i,2) + l-1)/nc;
                s(il,3) = (r(i,3) + m-1)/nc;
            end
        end
    end
end
end
scatter3(s(1:na,1),s(1:na,2),s(1:na,3),'filled'); % visualize all atoms in the unit
cell
```

# First assignment (evaluated)

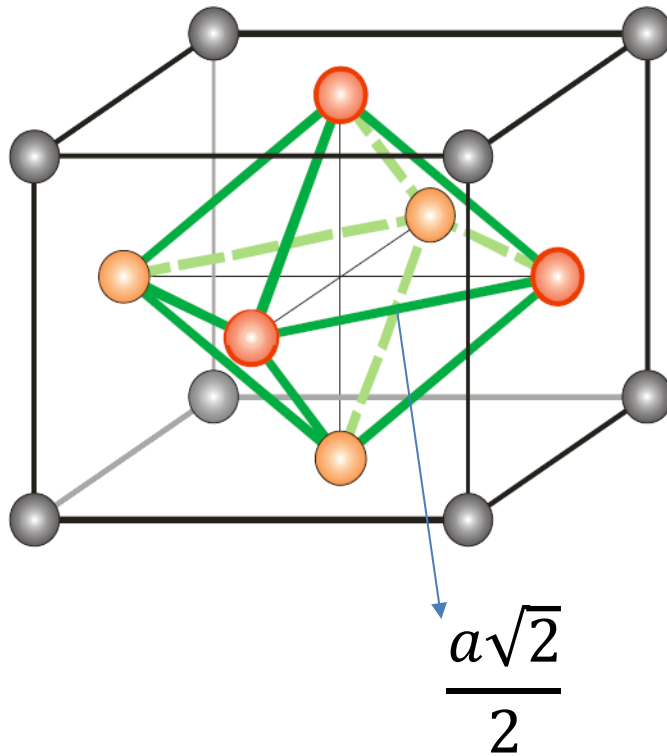
Diffusion of carbon in a homogeneous metal solid occurs as a fully random walk. The solid is made of pure FCC iron and carbon moves as an interstitial. Plot the probability distribution of the end-to-end distance after 500 steps.

Simulate then the effect of a large heat source positioned at one end of the crystal. How does the diffusion process change?

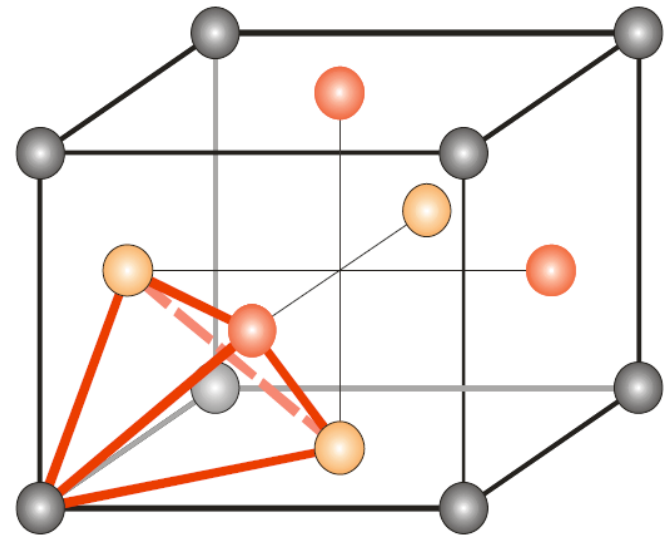
Compare the probability distribution of the end-to-end walk of the carbon atom in the solid at constant temperature with the solid subject to a thermal gradient.

# Interstitial sites in FCC

OCTAHEDRIC  
SITE



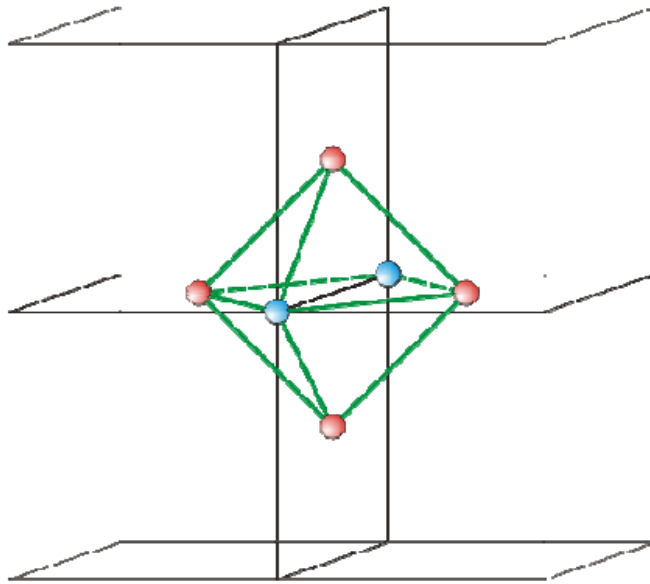
TETRAHEDRIC  
SITE



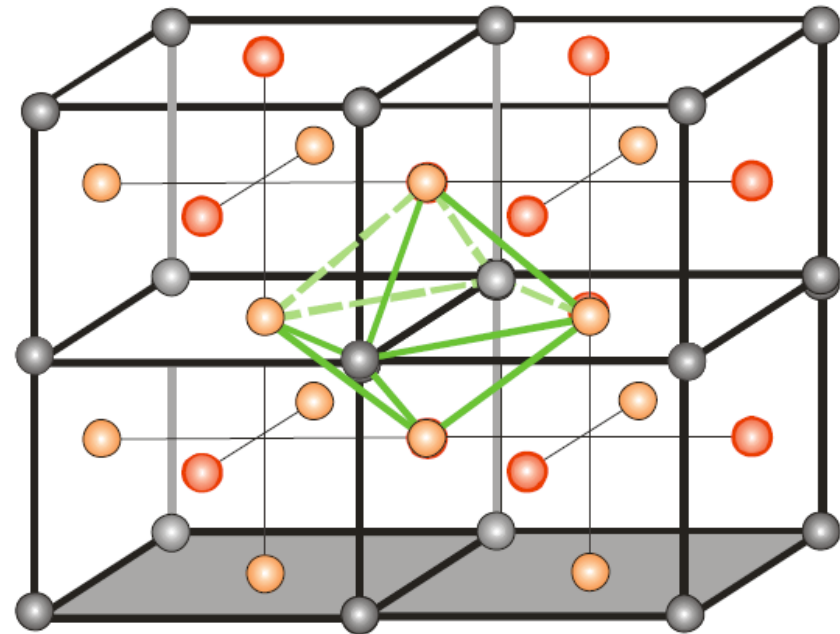


# Voids in FCC cells

Once we know the position of a void then we can use the symmetry operations of the crystal to locate the other voids. This includes lattice translations



Site for octahedral void



$$\left\{ \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right\} + \left\{ \frac{1}{2}, \frac{1}{2}, 0 \right\} = \left\{ 1, 1, \frac{1}{2} \right\} \equiv \left\{ 0, 0, \frac{1}{2} \right\}$$

Face centering translation

Equivalent site for an octahedral void

# Suggestions for binning

- 1) Divide the interval between max and min value of end-to-end distance in  $n_{bin}$
- 2) Calculate how many values of  $r_{ee}$  fall in each of the intervals
- 3) Careful to not 'loose' any of the values at the extremes
- 4) Plot the number of entries per bin divided by the number of total trials
- 5) Compare with the theoretical curve
- 6) Search for a reasonable  $n_{bin}$  to approach the theoretical curve