Section 3
Crystals

Gerhard Klimeck

gekco@purdue.edu

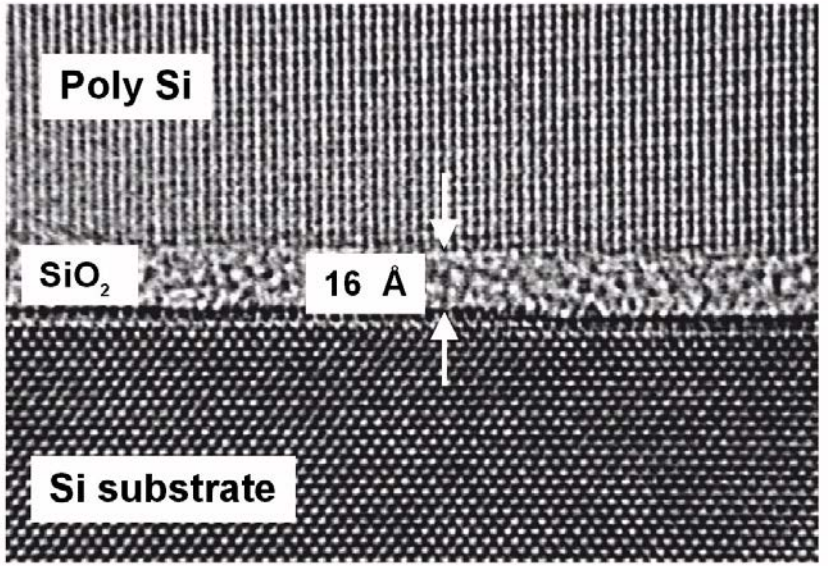
PURDUE UNIVERSITY

School of Electrical and Computer Engineering

Section 3
Crystals

One Video Segment

- 3.1 Crystal definitions



One Video Segment

- 3.2 Tables of Bravais Lattices

One Video Segment

- 3.3 Density Definitions and Applications to Common Materials

One Video Segment

- 3.4 Surfaces, Miller Index

Reference: Vol. 6, Ch. 1, ABACUS tool at nanohub.org/tools/abacus and "Crystal Viewer Lab, https://nanohub.org/resources/crystalviewer

Section 3
Crystals

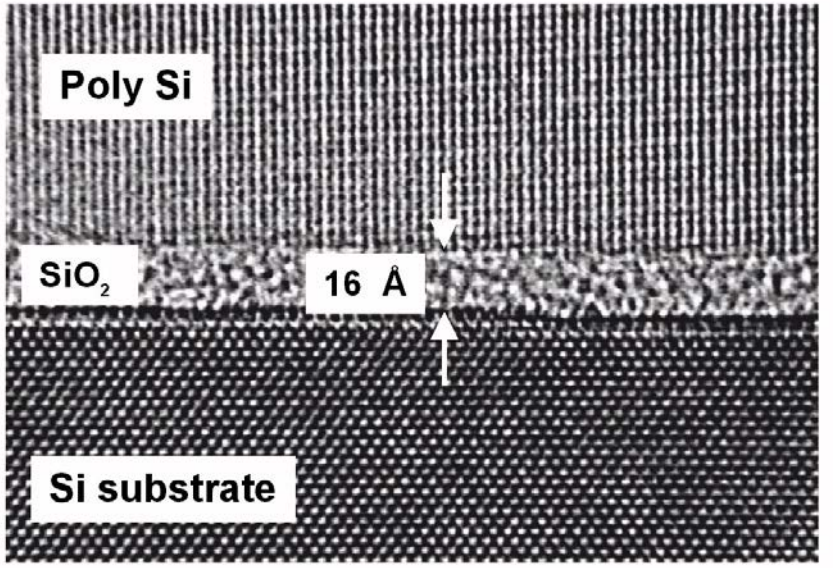
One Video Segment

One Video Segment

One Video Segment

One Video Segment

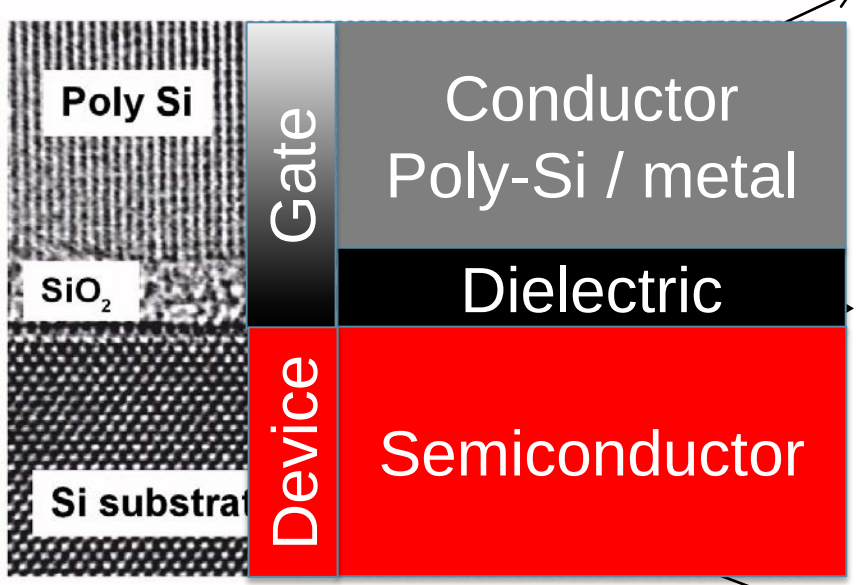
- 3.1 Crystal definitions
  - » One-dimensional Crystals – simple primitive cell
  - » Unit cells of a Periodic 2D Lattice
  - » Bravais lattice
  - » Bravais lattice with a basis
  - » Non-periodic repeated cells
  - » Definition of ONE Primitive Cell – Wigner-Seitz Cell
- 3.2 Tables of Bravais Lattices
  - » Bravais Lattices in 2D (5 types)
  - » Bravais Lattices in 3D (14 types)
  - » 3 Dominant Bravais Lattices in Nature
- 3.3 Density Definitions and Applications to Common Materials
  - » Number, Packing, and Areal Density
  - » Common Crystals – Non-Primitive Unit Cells (NaCl, GaAs, CdS)
- 3.4 Surfaces, Miller Index



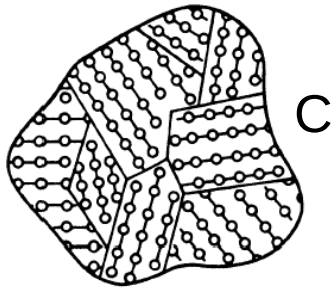
Reference: Vol. 6, Ch. 1, ABACUS tool at nanohub.org/tools/abacus and "Crystal Viewer Lab, https://nanohub.org/resources/crystalviewer

Crystals form the Core Device Material

Cross section of a MOSFET

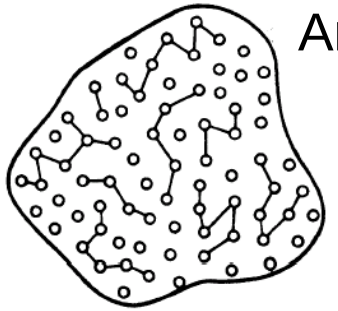


Device is a perfectly arranged crystal



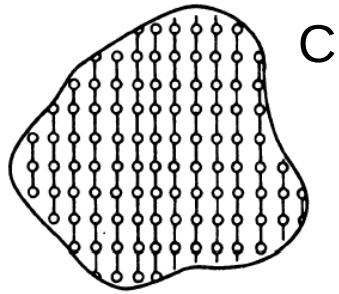
Poly-Crystalline

Conductive
Electron transport
Hold charge



Amorphous
Oxides

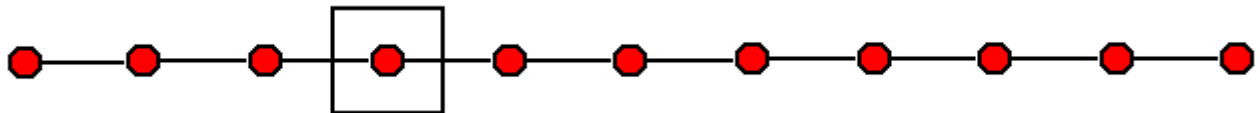
Non-Conductive
"NO" transport



Crystalline

Highly conductive
Electron transport

- Modern solid state devices use all forms these forms of materials
- Focus on Crystals first – start with 1D => 2D => 3D
- Transfer concepts of electronic behavior in crystals to other materials



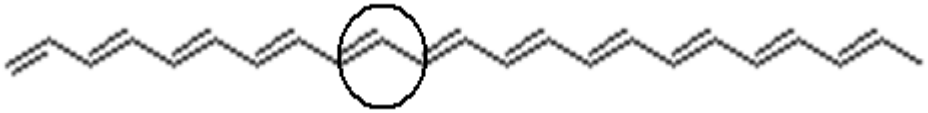
One-dimensional Crystals

There is exactly ONE primitive unit cell in a 1D system

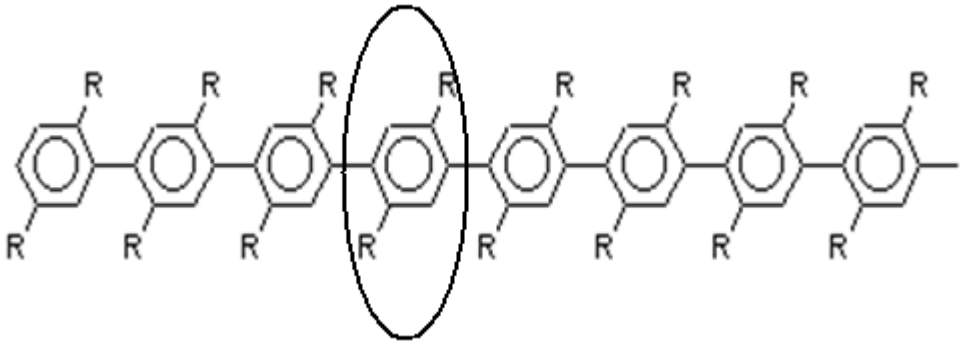
No realistic system is truly 1-D, but ….

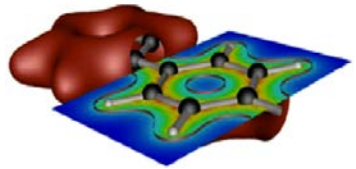
- 1D properties dominate behavior in some material and devices
  - Materials: e.g polymers,
  - Biology: e.g. DNA
  - Devices: e.g. 1D heterostructures (lasers, RTDs)
- Can often be solved analytically, many properties have 2D/3D analogs

Polyacetylene

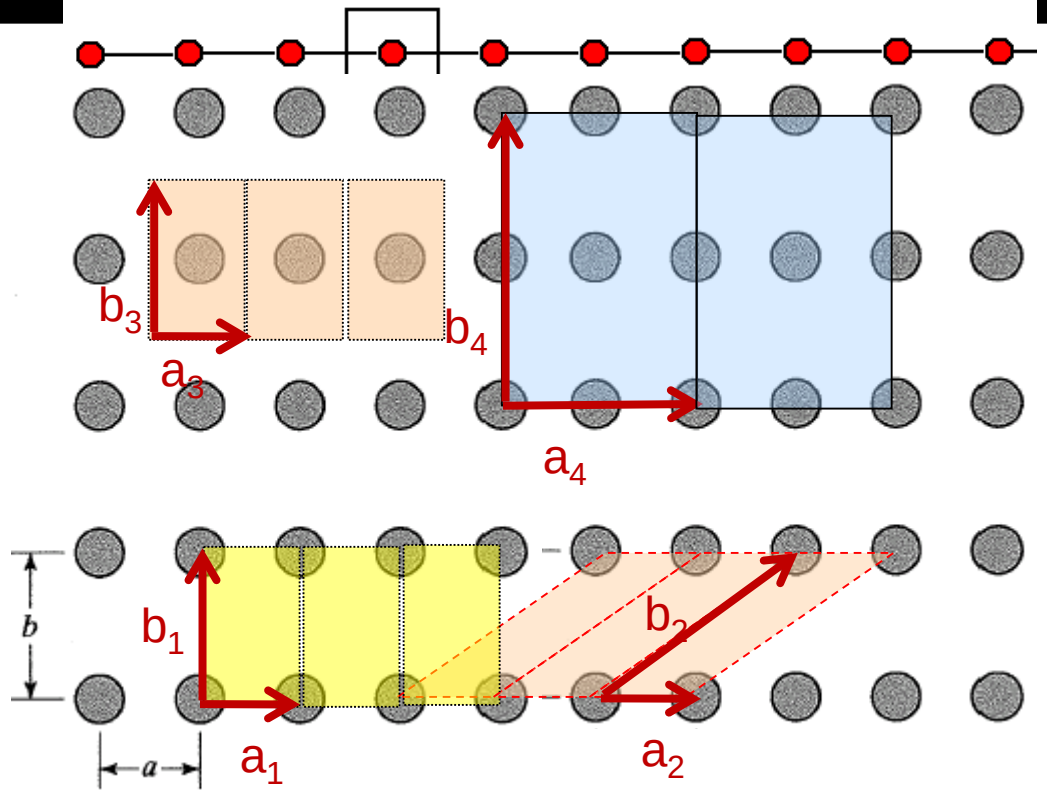


PPP





Unit cells of a Periodic 2D Lattice



"Infinitely" extended
2D shown
3D same concepts

⇒ N_A=6 x 10^{23}/mol
⇒ Can NEVER solve this, even on the largest computer
⇒ Simplify to a repeated (small) cell

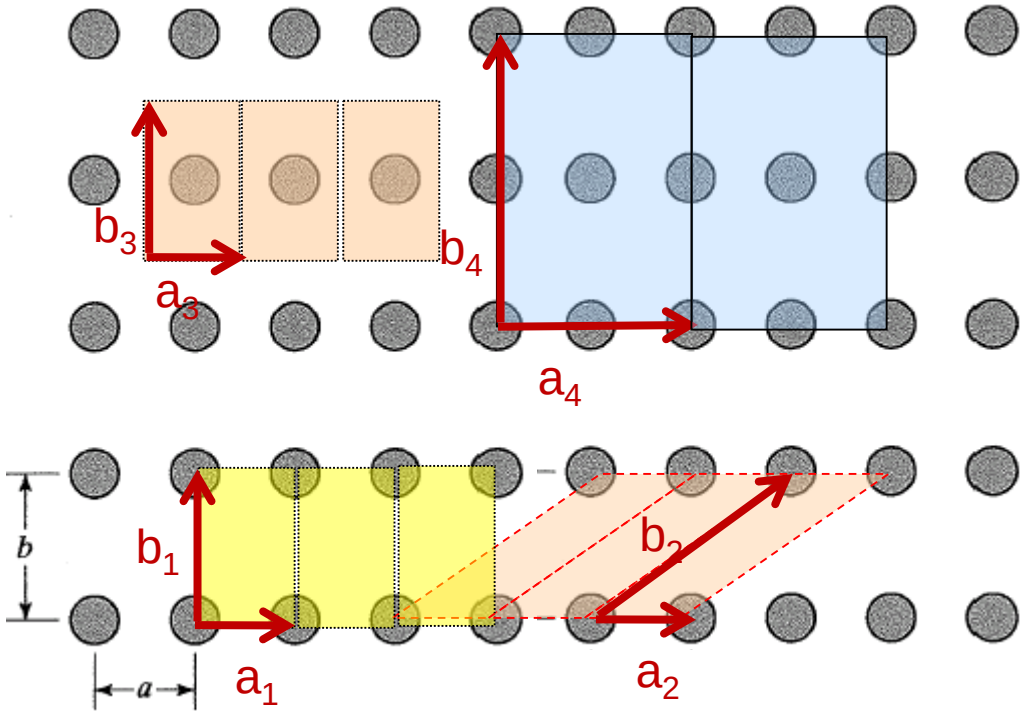
- Unit cells are *not* unique
- Unit cells can be Primitive or Non-primitive

- Property of ONE CELL defines the property of the solid

- Address every point in the lattice by integer translation of unit vectors

$$\vec{R} = h\vec{a} + k\vec{b}$$

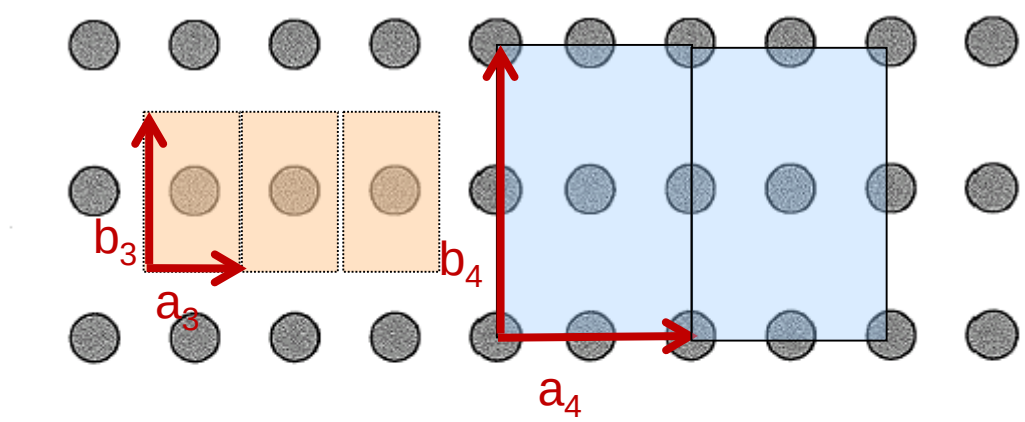
Bravais Lattice

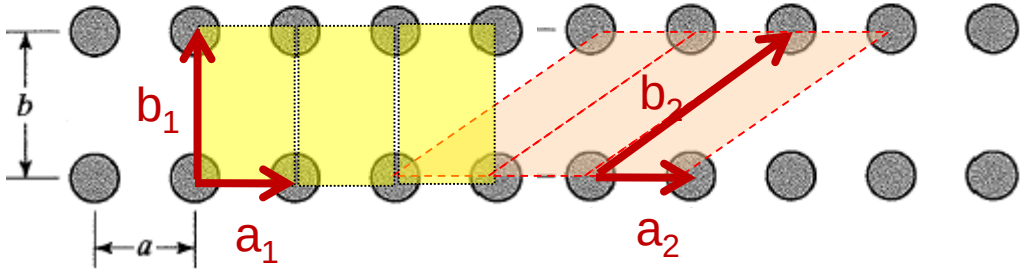


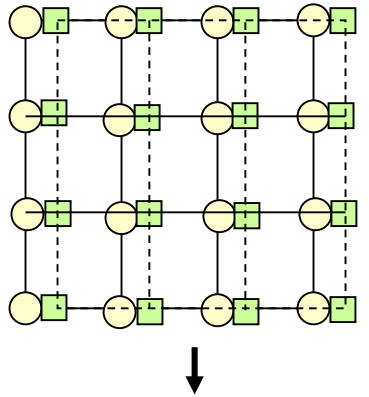
• Property of ONE CELL defines the property of the solid
• Address every point in the lattice by integer translation of unit vectors
• every point has the same environment as every other point (same number of neighbors, next neighbors, …)

$$\mathbf{R} = h\vec{a} + k\vec{b}$$

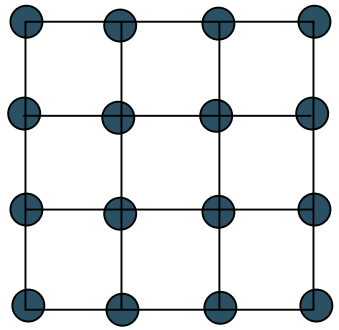
Bravais Lattice with a Basis







Non-Bravais lattice



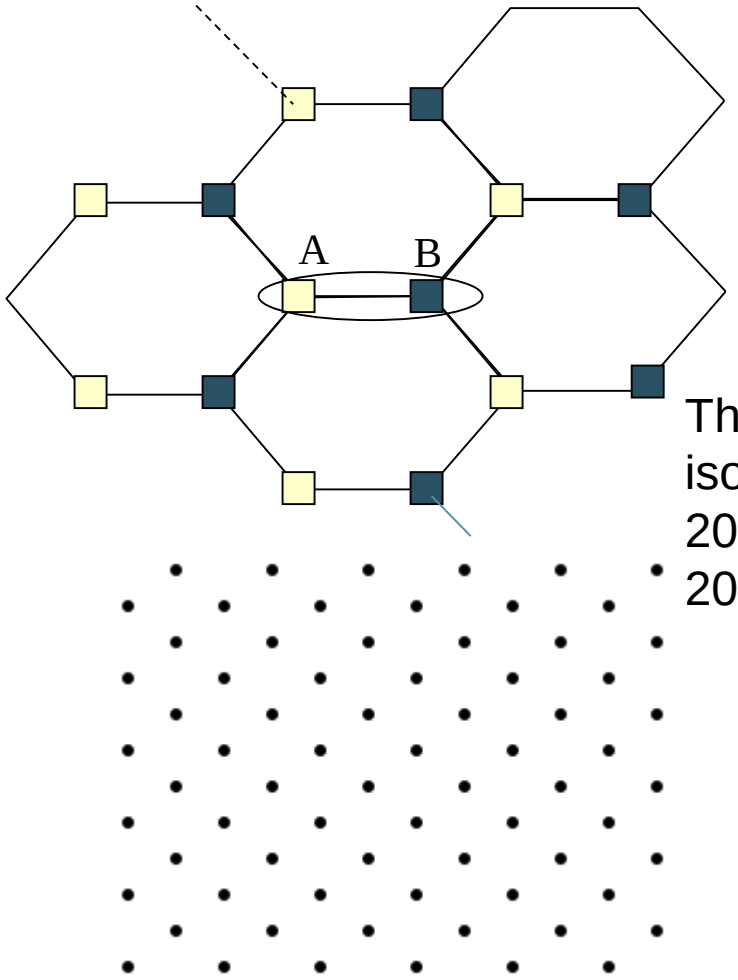
Bravais lattice with a basis

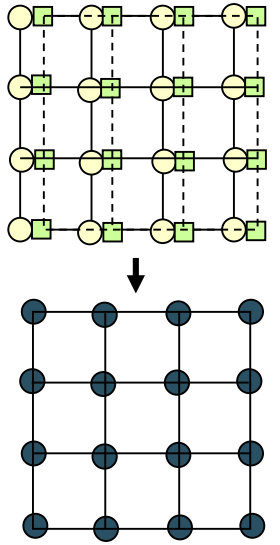
• Property of ONE CELL defines the property of the solid
• Address every point in the lattice by integer translation of unit vectors
• every point has the same environment as every other point (same number of neighbors, next neighbors, …)

$$\vec{R} = h\vec{a} + k\vec{b}$$

Graphene - Bravais Lattice with a Basis

A and B do not have identical environments





Non-Bravais lattice

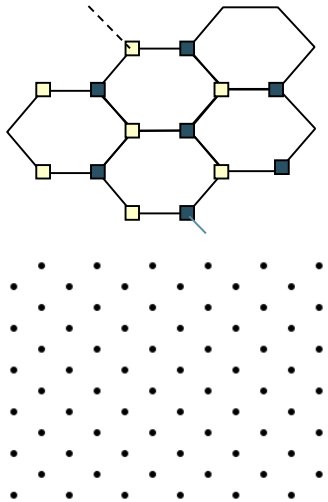
Bravais lattice with a basis

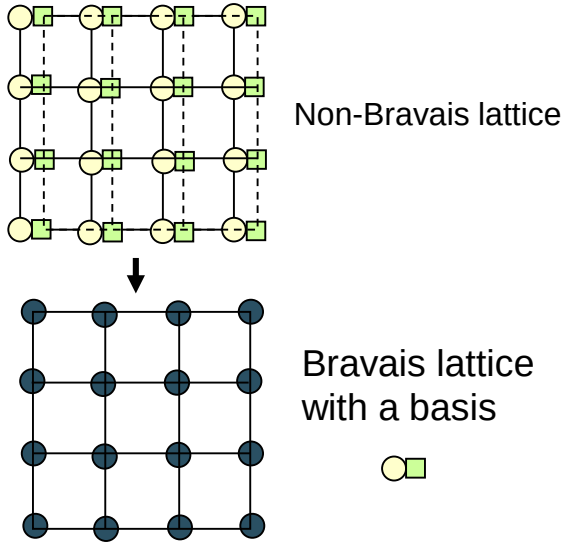
This is a Graphene sheet which has "recently" been isolated from Graphite by adhesive tape stamping.
2005 - Novoselov, Geim, et al. Nature, 438, 197.
2010 – Nobel Prize in Physics

Conversion into a Bravais lattice:
-Combine A and B into a single basis
-Obtain a rhombic Bravais lattice

Original image from: http://en.wikipedia.org/wiki/File:Rhombic_Lattice.svg

Bravais Lattice with a Basis





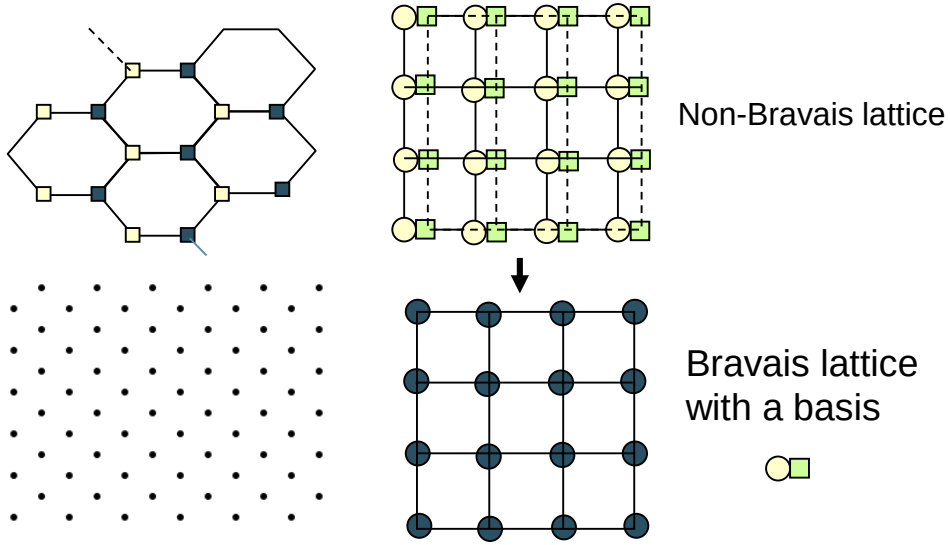
Conversion into a Bravais lattice:

- Combine complex components into a single repeated basis
- Establish basis vectors

• Property of ONE CELL defines the property of the solid
• Address every point in the lattice by integer translation of unit vectors
• every point has the same environment as every other point (same number of neighbors, next neighbors, …)

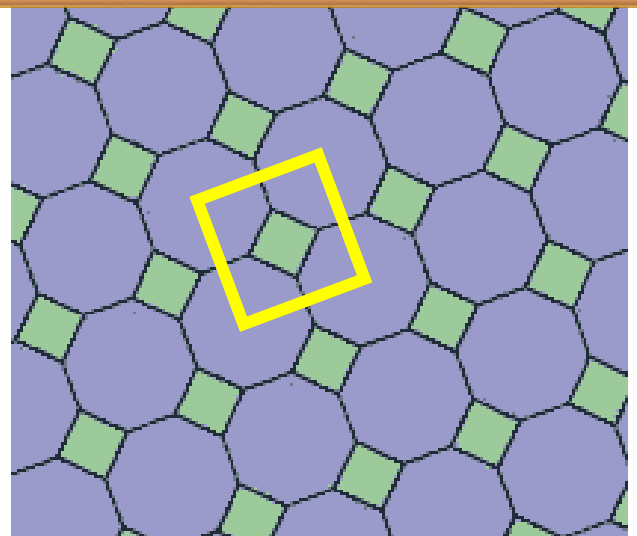
$$\mathrm{R} = \mathrm{h}\vec{a} + \mathrm{k}\vec{b}$$

Bravais Lattice with a Basis – in Art



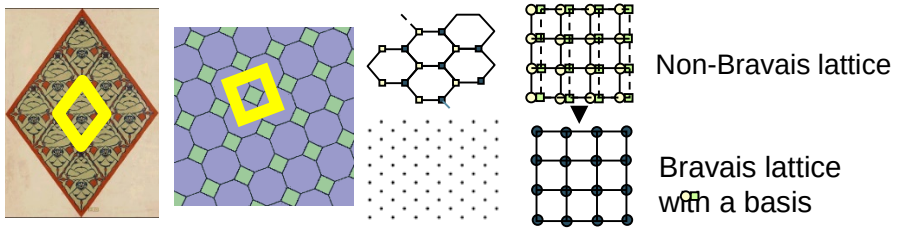
Conversion into a Bravais lattice:

- Combine complex components into a single repeated basis
- Establish basis vectors

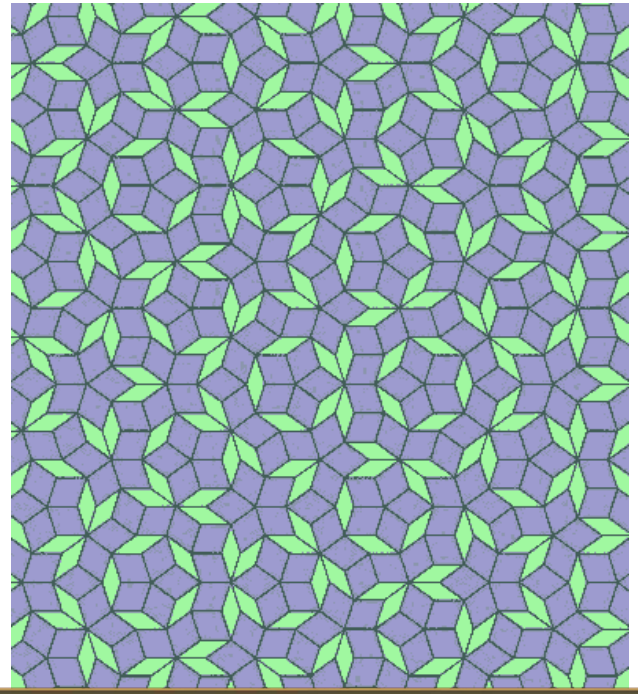


Kepler
Tiling

Non-Periodic Repeated Cells
NOT a Bravais Lattice



Penrose Tiles

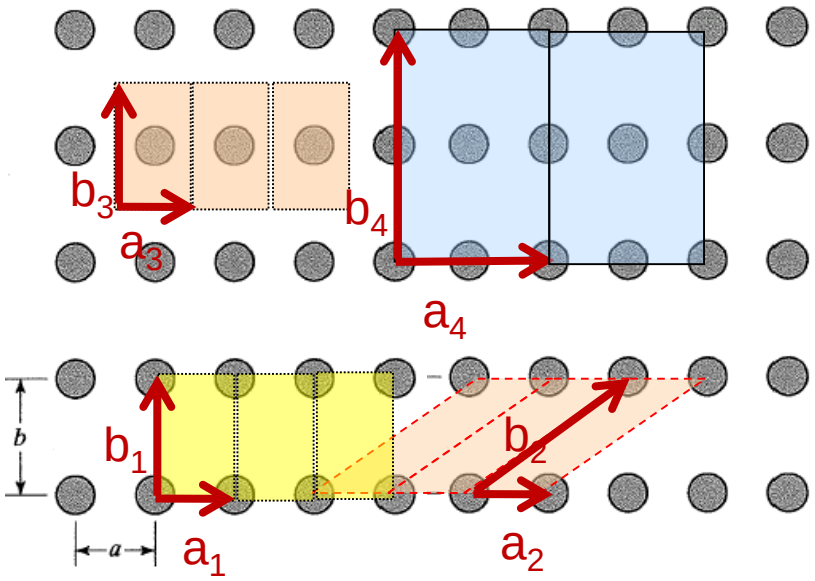


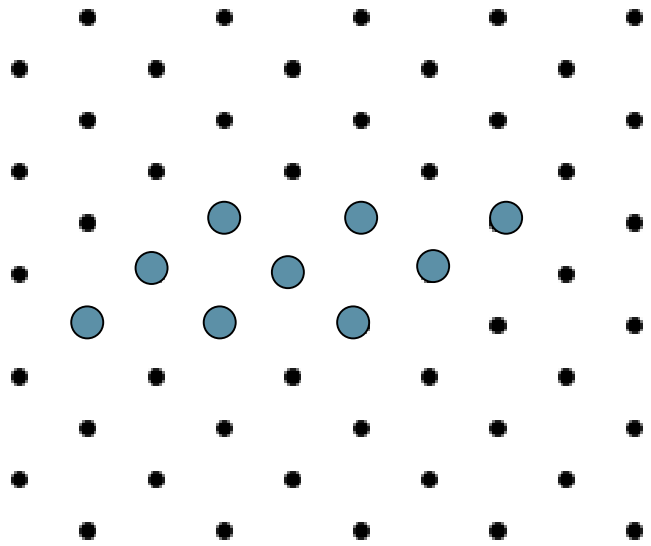
Ancient Tiles

… these CANNOT be transformed to Bravais lattice
ex. Aluminum-Manganese compounds, non-sticky coats

A Bravais Lattice must contain long-range order!

How to define ONE primitive cell?
Wigner-Seitz Primitive Cell





- Unit cells are *not* unique
- Unit cells can be Primitive or Non-primitive

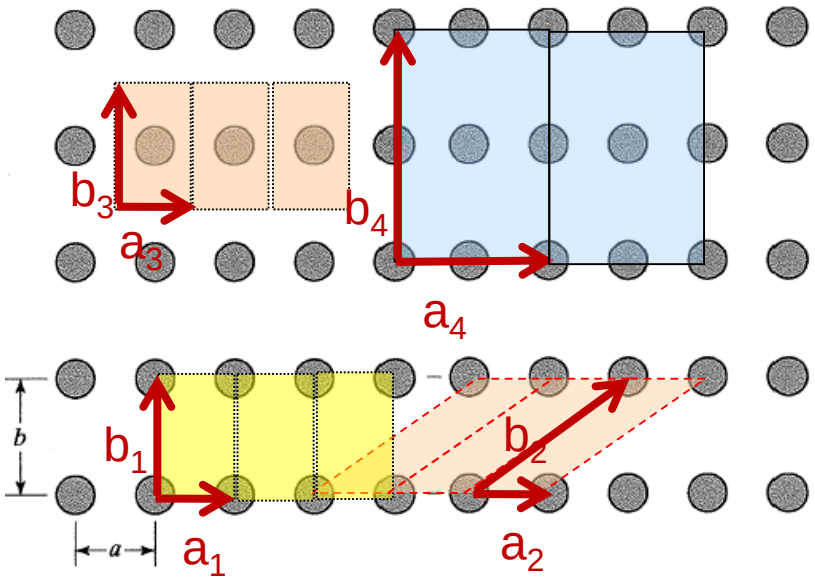
- Property of ONE CELL defines the property of the solid

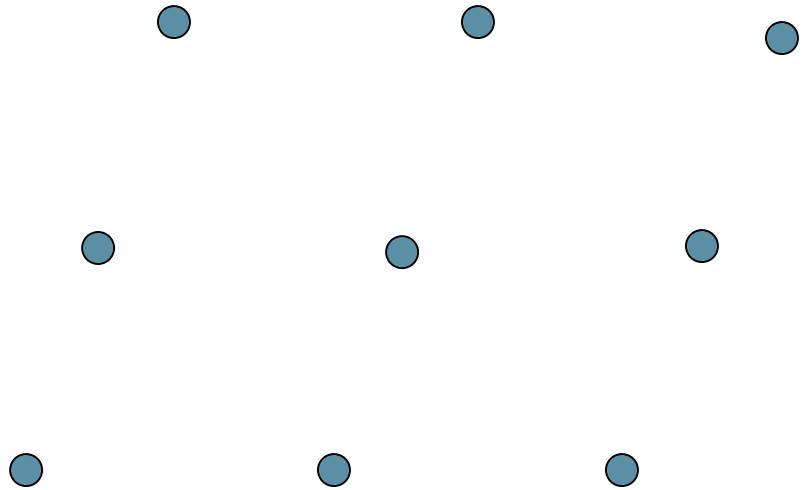
- Address every point in the lattice by integer translation of unit vectors

- every point has the same environment as every other point (same number of neighbors, next neighbors, …)

$$\mathrm{R} = h\vec{a} + k\vec{b}$$

How to define ONE primitive cell?
Wigner-Seitz Primitive Cell





Eg.: oblique

- Unit cells are *not* unique
- Unit cells can be Primitive or Non-primitive

- Property of ONE CELL defines the property of the solid

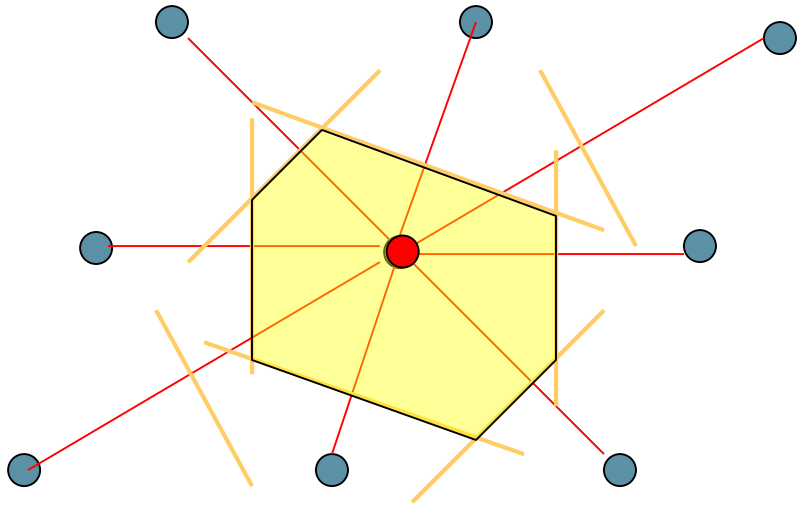
- Address every point in the lattice by integer translation of unit vectors

- every point has the same environment as every other point (same number of neighbors, next neighbors, …)

$$\mathrm{R} = h\vec{a} + k\vec{b}$$

How to define ONE primitive cell?
Wigner-Seitz Primitive Cell

- Choose a reference atom
- Connect to all its neighbors by straight lines
- Draw lines (in 2D) or planes (in 3D) normal to and at the midpoints of connecting lines
- Smallest area/volume enclosed is the Wigner-Seitz primitive cell



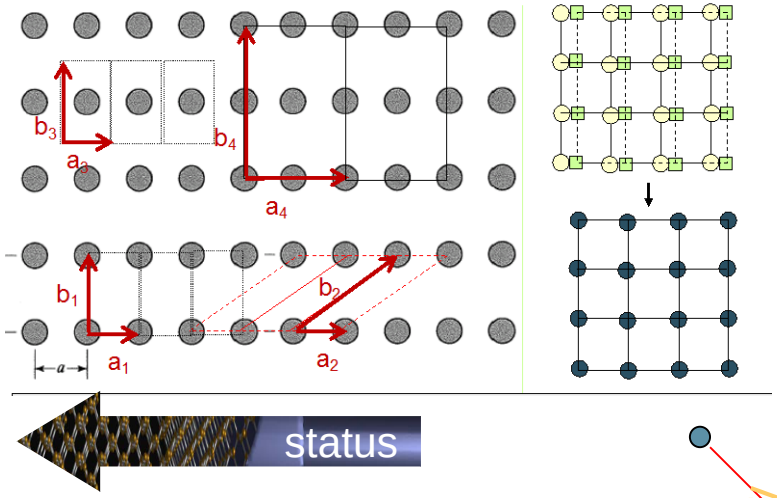
- Unit cells are *not* unique
- Unit cells can be Primitive or Non-primitive

Wigner-Seitz cell is ONE definition of a Unit Cell that always works
There are other ways of construction!

Section 3
Crystals

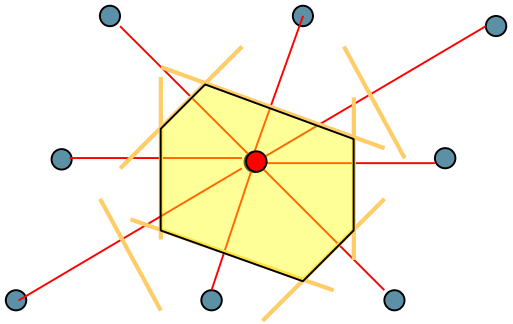
One Video Segment

- 3.1 Crystal definitions
  - » One-dimensional Crystals – simple primitive cell
  - » Unit cells of a Periodic 2D Lattice
  - » Bravais lattice
  - » Bravais lattice with a basis
  - » Non-periodic repeated cells
  - » Definition of ONE Primitive Cell – Wigner-Seitz Cell



One Video Segment

- 3.2 Tables of Bravais Lattices



One Video Segment

- 3.3 Density Definitions and Applications to Common Materials

One Video Segment

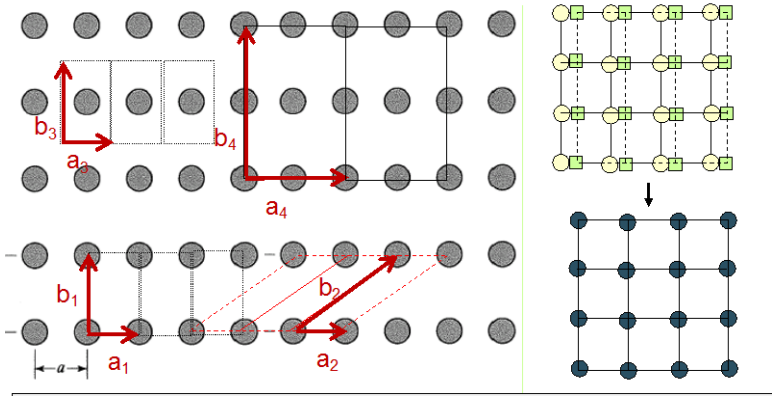
- 3.4 Surfaces, Miller Index

Reference: Vol. 6, Ch. 1, ABACUS tool at nanohub.org/tools/abacus and "Crystal Viewer Lab, https://nanohub.org/resources/crystalviewer

Section 3
Crystals

One Video Segment

- 3.1 Crystal definitions
  - » One-dimensional Crystals – simple primitive cell
  - » Unit cells of a Periodic 2D Lattice
  - » Bravais lattice
  - » Bravais lattice with a basis
  - » Non-periodic repeated cells
  - » Definition of ONE Primitive Cell – Wigner-Seitz Cell

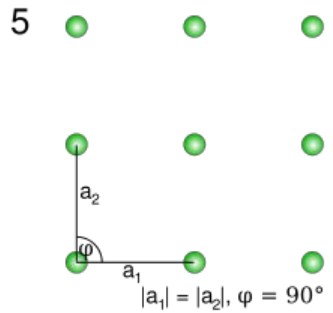


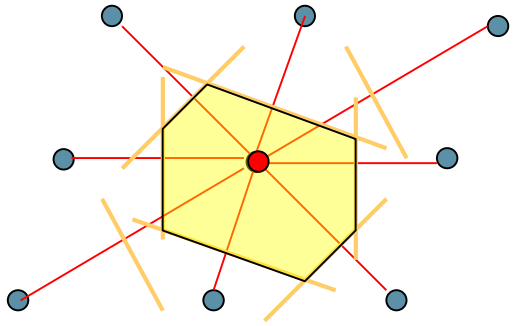
One Video Segment

- 3.2 Tables of Bravais Lattices

status

  - » Bravais Lattices in 2D (5 types)
  - » Bravais Lattices in 3D (14 types)
  - » 3 Dominant Bravais Lattices in Nature





One Video Segment

- 3.3 Density Definitions and Applications to Common Materials

One Video Segment

- 3.4 Surfaces, Miller Index

Reference: Vol. 6, Ch. 1, ABACUS tool at nanohub.org/tools/abacus and "Crystal Viewer Lab, https://nanohub.org/resources/crystalviewer