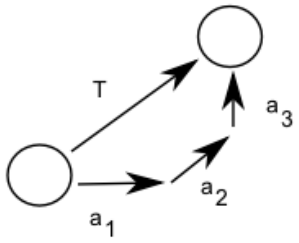
Topic 2-1: Lattice and Basis
Kittel Pages: 2-9

Summary: We begin our introduction of crystal structure by defining a few terms. The first is translational symmetry which explains the periodicity of a crystal. The next set of terms is the lattice and basis which represent the symmetry and the chemistry of the crystal respectively. Following this is the primitive and conventional cells which represent different ways to create the lattice through translation. Finally the bravias lattices are introduced and an example of a real world crystal is shown.

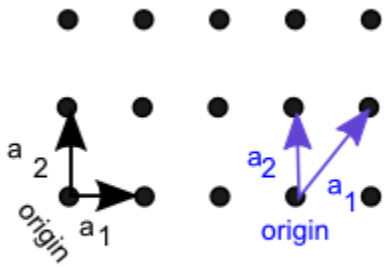
- Crystals- examples of macroscopic crystals include diamonds, table salt and snowflakes
  - Even aluminum is composed of crystals
- Crystals form from every bonding type (covalent, ionic, metallic, van der Waals). Most crystals are not obviously crystalline from a macroscopic perspective.
- Facet- one of the flat surfaces of a macroscopic crystal. As an example, here is pyrite (FeS_2), which forms as cubes.

- Microscopic crystal structure: atoms are arranged in a *periodic* manner with translational symmetry
- Translational symmetry (mathematical definition): A function f has translational symmetry described by $f(\vec{r})=f(\vec{r}+\vec{T})$, *if* we can construct some vector $\vec{T}$ such that $\vec{T}= u_1\vec{a}_1+u_2\vec{a}_2+u_3\vec{a}_3$ where $\vec{a}_i$ is a lattice vector and u_i is an integer.
  - This is a very general definition for anything with translational symmetry
  - Physically *f* could be the position of our atomic nuclei or the electron density

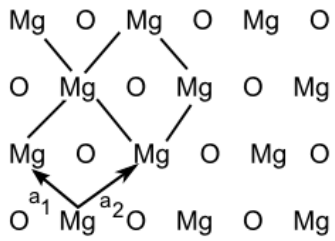
- Figure: If the crystal is periodic in $\vec{T}$ and has an atom at the origin (circle), then there *must* be a second atom at $\vec{a}_1+\vec{a}_2+\vec{a}_3$



- Given that crystals have translational symmetry, there must be some **repeat unit**, called the **unit cell**, which describes the crystal chemistry as well as its symmetry
- Lattice - set of *points* created by $\vec{T}$; the lattice reflects the symmetry of the crystal
- Basis - describes the chemical constituents within the crystal. The basis is applied to the lattice points.
- Constructive approach to building a crystal:
  - Using $\vec{T}$ we can populate space with a framework of points, creating a lattice.
  - Subsequently, we will decorate the lattice with a basis

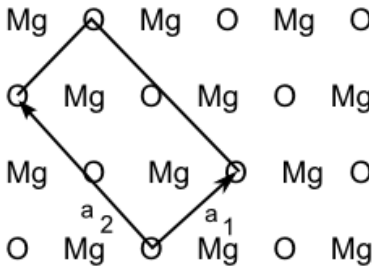


- $\vec{a}_1$ and $\vec{a}_2$ along with the origin are not unique
- Only constraint is that the lattice, when translated, must create the crystal
- Basis- how we decorate each lattice point
- Now that we have our lattice pointe, as shown above, we can decorate these points with atoms using our basis, below is an example of a MgO basis



Basis
Mg=0,0
O= ½, ½

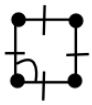
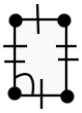
- In the above configuration the other magnesium atoms are created through translation (those not included in the basis)
    - Be careful when creating a primitive cell, there should not be two atoms at the same lattice point when the cell is tiled across the crystal.

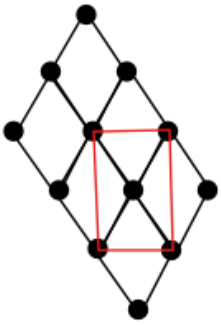


Basis
O= 0,0
O= 0, ½
Mg= ½ , ¼
Mg= ½ , ¾

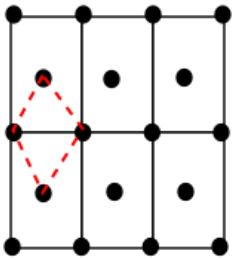
- Basis is also not unique. For example, the figure above shows the same crystal, but by picking different lattice vectors $\vec{a}_1$ and $\vec{a}_2$, the basis has changed.
- 2 types of lattice
    - Primitive- smallest area or volume cell that still spans free space upon translation
        - Pick primitive cell that reflects highest symmetry of cell (in above example this would be the square)
    - Conventional cell – larger than the primitive cell, has attractive geometric features that the primitive cell may not include. Contains more than one lattice point from the primitive $\vec{T}$
- **Bravais lattices -** infinite array of discrete points generated by a set of discrete translation operations described by: $\vec{T}= u_1\vec{a}_1+u_2\vec{a}_2+u_3\vec{a}_3$ where u_i are any integers and $\vec{a}_i$ are known as the primitive vectors which lie in different directions and span the lattice. This discrete set of vectors must be closed under vector addition and subtraction. For any choice of position vector $\vec{T}$, the lattice looks exactly the same.

Bravais Lattice in 2D

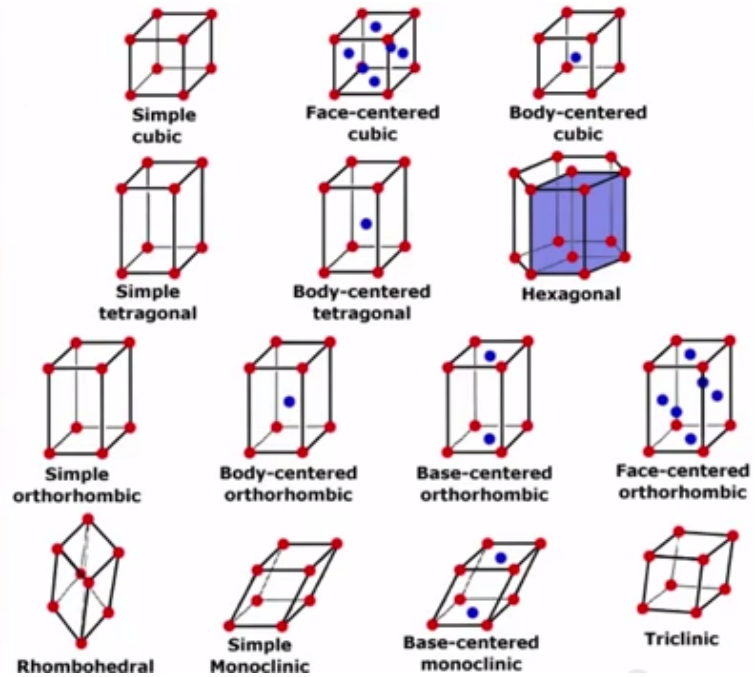
- Square  θ= 90
- Hexagonal  θ= 60
- Oblique  θ≠ 90
- Rhombic  θ≠ 90, 60
- Rectangular  θ = 90
- Can take a rhombic lattice and make a centered rectangular lattice
    - When talking about a centered lattice we mean that there is an atom centered within the cell. In this case that means that there is a lattice point at the center of the rectangular cell



- The centered rectangular lattice then looks like so

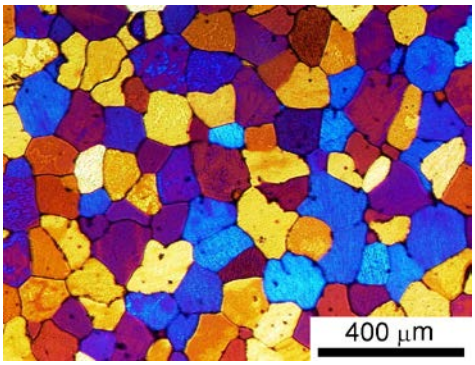


- While a rhombic cell works to span all space, the centered rectangular cell makes the 180 degree symmetry more obvious
    - This is an example of a conventional cell
    - Conventional cells better represent the symmetry and tend to be easier to work with
- Cannot center all bravais lattices
    - Cannot center a square lattice because it gives no additional information about the lattice
- Also have bravais lattices in 3D



- 3 types of centering in 3D: base, face and body
- When you see facets of macroscopic structures you are really seeing the exposed planes of the unit cell all lined up
- An example of this is pyrite which has a cubic unit cell and also looks like a cube in its macroscopic form (seen in the picture at the beginning of the notes)
- Metals like aluminum are composed of many small crystals in different orientations
    - While aluminum has no facets it does have a microscopic crystal structure
    - Figure below shows a cross-section through a ‘polycrystalline’ (multiple single crystals together) piece of Al. Within each grain (colored region), the crystal

displays translational symmetry $\vec{T}$. However, there is no guarantee of an orientational relationship between grains.

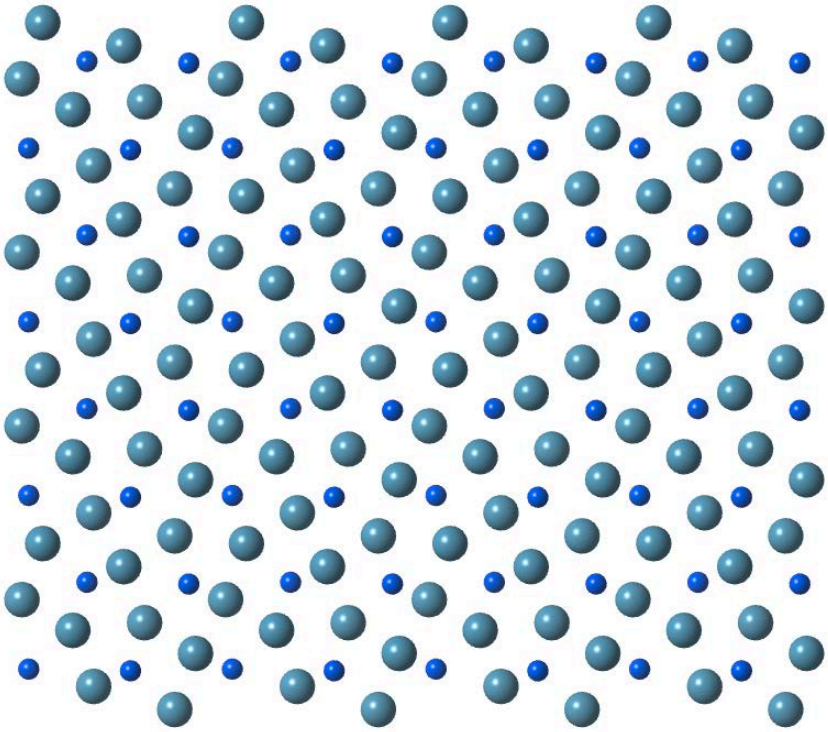


http://core.materials.ac.uk/search/detail.php?id=1741

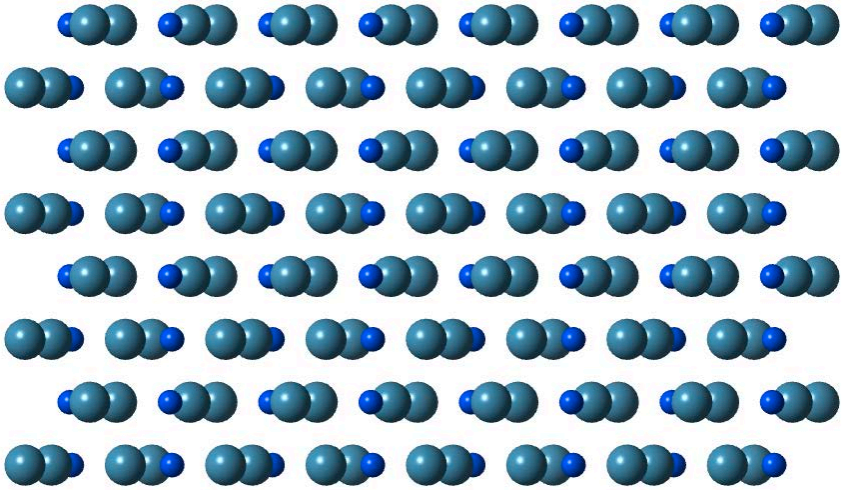
Questions to Ponder

1. Why wouldn't it make sense to have a base centered tetragonal cell?

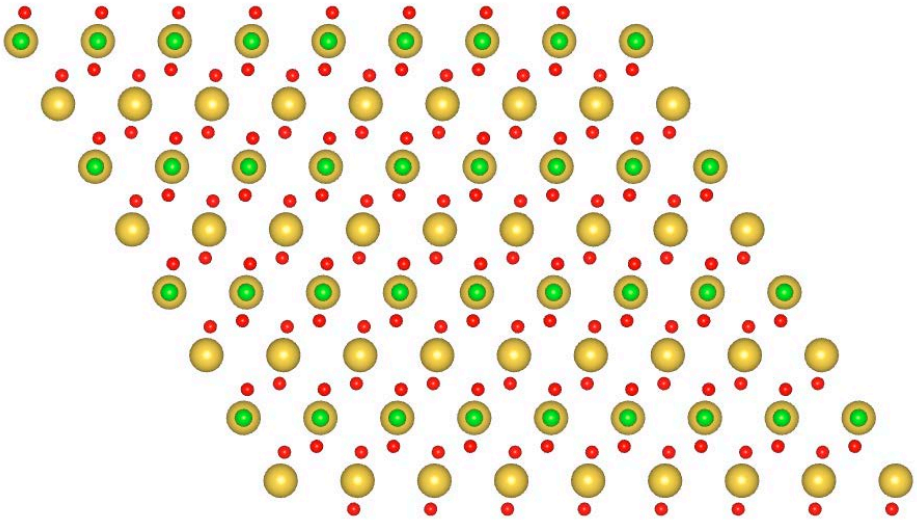
2. Here's Ca_2Si, viewed along one of its crystallographic axes ($\vec{a}_1$). Can you identify $\vec{a}_2$ and $\vec{a}_3$ vectors that capture the translational symmetry?



3. Here's the same Ca_2Si material, but viewed along $\vec{a}_2$. Can you identify $\vec{a}_1$ and $\vec{a}_3$ vectors that capture the translational symmetry?



4. Here is NaClO2 (monoclinic, $\vec{a}_3$ perpendicular to $\vec{a}_1$ and $\vec{a}_2$) viewed down $\vec{a}_3$; can you identify 3 distinct ways to define $\vec{a}_1$ and $\vec{a}_2$?



5. Find lattice points and vectors for each of the following wallpaper motifs.