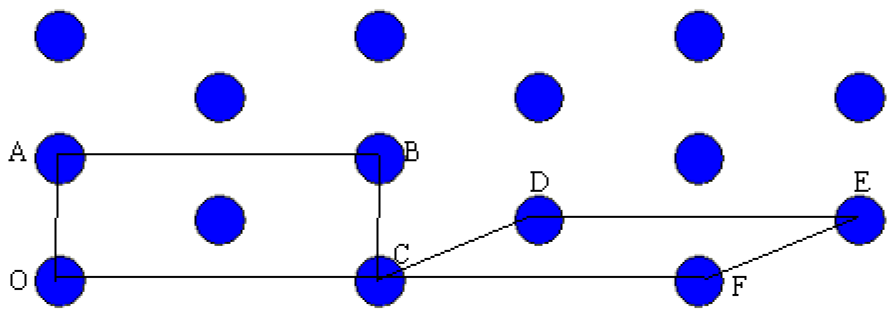
Lecture 7: Conventional Unit Cell, Bravais Lattice Classification, and Symmetry Groups

1. Conventional Unit Cell

As mentioned previously, the smallest repeating cell in a lattice is called the primitive cell. However, it is important to emphasize that the primitive cell does not necessarily exhibit the full symmetry of the crystal.



In the figure, the cell CDEF is a primitive cell, but it does not display the complete symmetry of the crystal. If instead we choose the cell OABC, we observe that this cell possesses the full symmetry of the crystal. **Nevertheless, this cell is not a primitive cell.**

A unit cell that exhibits the full symmetry of the crystal, but is not necessarily the smallest possible cell, is called the ***conventional unit cell***.

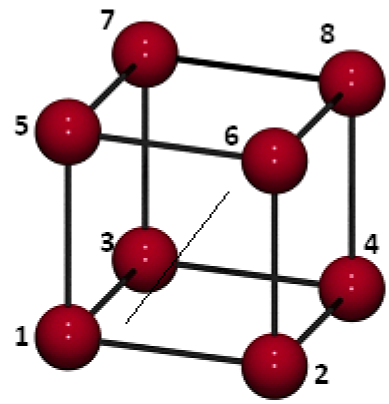
The main advantage of using the conventional unit cell is that it allows us **to clearly visualize the crystal's full symmetry.**

It should also be noted that the **Miller indices** of planes defined using the primitive cell are not necessarily the same as those defined using the conventional unit cell.

2. Bravais Lattice Classification

In this section, we explain how Bravais lattices can be classified from the viewpoint of symmetry (rather than from the structure point of view). A Bravais lattice can be classified according to the limited set of symmetry operations that leave the lattice invariant.

- ✓ For example, a cube may be rotated by a certain angle (π/2) about an axis passing through its center and still coincide with itself.



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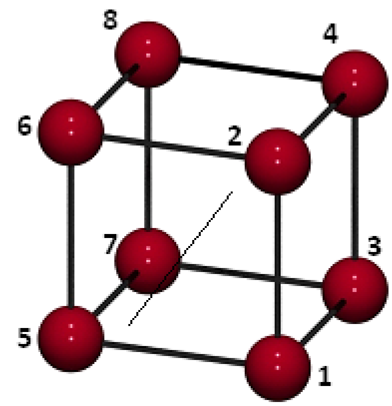
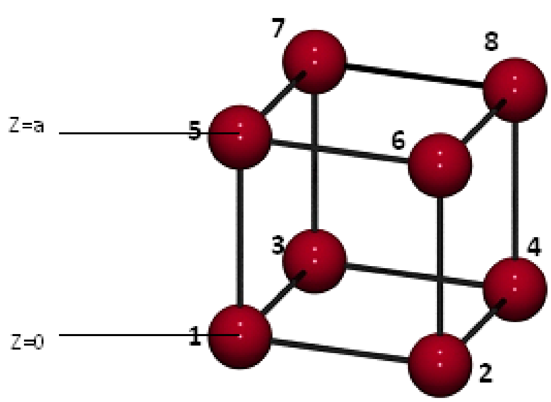
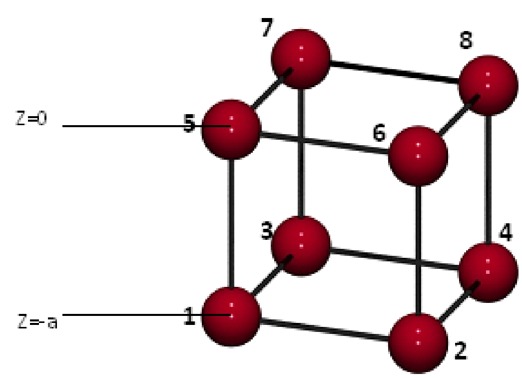
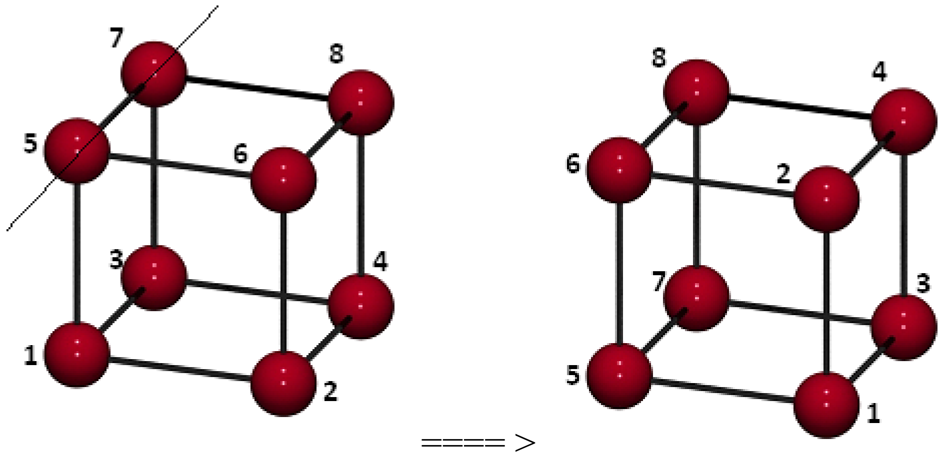


- ✓ In another example, the cube may be translated by a Bravais lattice vector ($\vec{R} = -a\hat{z}$) and remain unchanged.





- ✓ Similarly, rotating the cube by π/2 about an axis passing through atoms labeled 5 and 7 leaves these atoms unchanged, indicating a valid symmetry operation.

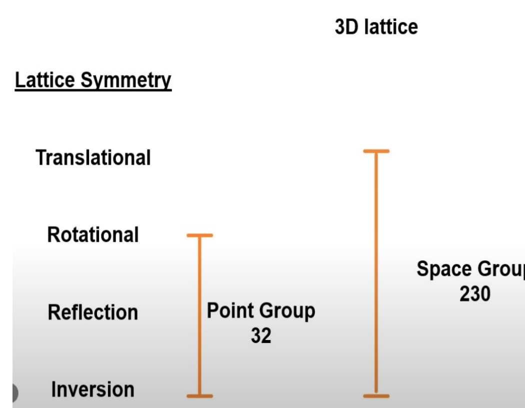


Therefore, any symmetry operation of a Bravais lattice can be classified as one of the following:

- **Rotation about an axis.**
- **Translation by a Bravais lattice vector.**
- **A rigid operation that leaves at least one part of the lattice unchanged.**

3. Point Groups and Space Groups

- Symmetry operations that leave at least one point in the lattice unchanged are called **point-group** symmetry operations. These usually include **rotation, reflection, and inversion.**
- It has been shown that there are exactly 32 possible crystallographic point groups.
- When **translational symmetry** is included along with point-group symmetry operations, the resulting set of symmetries is called **a space group.**



➢ There are 230 distinct space groups in three-dimensional crystals.