Exercises 2b 25.02.2025 - Solutions

1

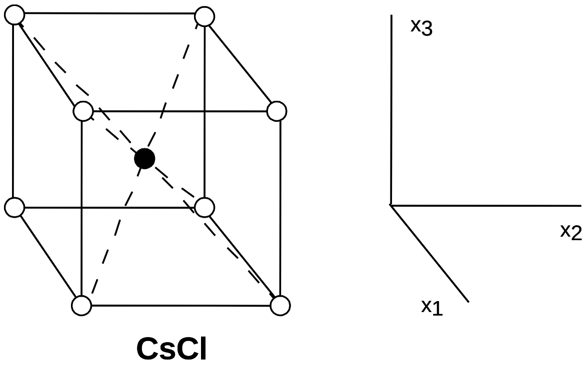


Fig.1.1

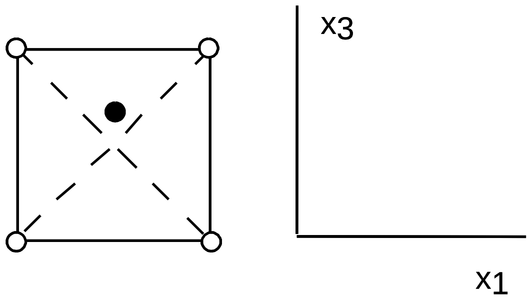
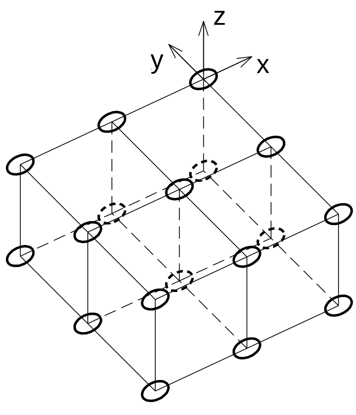


Fig.1.2

The centrosymmetric CsCl structure is cubic (with four atoms of one of the species occupying the cube corners and an atom of the other species occupying the centre of the cube) thus has the full cubic symmetry, $m\bar{3}m$. During the phase transition the structure becomes polar, leading to disappearance of all 3-fold symmetry axes along <111> directions, as well as 4-fold axes directed along x_1 and x_2 directions. The 4-fold symmetry along x_3 direction is kept unbroken. Other symmetry elements that stay in the structure are mirror planes having normal along (1,0,0), (0,1,0), (1,1,0) and (1,-1,0). Hence the structure exhibits the point symmetry *4mm*.

2



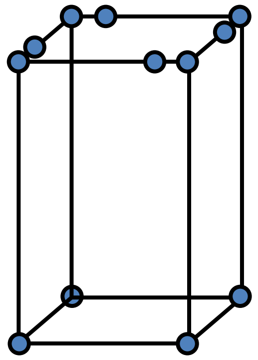
The “crystal” structure represented above consists of a cubic lattice with oval, bi-dimensional objects placed at the lattice points. As the ovals are placed on the *xy* plane, it immediately follows that this is a mirror plane. Additionally, each bi-dimensional oval possesses two other mirror planes -- *xz* and *yz*. The symmetry is then *mmm*.

3

To reduce the symmetry from $m\bar{3}m$ to *mmm*, we should modify the cell in Fig.1.1 in such a way that all 4-fold axes become 2-fold and all 3-fold axes disappear. This time we keep the central atom in the centre of the unit cell and we transform a cell from a cube to a parallelepiped ($a \neq b \neq c$). This way only two-fold axes and mirror planes will be the symmetry elements of the structure as required for *mmm* structure.

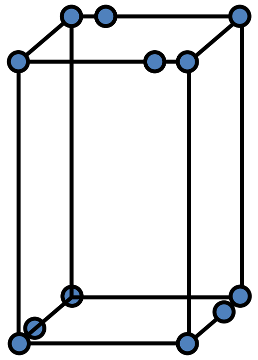
4

The aim is to create an object which has a four-fold rotation symmetry axis (*4*), but not mirror symmetry. We can propose a structure based on a square prism from *slide 54* (with $a=b\neq c$), the mirror symmetry can be broken e.g. by placing an additional sphere close to the top-right corner of each lateral face:



- $\bar{4}$:

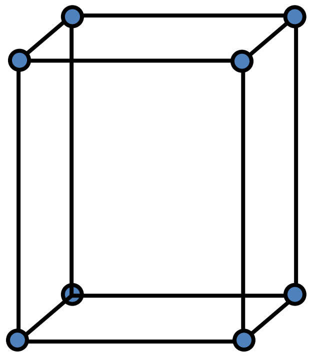
Similar to the previous example, this object can be constructed from a square prism by placing an additional sphere on each lateral face of the prism. However, now the atoms alternate between the top and the bottom corners in order to display $\bar{4}$ symmetry:



5

- ***mmm*:**

Such object can be obtained by stretching the square prism to orthorhombic parallelepiped with $a \neq b \neq c$:



- ***222*:**

This object is less intuitive. It is necessary to obtain the *2* symmetries while avoiding the mirror symmetries. The object is also a parallelepiped, but now there are only two spheres in each face, placed on opposed corners: