

## Answers to Examples Class 2

### Calcium Chloride

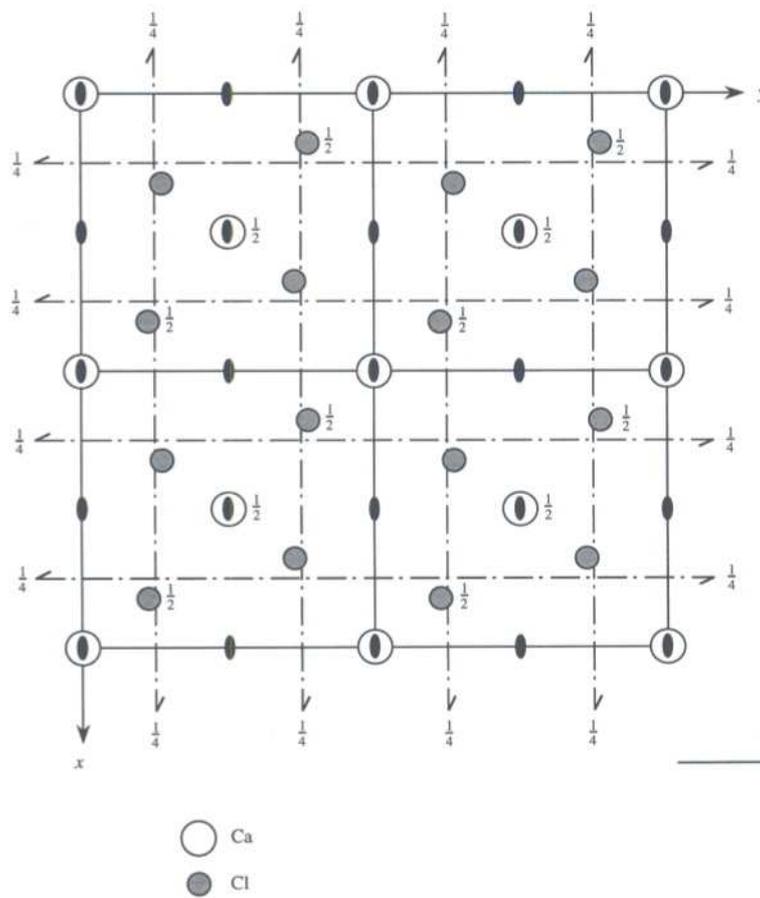


Figure 1: Structure projected along  $[001]$ . The Bravais lattice is  $P$  (the Ca at the origin has a different environment to that at the centre of the unit cell. Diads parallel to  $[001]$  go through each Ca and down the centres of the four sides of the cell containing  $[001]$ .  $(002)$  planes at  $z = 0$  and  $\frac{1}{2}$  are mirrors.  $(200)$  diagonal glide ( $n$ ) planes cut at  $x = \frac{1}{4}$  and  $x = \frac{3}{4}$ .  $(020)$  diagonal glide ( $n$ ) planes cut at  $y = \frac{1}{4}$  and  $y = \frac{3}{4}$ .  $2_1$  screw axes lie in the glide planes at heights  $z = \frac{1}{4}$  and  $z = \frac{3}{4}$  (only the former is illustrated).

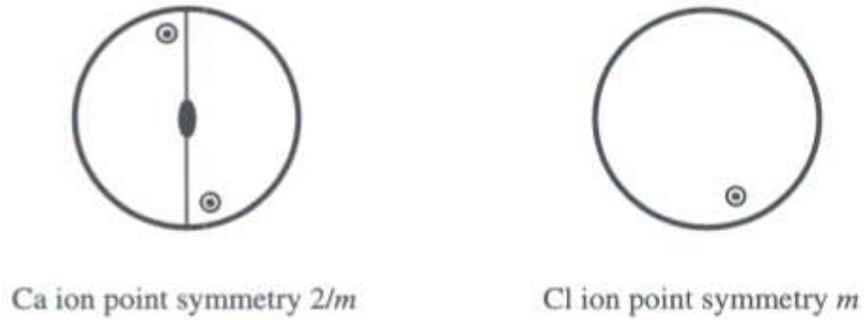


Figure 2: Translational symmetry neglected in determining point group, which is  $mmm$ . Point symmetry of Ca is  $2/m$  and that of Cl is  $m$ .

## Martensite

The strain which transforms the structure of austenite into martensite is the Bain strain, which involves a compression along one edge and uniform expansion along the other two edges of the unit cell of austenite.

Suppose that the austenite is represented as a sphere with its unit cell edges denoted by the vectors  $\mathbf{a}_i$  with  $i = 1, 2, 3$ , as illustrated in Fig. 3a,b. The Bain strain changes the sphere into an ellipsoid of revolution about  $\mathbf{a}_1$ . There are no lines in the  $(0\ 0\ 1)_\gamma$  plane which are undistorted. However, it is possible to find lines such as  $wx$  and  $yz$  are undistorted by the deformation, but are rotated to the new positions  $w'x'$  and  $y'z'$ . Since they are rotated by the Bain deformation they are not invariant-lines. In fact, the Bain strain does not produced an invariant-line strain. It can be converted into an invariant-line strain by adding a rigid body rotation as illustrated in Fig. 3c.

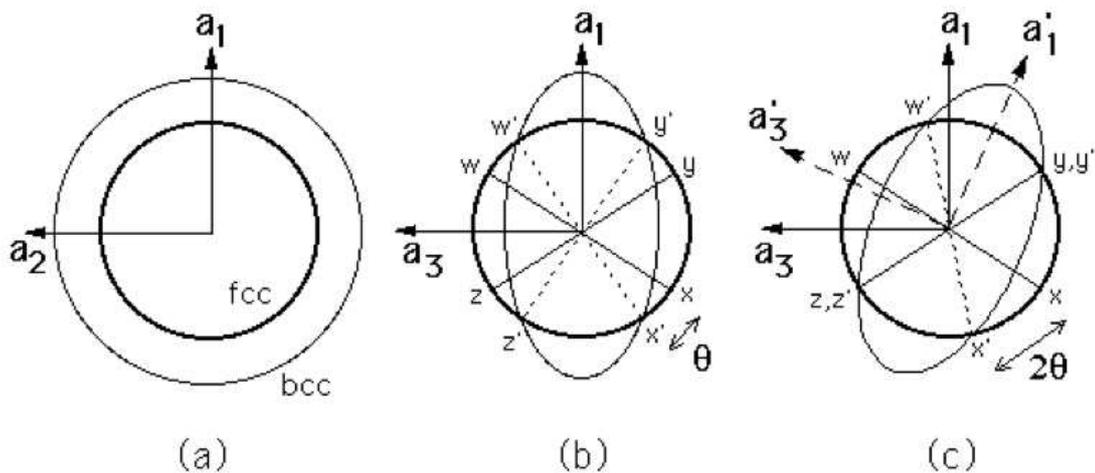


Figure 3: Bain strain and rigid body rotation.

It is also apparent from Fig. 3c that there is no possible rotation which would convert  $\mathbf{B}$  into an invariant-plane strain because there is no rotation capable of making two of the non-parallel undistorted lines into invariant-lines. Thus, it is impossible to convert austenite into  $\alpha'$  martensite by a strain which is an invariant-plane strain. A corollary to this statement is that the two crystals cannot ever be joined at an interface which is fully coherent and stress-free.

## Orientation Relationships

Inspection of the matrix reveals that

$$J_{11} + J_{22} + J_{33} = 1 + 2 \cos \theta \quad (1)$$

and the components of the unit vector  $\mathbf{u}$  along the axis of rotation are given by

$$\begin{aligned} u_1 &= (J_{23} - J_{32})/2 \sin \theta \\ u_2 &= (J_{31} - J_{13})/2 \sin \theta \\ u_3 &= (J_{12} - J_{21})/2 \sin \theta \end{aligned} \quad (2)$$

It follows that the matrix describes a rotation of  $90^\circ$  about  $[001]_X$ , and hence represents a symmetry operation so that  $\Sigma = 1$ .