Examples Class 2

Calcium Chloride

The orthorhombic unit cell of $CaCl_2$ has $a = 0.624\,\text{nm}$, $b = 0.643\,\text{nm}$ and $c = 0.420\,\text{nm}$ with ion positions at

Ca: 0,0,0 $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

Cl: $x, y, 0$ $\overline{x}, \overline{y}, 0$ $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2}$ $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2}$

with $x = 0.325$ and y= 0.275. Fig. 1 is an accurate projection of this structure on (001).

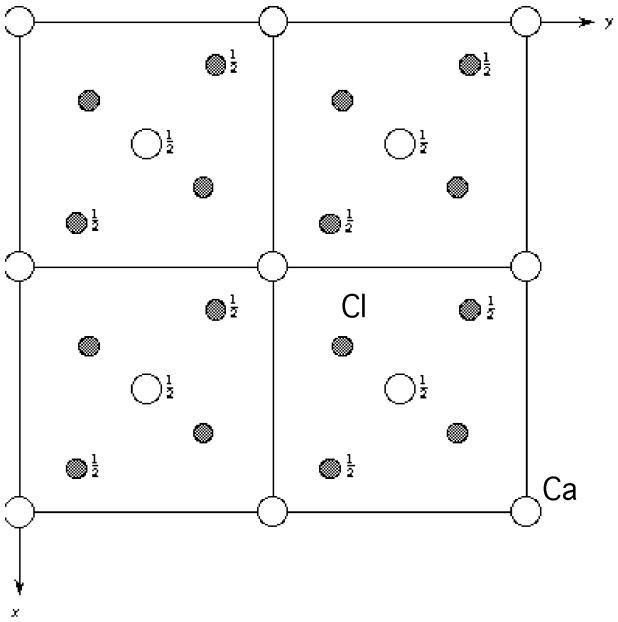

Figure 1: The structure projection for calcium chloride

1. What is the Bravais lattice of this structure?
2. Locate all symmetry elements present in the structure and hence determine those along [100], [010] and [001]. What is the point group of the crystal structure?
3. Determine the point symmetries of the Ca and Cl ions and express them on sketch stereograms.

Martensite

Show diagramatically that it is impossible to obtain a fully coherent boundary between austenite and martensite.

Orientation relationships

A rotation matrix can be used to describe the orientation relationship between two grains with identical crystal structure. It can also be described by an axis of rotation and a right–handed angle of rotation (an axis–angle pair).

The general rotation matrix relating the two cubic lattices for a right–handed rotation θ about a unit axis $[u_1\ u_2\ u_3]$ is given by:

$$(\mathrm{Y\ J\ X}) = \begin{pmatrix} u_1u_1(1-m)+m & u_1u_2(1-m)+u_3n & u_1u_3(1-m)-u_2n \\ u_1u_2(1-m)-u_3n & u_2u_2(1-m)+m & u_2u_3(1-m)+u_1n \\ u_1u_3(1-m)+u_2n & u_2u_3(1-m)-u_1n & u_3u_3(1-m)+m \end{pmatrix} \tag{1}$$

where $m = \cos\theta$ and $n = \sin\theta$

Show how you might deduce the axis–angle pair from this matrix. Hence derive the axis–angle pair for the rotation matrix

$$(\mathrm{Y\ J\ X}) = \begin{pmatrix} 0 & 1 & 0 \\ \overline{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{2}$$

What is the Σ value relating these two grains?