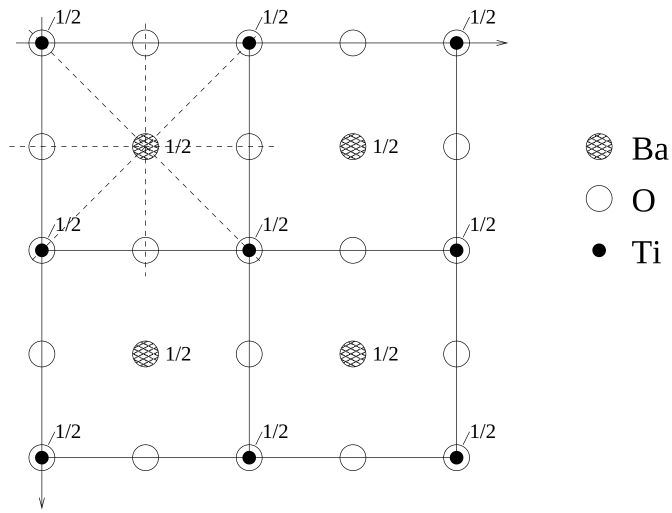
Question A2, 1998:
**rotation axis**: The axis, of order $n$, about which rotation by a given fraction $1/n$ of a complete rotation brings an objecct back into coincidence with itself.
**mirror plane**: A plane through which reflection of an object brings it back into coincidence with itself.
**centre of symmetry**: A point through which an object can be inverted (*ie* all points $x, y, z$ are transformed into $\overline{x}, \overline{y}, \overline{z}$) to bring the object into coincidence with itself.
**$BaTiO_3$**:




Rotation axis through $\frac{1}{2}\frac{1}{2}0$ is $n = 4$, rotation axis through $\frac{1}{2}00$ is $n = 2$. One centre of symmetry is $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.
**Pyroelectricity** property whereby a change in temperature produces a change in the dielectric polarisation of a material.
**Piezoelectricity** property whereby the application of a stress produces a change in the dielectric polarisation of a material, or conversely when application of an electric field produces a first-order strain of the crystal.
**Ferroelectricity** the generation of a reversible dielectric polarisation of a crystal on cooling below a specific temperature. A ferroelectric phase transition is an example of displacive phase transition.
A structure with a centre of symmetry cannot have a permanent electric dipole moment. However, the lack of centre of symmetry is not the only requirement to have a dipole moment, a *principal axis* not perpendicular to a mirror plane or to a rotation axis is also needed.
Below 120$^o$C, $BaTiO_3$ is tetragonal. Therefore displacement of Ti must keep $n = 4$ axis, displacement is along [001]. There are no centre of symmetry and the mirrors which are not parallel to [001] are no longer.
The polarisation per unit volume for the tetragonal phase is:

$$\frac{1}{V_{\text{unit cell}}}(4e \times \delta z_{Ti} + 2e \times \delta z_{Ba} + 3 \times 2(-e)\delta z_O)$$

giving 0.18 C.m$^{-2}$.