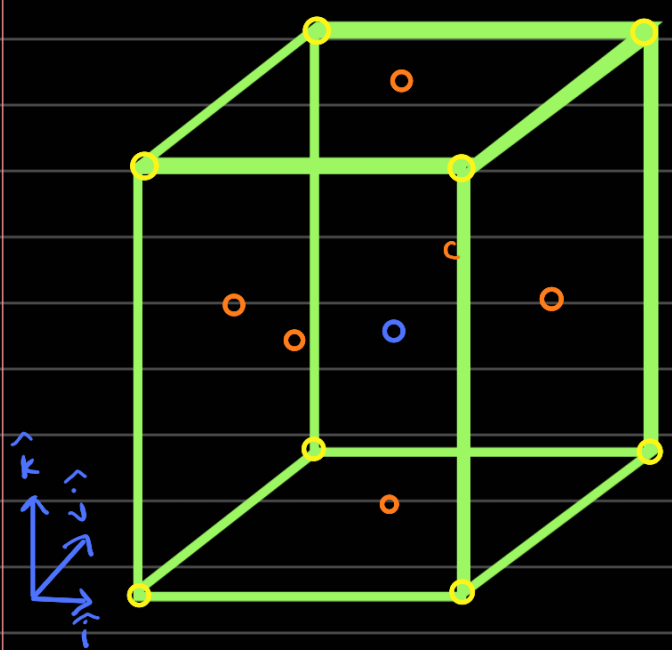
Assignment-3

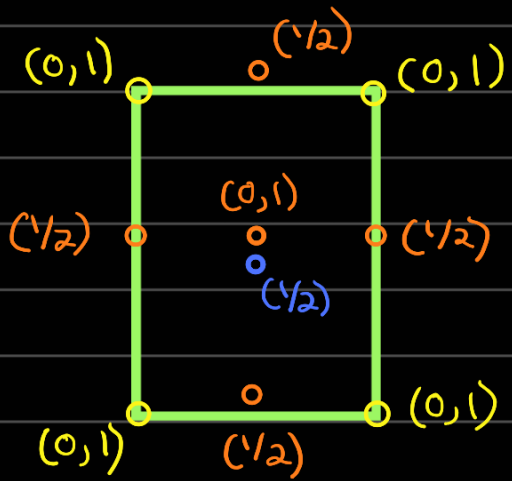
$BaTiO_3$ → distorted perovskite

tP lattice: Ba at (0,0,0)
Ti at (0.5, 0.5, 0.482)
O at (0.5, 0.5, 0.016, 0.5, 0, 0.515),
(0, 0.5, 0.515)

$a = 0.3999$ nm, $c = 0.4018$ nm



- [0 1 0] projection of the crystal



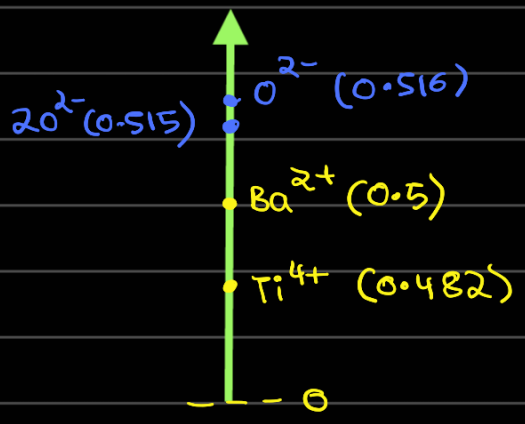
- Electric polarisation

Centre of charge of Ba^{2+} is at the centre of the tP lattice $\longrightarrow$ (0.5, 0.5, 0.5)

$Ti^{4+} \longrightarrow$ (0.5, 0.5, 0.482)

Centre of charge of the 4 O^{2-} ($4 \times 1/2 = 2$ effective O^{2-}) which lie on planes ⊥ to c-axis lies on (0.5, 0.5, 0.515)

Centre of charge of the 2 O^{2-} ($2 \times 1/2 = 1$ effective O^{2-}) which lie on the c-axis lies on (0.5, 0.5, 0.516)



Centre of +ve charge $= \dfrac{0.482 \times 4 + 0.5 \times 2}{4 + 2}$

$= \dfrac{2.928}{6}$

$= 0.488$

Centre of −ve charge $= \dfrac{4 \times 0.515 + 2 \times 0.516}{4 + 2}$

$= \dfrac{2 \times 0.515 + 0.516}{2 + 1}$

$= \dfrac{1.546}{3}$

$\simeq 0.5153$

So $u = 9 \times d$

$$= 6q \times c(0.5153 - 0.488)$$

$$= 6 \times 1.602 \times 10^{-19}\ C \times 0.4018 \times 10^{-9} \times 0.0273\ Cm$$

$$= \frac{6 \times 1.602 \times 0.4018 \times 0.0273 \times 10^{-28}}{3.33564 \times 10^{-30}}\ Debye$$

$$\simeq 3.1609\ D$$

$\therefore$ Electric polarisation $= \frac{\mu}{V}$

$$= \frac{3.1609}{a^2 \times c}$$

$$= \frac{3.1609 \times 3.33564 \times 10^{-30}}{(0.3999)^2 \times 0.4018 \times 10^{-27}}\ Cm^{-2}$$

$$\simeq 0.1641\ Cm^{-2}\ (\text{coulomb per metre squared})$$