

SSC3473 Solid State Chemistry – Crystal Chemistry

1. Copper metal is face centred cubic with $a=3.615 \text{ \AA}$. Assuming the atoms touch along the face diagonal, calculate the metallic radius of copper.
2. The metallic radius of gold is 1.44 \AA , and its structure is face-centred cubic. What is the unit cell parameter, a , for gold?
3. The metallic radius of chromium is 1.25 \AA and its structure is body centred cubic. What is the unit cell parameter, a , for chromium?
4. NaCl is face centred cubic with $a = 5.64 \text{ \AA}$. Assuming the radius of the chloride ion is 1.80 \AA , calculate the radius for Na^+ . Are the chloride ions in contact in NaCl?
5. Calculate the d-spacing of the (1 2 3) planes in a cubic crystal with $a=b=c=8.00 \text{ \AA}$. Calculate the d-spacing of the same planes in an orthorhombic crystal with $a=7.00 \text{ \AA}$, $b=8.00 \text{ \AA}$ and $c=9.00 \text{ \AA}$.
6. Li_2O has a cubic structure with unit cell edge 4.61 \AA .
The atomic coordinates are:

Li	$\frac{1}{4} \frac{1}{4} \frac{1}{4}$	$\frac{3}{4} \frac{3}{4} \frac{3}{4}$	$\frac{1}{4} \frac{1}{4} \frac{3}{4}$	$\frac{1}{4} \frac{3}{4} \frac{3}{4}$
	$\frac{1}{4} \frac{3}{4} \frac{1}{4}$	$\frac{3}{4} \frac{1}{4} \frac{3}{4}$	$\frac{3}{4} \frac{1}{4} \frac{1}{4}$	$\frac{3}{4} \frac{3}{4} \frac{1}{4}$
O	$0 \ 0 \ 0$	$\frac{1}{2} \ \frac{1}{2} \ 0$	$0 \ \frac{1}{2} \ \frac{1}{2}$	$\frac{1}{2} \ 0 \ \frac{1}{2}$

Draw a projection of the structure onto the xy plane. Indicate the coordination environments of Li and O. Calculate the Li-O bond length. What is the name for this structure type?
7. CsCl is primitive cubic with unit cell $a = 4.115 \text{ \AA}$. Using the d-spacing equation, calculate the spacing of (a) the 110 planes and (b) the 111 planes.
8. X-rays of wavelength $\lambda = 1.50 \text{ \AA}$ are reflected from the (2 2 2) planes of a cubic crystal with unit cell $a = 5.00 \text{ \AA}$. Calculate the Bragg angle, θ , for $n=1$.