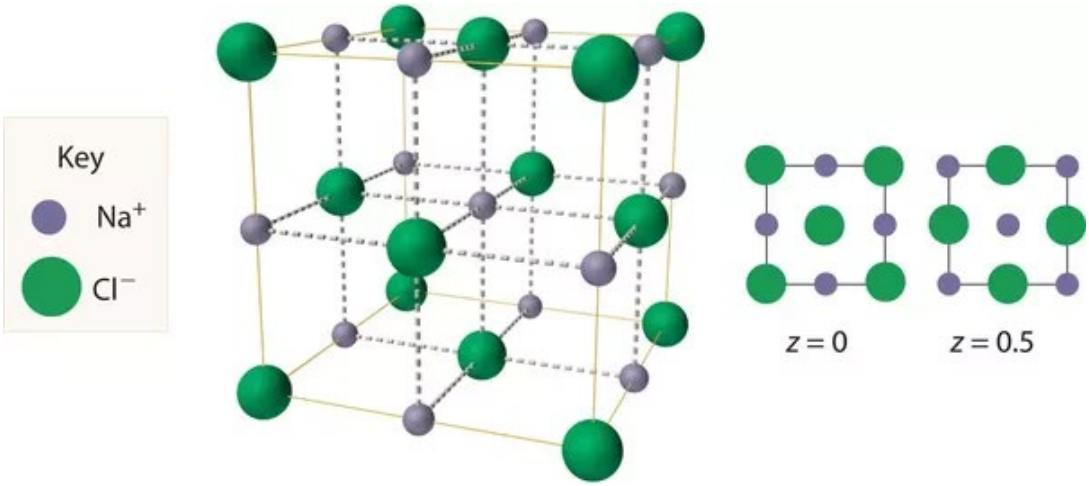
Example- Calculate some quantities for sodium chloride/NaCl (AKA salt) crystal.

Per Wikipedia, sodium chloride (NaCl) has a face-centered cubic lattice/unit cell crystal structure (see below) with a lattice constant of 564 pm = 5.64 Å.



We can see that it can be broken into primitive cells with a simple cubic lattice with Na and Cl atoms occupying alternate corners with a lattice constant of 282 pm = 2.82 Å.

The atomic surface density (*asd*) of the top face of the cubic lattice would be:

$$asd_{top} = \frac{\#\text{ atoms on top}}{\text{area of top}} = \frac{4\,(0.25)}{\left(282*10^{-12}\right)^2}$$

$$\Rightarrow \quad \underline{\boldsymbol{asd_{top} = 1.2575 \times 10^{19}\ \text{atoms/m}^2 = 1.2575 \times 10^{15}\ \text{atoms/cm}^2}}.$$

The atomic volume density (*avd*) of the NaCl cubic lattice would be:

$$avd_{\text{NaCl}} = \frac{\#\text{ atoms in cell}}{\text{volume of cell}} = \frac{8\,(0.125)}{\left(282*10^{-12}\right)^3}$$

$$\Rightarrow \quad \underline{\boldsymbol{avd_{\text{NaCl}} = 4.459 \times 10^{28}\ \text{atoms/m}^3 = 1.2575 \times 10^{22}\ \text{atoms/cm}^3}}.$$

The atomic volume density (*avd*) of the Na and Cl atoms would be:

$$avd_{\text{Na}} = avd_{\text{Cl}} = 0.5\, avd_{\text{NaCl}}$$

$$\Rightarrow \underline{\boldsymbol{avd_{\text{Cl}} = avd_{\text{Cl}} = 2.23 \times 10^{28}\ \text{atoms/m}^3 = 2.23 \times 10^{22}\ \text{atoms/cm}^3}}.$$

To get the mass density (md_{NaCl}), we need the atomic number for Na (22.99) and Cl (35.45) as well as Avogadro's constant N_A.

$$md_{\text{NaCl}} = \frac{avd_{\text{Na}}\ (\text{atomic weight of Na}) + avd_{\text{Cl}}\ (\text{atomic weight of Cl})}{N_A}$$

$$= \frac{2.23*10^{28}\ (22.99) + 2.23*10^{28}\ (35.45)}{6.02214*10^{23}}$$

$$\Rightarrow \quad \underline{\boldsymbol{md_{\text{NaCl}} = 2.16 \times 10^{6}\ \text{g/m}^3 = 2.16\ \text{g/cm}^3}}.$$