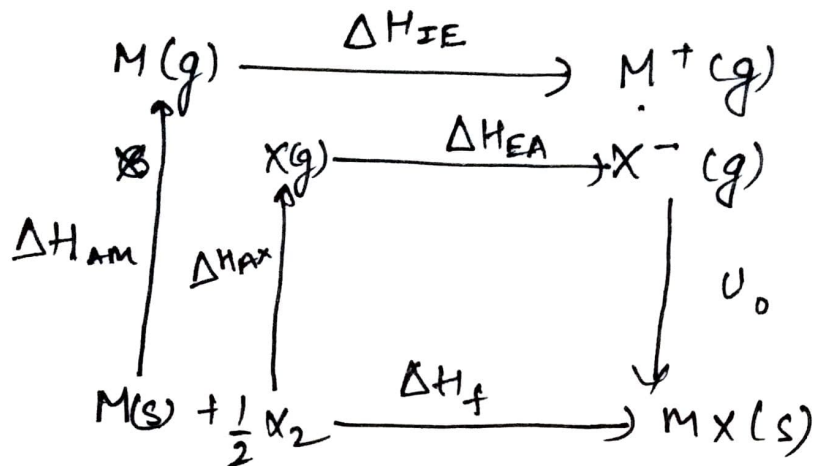


The lattice energy of ionic crystal is determined by using Born-Haber cycle which can represent diagrammatically as:-



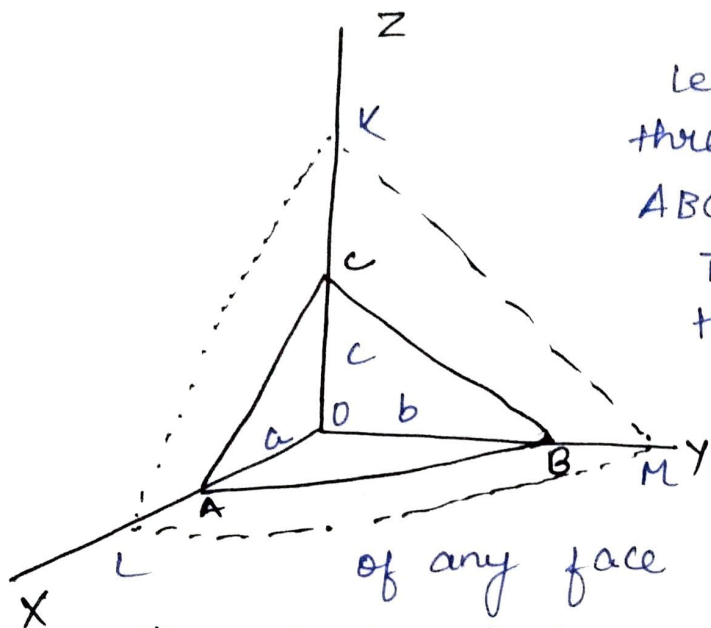
$$\Delta H_f = \Delta H_{AM} + \Delta H_{AX} + \Delta H_{IE} + \Delta H_{EA} + U_0$$

ΔH_{AM} and ΔH_{AX} are the enthalpy of atomization of metal and non metal.

ΔH_{IE} is the energy of ionization / enthalpy of ionization and ΔH_{EA} is the electron affinity of metal and non-metal respectively.

Law of Rational Indices

This law states that the intercept of any face of crystal lattice along the crystallographic axes are either to the unit intercepts (a, b, c) or some simple whole number multiples of them e.g. $na, n'b, n''c$ etc. where n, n', n'' are simple whole numbers.



Let OX, OY, OZ are representing three crystallographic axes and ABC be the unit plane.

The unit intercepts will be then a, b, c .

According to the law of rational Miller indices the intercepts

of any face such as KLM , on the same three axes will be a simple whole number multiple of a, b and c .

Miller Indices: Miller indices are a set of integers (h, k, l) which are used to describe a given plane in a crystal. The miller indices of a face of a crystal are inversely proportional to the intercept of that face on various axes.

The steps for determination of miller indices is given by.

- ① Prepare a three column table with unit cell axes at the top of column.
- ② Enter intercept in each column of the plane of these axes.
- ③ Invert all numbers.
- ④ Clear fractions to get h, k, l .

Q calculate the Miller indices of crystal plane which cut through crystal axes at $(2a, 3b, c)$.

- ①
- | | | | | |
|-----|-----|-----|---|---|
| a | b | c | } | Prepare the table and enter the intercept |
| 2 | 3 | 1 | | |
- ②
- | | | | |
|---------------|---------------|-----|----------------------|
| $\frac{1}{2}$ | $\frac{1}{3}$ | 1 | → invert the number. |
|---------------|---------------|-----|----------------------|
- ③ Multiply by ⑥ to get clear fraction & obtain h, k, l .
- | | | | |
|-----|-----|-----|------------------------|
| 3 | 2 | 6 | Miller indices (326) |
|-----|-----|-----|------------------------|

Interplanar spacing in crystal system

In a crystal system, the interplanar distance d_{hkl} is given by

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

where h, k, l are Miller indices and a, b, c are plane intercepts.

① For cubic system,

$$a = b = c$$

$$\text{so } \frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{a^2} + \frac{l^2}{a^2}$$

$$= \frac{1}{a^2} (h^2 + k^2 + l^2)$$

$$\text{or } d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Assignment

- Q1. Find miller indices for crystal planes that cut crystal axes at (i) a, b, c (ii) $6a, 2b, 3c$ and $(3a, -2b, -3c)$
- Q2. Derive interplanar spacing in crystal as for tetragonal and orthorhombic system.
- Q3. Density of Li is 0.56 g cm^{-3} and separation of (100) plane of metal is 350 pm .
 $M(\text{Li}) = 6.941 \text{ g mol}^{-1}$
Find whether it is fcc or bcc.

* submit assignment on ankitagha26@gmail.com
before 19.07.2020. Okul
17/7/2020