1. Determine the boundaries of the first Brillouin zone for potassium which has a bcc structure and a lattice constant of 5.32 Å.

Answer : Calculate the boundaries of brillouin zone for potassium as follows:

The direct lattice boundaries are given as:

$$a_1 = \frac{a}{2}(1,1,1)$$

$$a_2 = \frac{a}{2}(-1,1,1)$$

$$a_3 = \frac{a}{2}(-1,-1,1)$$

Here a is the lattice constant .

Substitute 5.32 $A°$ for a.

$$a_1 = \frac{5.32\ A°}{2}(1,1,1) = (2.66,2.66,2.66)\ A°$$

$$a_2 = \frac{5.32\ A°}{2}(-1,1,1) = (-2.66,2.66,2.66)\ A°$$

$$a_3 = \frac{5.32\ A°}{2}(-1,-1,1) = (-2.66,-2.66,2.66)\ A°$$

Calculate the reciprocal of lattice vector by the relation as follows:

$$b_1 = \frac{2\pi}{a}(1,0,1)$$

$$b_2 = \frac{2\pi}{a}(-1,1,0)$$

$$b_3 = \frac{2\pi}{a}(0,-1,1)$$

Here a is the lattice constant .

Substitute 5.32 $A°$ for a

$$b_1 = \frac{2\pi}{a}(1,0,1) = \frac{2(3.14)}{5.32\ A°}(1,0,1) = (1.18\ ,0\ ,1.18)/A°$$

$$b_2 = \frac{2\pi}{a}(-1,1,0) = \frac{2(3.14)}{5.32\ A°}(-1,1,0) = (-1.18\ ,1.18\ ,0)/A°$$

$$b_3 = \frac{2\pi}{a}(0,-1,1) = \frac{2(3.14)}{5.32\ A°}(0,-1,1) = (0\ ,-1.18\ ,1.18)/A°$$

Answer:

$$a_1 = (2.66,2.66,2.66)$$

$$a_2 = (-2.66,2.66,2.66)\ A°$$

$$a_3 = (-2.66,-2.66,2.66)\ A°$$

$$b_1 = (1.18\ ,0\ ,1.18)/A°$$

$$b_2 = (-1.18\ ,1.18\ ,0)/A°$$

$$b_3 = (0\ ,-1.18\ ,1.18)/A°$$