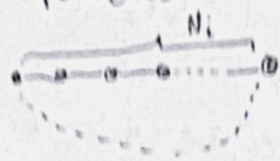


\* <sup>boundary</sup> Born - von Karman condition  $\lambda$  number of electrons per unit cell

Born - von Karman  
The boundary condition is the condition that implies the wavefunction was eigenstates of  $\hat{H}$  are periodic



$$\psi(\vec{r} + \underbrace{N_i \vec{a}_i}_{\substack{\uparrow \\ \text{primitive vector } \vec{a}_i}}) = \psi(\vec{r}) \quad (*)$$

$N_1 N_2 N_3 = N$   
number of primitive cells in the crystal.

the largest translation that's we can go from vector  $\vec{a}_i$

$$(*) \Leftrightarrow e^{i \vec{k} \cdot N_i \vec{a}_i} = 1 \quad \Leftrightarrow \vec{k} = \sum \frac{N_i \vec{a}_i}{N_i} \cdot \vec{b}_i$$

$\Rightarrow$  The smallest volume that contains one point  $\vec{k}$  is

$$\Delta K = \frac{1}{N_1 N_2 N_3} \underbrace{b_1 \cdot (b_2 \times b_3)}$$

$V_{BZ}$  : volume of the Brillouin zone

$$= \frac{V_{BZ}}{N}$$

$\rightarrow$  In the Brillouin zone, number of  $\vec{k}$  points that's we can have

$$\boxed{\frac{V_{BZ}}{\Delta K} = N} \quad \checkmark$$

• In the class, we mentioned about number of valence electrons. what the teachers means is number of valence electrons per unit cell

In total, number of valence electrons that's we have

$$n_e \cdot N_{\text{unit-cell}} \equiv N$$

Inside the Brillouin zone, we have all of  $k$ -points in our  $k$  space, because the points that's outside this volume have the correspondence inside this region.

so that,  
We For each band to full fill, we just need 1 valence electron.

below  
In the class, Lilia showed the Fermi level, we have 3 band, so that if we have more than 6 valence electrons, we will fill the band that's higher than the Fermi level.