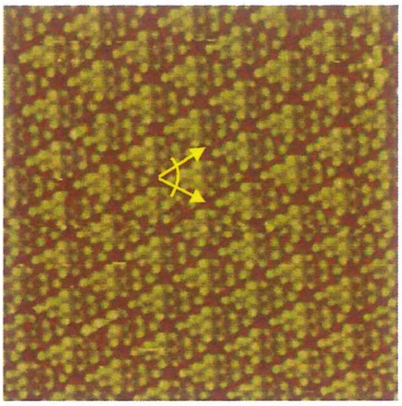
**Question 1: Crystal structure and X-ray scattering**

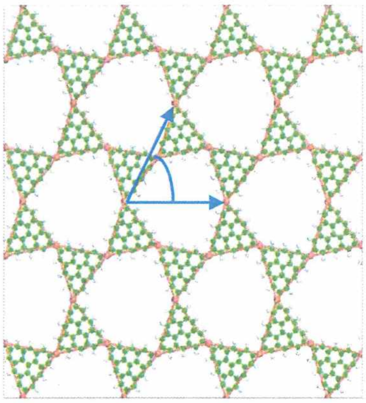
*Note that a rough hand sketch is sufficient, don't spend your time making good-looking drawings!*

1. (10p) Apply the idea of repeating environment to the following 2D patterns, identify the underlying Bravais lattice. Find the relationship between the translation vector **a**, **b**, and the θ between them (say |**a**| = |**b**|, and θ = 90°).

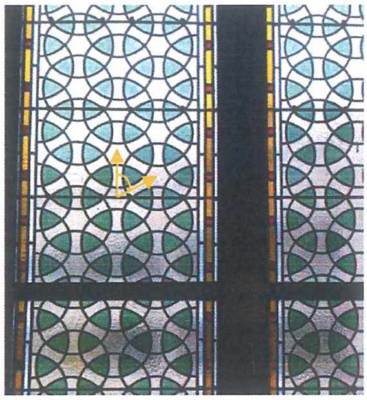
A



B



C



|**a**| = |**b**|, θ = 120° (60°)
hexagonal

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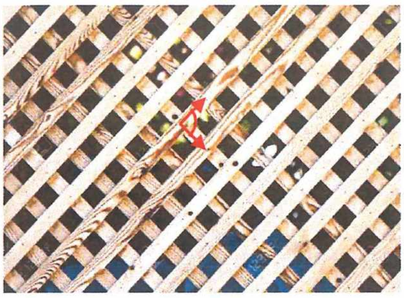
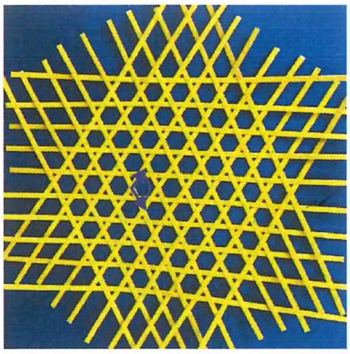
D

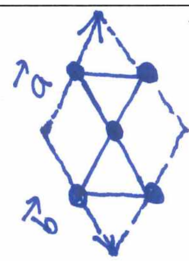


|**a**| = |**b**|, θ = 90°
square

2. (3p) The so-called Kagome lattice shown



|**a**| = |**b**|, θ = 120° (60°)
hexagonal

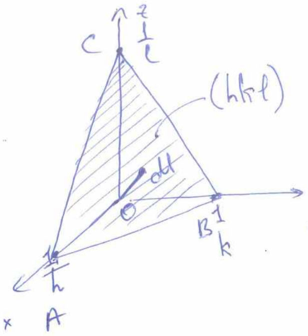


$1 + 4 \times \frac{1}{2} = 3$

below can be viewed as a 2D Bravais lattice. Identify the primitive cell of the Kagome lattice if each crossing point of two bamboo ribbons can be regarded as a lattice site. Count the number of lattice sites in a primitive cell.

3. (5p)
   a) Show that a reciprocal lattice vector $\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$ is orthogonal to the lattice plane ($hkl$).

$G = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 \quad \perp \quad (hkl)$




Any vector $\vec{v} \perp$ to the plane is collinear with normal vector $\vec{n}$ to this plane, means $\perp$ to any two vectors in this plane $\vec{v}_1, \vec{v}_2$.
Vector, perpendicular to $\vec{v}_1$ and $\vec{v}_2$ can be otained as $\vec{v}_1 \times \vec{v}_2$:
Let's choose any 2 vectors in a plane (hkl)

$\vec{v}_1 = \vec{AB} = \left(-\frac{1}{h}, \frac{1}{k}, 0\right)$ and $\vec{v}_2 = \vec{BC} = \left(0, -\frac{1}{k}, \frac{1}{l}\right)$

$A = \left(\frac{1}{h}, 0, 0\right)$
$B = \left(0, \frac{1}{k}, 0\right)$
$C = \left(0, 0, \frac{1}{l}\right)$

$$[\vec{v}_1 \times \vec{v}_2] = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ -\frac{1}{h} & \frac{1}{k} & 0 \\ 0 & -\frac{1}{k} & \frac{1}{l} \end{vmatrix} = \left(\frac{1}{kl}\right)\vec{i} + \left(\frac{1}{hl}\right)\vec{j} + \vec{k}\left(\frac{1}{hk}\right) = \vec{n} \quad \Big| hkl$$

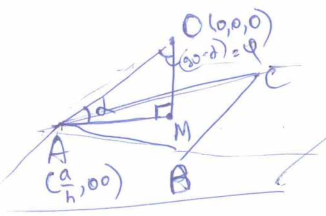
$$\vec{n} = (h, k, l) \Rightarrow \vec{n} \parallel \vec{G}$$

in s.cubic $b_1 \parallel a_1 \parallel x$ $\vec{i}$
$b_2 \parallel a_2 \parallel y$ $\vec{j}$
$b_3 \parallel a_3 \parallel z$ $\vec{k}$

b) Show that the distance $d_{hkl}$ of two lattice planes with Miller indices ($hkl$) is given by $d_{hkl} = 2\pi N / |h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3|$.

Regarding to the image above, let's find $d_{hkl}$ as $OM$

$d = OM$




$AO = \frac{d}{\sin\alpha}$ $\quad \vec{d} = \vec{OM} =$ projection of $\vec{AO}$ on $\vec{n} \Rightarrow$

$\alpha(hkl) \Rightarrow d = |AO|\cos\varphi \Rightarrow \vec{AO}\cdot\vec{n} = \underbrace{|\vec{AO}|}\cdot|\vec{n}|\cdot\cos\varphi$

$AO\cos\varphi = d$

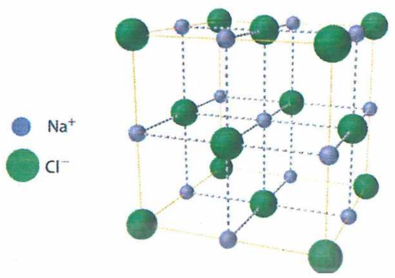
$$d = |\vec{AO}|\cos\varphi = \frac{\vec{AO}\cdot\vec{n}}{|\vec{n}|} = \frac{\left(\frac{a}{h}, 0, 0\right)(h, k, l)}{\sqrt{h^2+k^2+l^2}} = \frac{a}{\sqrt{h^2+k^2+l^2}} = $$

in SC $\quad \vec{b}_1 = \frac{2\pi}{a_1} \to |b_1| = \frac{2\pi}{a_1} \qquad |\vec{G}| = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2}$

$$G = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 = 2\pi\left(\frac{h}{a_1} + \frac{k}{a_2} + \frac{l}{a_3}\right) = \frac{2\pi}{a}\left(h\vec{i} + k\vec{j} + l\vec{k}\right) \Rightarrow \quad = \frac{2\pi}{|h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3|}$$

, N is coming from distance between planes (first order, 2nd etc)

4. (8p) By analyzing the structure factor of NaCl, show the lattice planes $h,k,l$, from which diffraction peaks are expected. (*hint*: NaCl has two kinds of atoms in a cubic system, which can be considered as 4 Na at 000 FCC structure + 4 Cl at ½ ½ ½ FCC structure).




$$F_{hkl} = \left[1 + e^{2\pi i\left(\frac{h+k}{2}\right)} + e^{2\pi i\left(\frac{k+l}{2}\right)} + e^{2\pi i\left(\frac{h+l}{2}\right)}\right] \times \left(f_{Na} + f_{Cl}\, e^{2\pi i\left(\frac{h+k+l}{2}\right)}\right)$$

Invisible $\quad F_{hkl} = 0 \times \left(f_{Na} + f_{Cl}\, e^{2\pi i\left(\frac{h+k+l}{2}\right)}\right)$ if $h,k,l$ mixed $\quad 0$

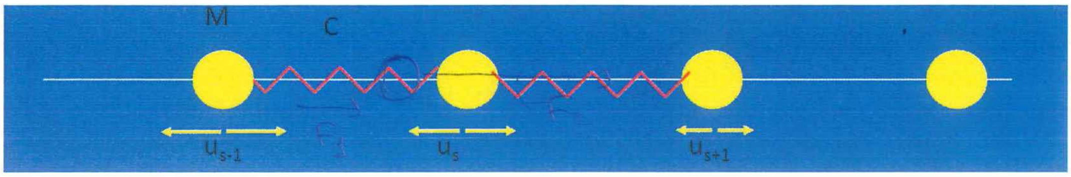
Visible

$F_{hkl} = 4 \times \left(f_{Na} + f_{Cl}\, e^{2\pi i\left(\frac{h+k+l}{2}\right)}\right)$ $=1$ if $h,k,l$ even $\quad 4(f_{Na} + f_{Cl})$

$F_{hkl} = 4 \times \left(f_{Na} + f_{Cl}\, e^{2\pi i\left(\frac{h+k+l}{2}\right)}\right)$ $=-1$ if all odd $\quad 4(f_{Na} - f_{Cl})$

## Question 2: Phonons and thermal properties.

As shown below, consider a linear chain of $N$ atoms all with mass $M$, and the force constant is $C$.



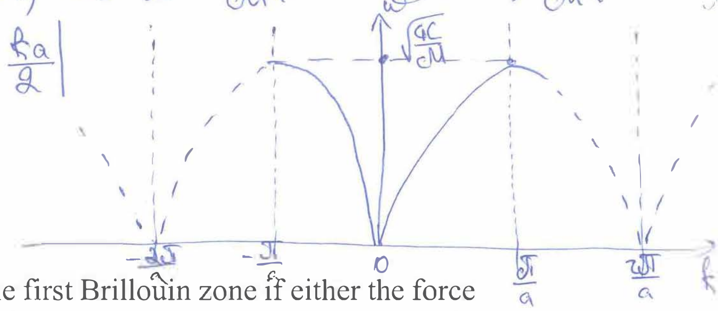

1) (8p) Calculate and sketch the dispersion relation in the first Brillouin zone for the chain above.

$$M\ddot{u}_s = C(u_{s+1}-u_s) + C(u_{s-1}-u_s) = C(u_{s+1}+u_{s-1}-2u_s)$$

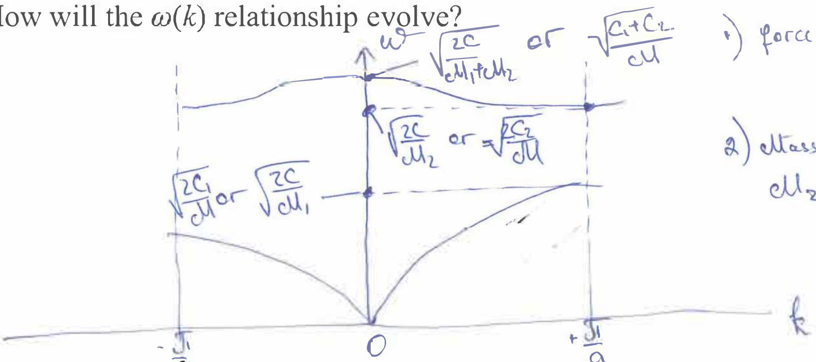
$$u_s = u_0 e^{iska} e^{-i\omega t} \Rightarrow u_{s\pm1} = u_0 e^{iska} e^{\pm ika - i\omega t}$$

$$-M\omega^2 u_s = C(u_s e^{ika} + u_s e^{-ika} - 2u_s) \Rightarrow \omega^2 = \frac{C}{M}\left(2-(e^{ika}+e^{-ika})\right) = \frac{2C}{M}(1-\cos ka)$$

$$\Rightarrow \omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{ka}{2}\right|$$




2) (6p) Sketch the dispersion relationship in the first Brillouin zone if either the force constant or the mass of atoms changes. The mono-atomic chain becomes a di-atomic chain. How will the $\omega(k)$ relationship evolve?



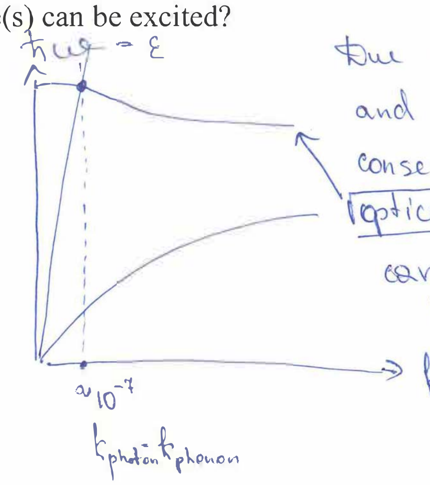

1) force const $C_1, C_2$, $C_2 > C_1$

2) Masses : $M_1, M_2$, $M_2 < M_1$

3) (6p) Suppose a green laser light (532 nm) illuminate the chain. Based on the sketch in the 2), estimate which vibrational mode(s) can be excited?

$\mathcal{E} = ck$ for photons

$k_{photon} = \frac{1}{\lambda} \approx 10^{-7} \left(\frac{1}{cm}\right)$ - very small




Due to energy ($\hbar\omega$) and momentum ($k$) conservation, only $\boxed{\text{optical branches}}$ can be excited by photons

$\frac{d\omega}{dk} = -2kA$

$k = \left(\frac{\omega_0 - \omega}{A}\right)^{\frac{1}{2}}$

4) (6p) Suppose the optical branch has the form of $\omega(K) = \omega_0 - AK^2$ near $K = 0$, where $\omega_0$ is a constant. In three-dimension case, show that $D(\omega) = \left(\frac{L}{2\pi}\right)^3 \frac{2\pi}{A^{\frac{3}{2}}} \sqrt{\omega_0 - \omega}$ for $\omega < \omega_0$, and $D(\omega) = 0$, for all $\omega > \omega_0$.

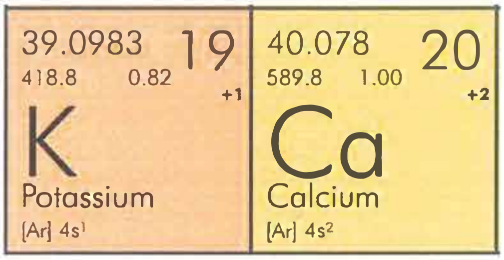
$D(\omega) = \frac{dN}{d\omega} = \frac{dN}{dk}\cdot\frac{dk}{d\omega} = \frac{dN}{dk}\cdot\frac{1}{\frac{d\omega}{dk}}$; $N = \frac{4\pi k^3}{3(2\pi)^3} L^3 \Rightarrow \frac{dN}{dk} = \frac{\cancel{3}\cdot 4\pi k^2 L^3}{\cancel{3}(2\pi)^3}$

$\Leftrightarrow \frac{2k^2}{(2\pi)^2} L^3 \cdot \frac{1}{2kA} = \frac{L^3}{2\pi^2}\cdot\frac{k}{A} = \left(\frac{L}{2\pi}\right)^3 \cdot \frac{2\pi}{A^{\frac{3}{2}}}\sqrt{\omega_0 - \omega}$

$\sqrt{\omega_0 - \omega}$ = real, $\omega < \omega_0$ ; im, $\omega > \omega_0$ $\rightarrow$


**Question 3: Free electrons in potassium and calcium**

Consider two crystals: K (1 valence $e$) and Ca (2 valence $e$). Both are 3D simple cubic. Suppose we can slice the single crystals and isolate atomic planes, both K and Ca can form 2D square lattices of constant $a$ and $b$, respectively




1) (6p) Calculate the 3D density of state ($D_{3D}(E)$) and 2D density of states ($D_{2D}(E)$), We assume the size of the specimen is $L^3$ and electron mass is $m_e$. ($L = N_x a$ or $N_x b$ for K and Ca, respectively).

$DOS(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{dN}{dk}\cdot\frac{dk}{d\varepsilon}$; $N = \frac{2\cdot V}{V_s}$; $\varepsilon = \frac{\hbar^2 k^2}{2m}$; $\frac{d\varepsilon}{dk} = \frac{\cancel{2}\hbar^2 k}{\cancel{2}m}$

3D:

$N = 2\frac{4\pi k^3}{3(2\pi)^3} L^3$

$\frac{dN}{dk} = \frac{8\cdot 3\pi k^2}{3\cdot 8\cdot \pi^3}\cdot L^3$

$DOS(k) = \frac{k^2 L^3}{\pi^2}\cdot\frac{m}{\hbar^2 k} = \frac{L^3}{\pi^2}\cdot\frac{mk}{\hbar^2}$

$DOS(\varepsilon) = \frac{L^3 m}{(\pi\hbar)^2}\cdot\frac{\sqrt{2m\varepsilon}}{\hbar} \sim \sqrt{\varepsilon}$

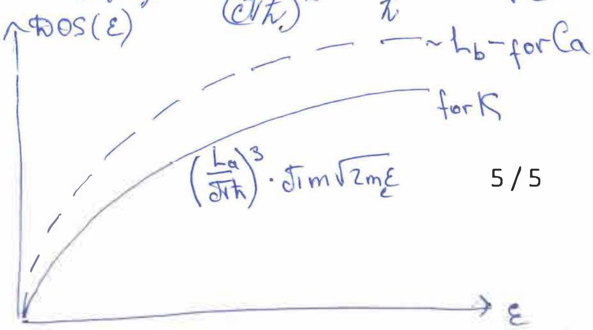
2D:

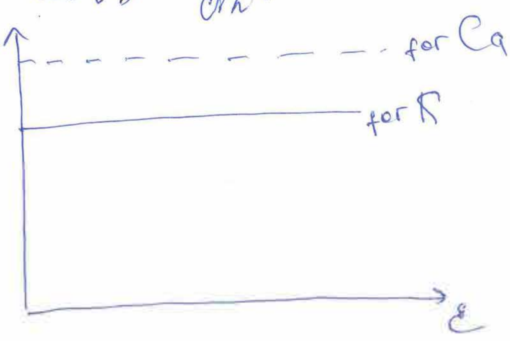
$N = 2\frac{\pi k^2}{(2\pi)^2} L^2$

$\frac{dN}{dk} = \frac{2k L^2}{2\pi}$

$DOS(k) = \frac{L^2}{\pi}k\cdot\frac{m}{\hbar^2 k} = \frac{L^2 m}{\pi\hbar^2}$

$DOS(\varepsilon) = \frac{L^2 m}{\pi\hbar^2}$ = const

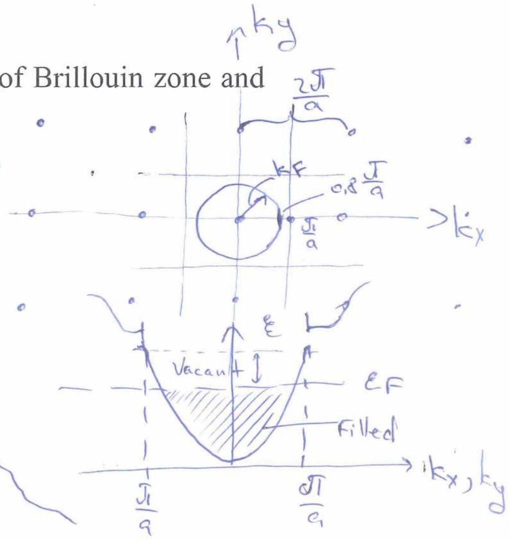


2) (12p)

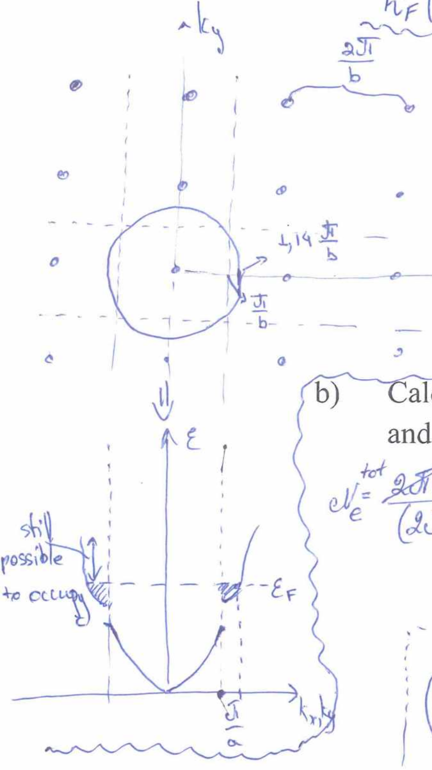
a) Argue why both of them are metals (use the concept of Brillouin zone and Fermi surface).

$k_F(K) \approx 0{,}8\frac{\pi}{a}$, $k(BZ\ edge) = \frac{\pi}{a}$ $\Longrightarrow$




$k_F(Ca) \approx 1{,}12\frac{\pi}{b}$

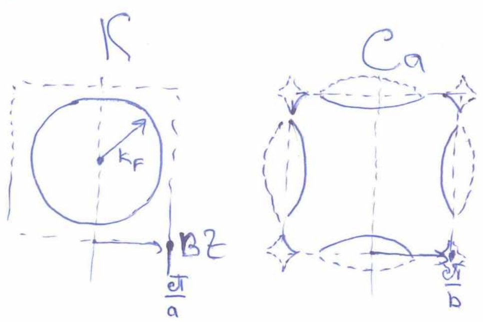
$\Longleftarrow$ $k(BZ\ edge) = \frac{\pi}{b}$




b) Calculate and sketch the size and shape of the Fermi surface for the 2D K and Ca (assume no modification due to the periodic potential of $K^+$ and $Ca^+$).

$N_e^{tot} = \frac{2\pi k_F^2 L^2}{(2\pi)^2} = NZ$ $\quad k_F^2 = \frac{2\pi N Z}{L^2} = \frac{2\pi N Z}{N a^2} \Rightarrow \sqrt{\frac{2Z}{\pi}}\cdot\frac{\pi}{a} = k_F(K) = \sqrt{\frac{2}{\pi}}\cdot\frac{\pi}{a} \approx 0{,}8\frac{\pi}{a}$

$\sqrt{\frac{2Z}{\pi}}\cdot\frac{\pi}{b} = k_F(Ca) = \sqrt{\frac{4}{\pi}}\cdot\frac{\pi}{b} \approx 1{,}12\frac{\pi}{b}$




3) (8p) Suppose the scattering time $\tau$ is identical for K and Ca. From Drude's model briefly compare the difference between 2D K and Ca in electrical conductivity and thermal conductivity $K = \frac{1}{3} c_{el} v^2 \tau$, and their ratio $K/\sigma T$ (which is called the Wiedemann-Franz law).

$$C_{el} = \frac{\pi^2 n k_B^2}{2E_F} T \ (\mathrm{JK^{-1}m^{-3}}), \quad \vec{j} = \frac{ne^2\tau}{m_e}\vec{E}$$

$v$ is the velocity of electron, $n = N/V$, $mv_F^2 \approx 2E_F$, where $v_F$ is the Fermi velocity.

$\sigma = \frac{ne^2\tau}{m} = ne\mu$, $n = \frac{Q}{V} = \frac{N_e}{(L)^2}$ $\quad n(K) = \frac{1}{a^2}$, $n(Ca) = \frac{2}{b^2}$

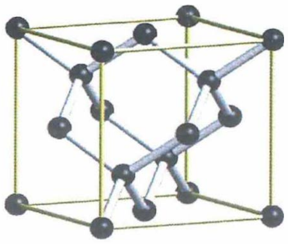
$\boxed{\frac{\sigma_K}{\sigma_{Ca}} = \frac{n_K}{n_{Ca}} = \left(\frac{b}{2a}\right)^2}$ $\quad K = \frac{1}{3}\frac{\pi^2 n k_B^2}{\cancel{2E_F}}T\cdot\cancel{v_F^2}\tau \quad (v_F^2 \sim 2E_F\frac{1}{m}) \quad = \frac{1}{3}\frac{\pi^2 n k_B^2 T\tau}{m}$

$\frac{K(K)}{K(Ca)} = \frac{n_K}{n_{Ca}} = \left(\frac{b}{2a}\right)^2$

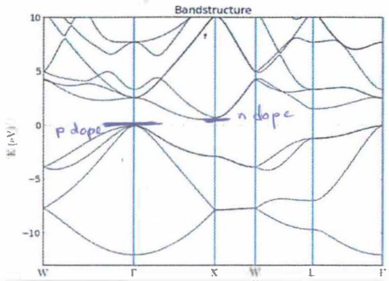
Ratio $\frac{K}{\sigma T} = \frac{\frac{1}{3}\pi^2 \cancel{n} k_B^2 T \cancel{\tau}\cdot\cancel{m}}{\cancel{m}\cdot\cancel{n}e^2\cancel{\tau}} = $ const for any metal, the same.

## Question 4: Semiconductor and superconductivity

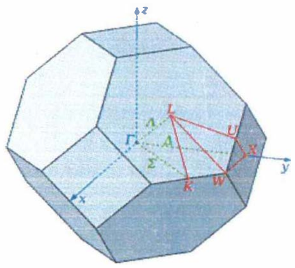
Silicon (Si) is arguably the most important material of the last century, which is frequently referred as the Silicon age.



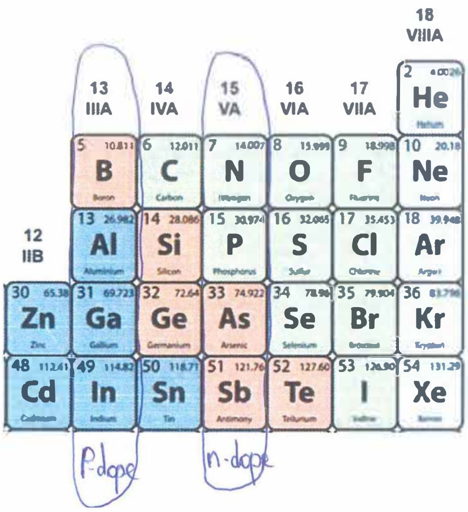
Crystal Structure




$E\,(k)$ relationship of Silicon

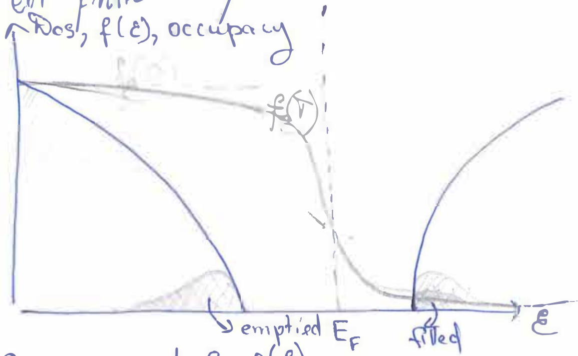



Wigner-Seitz cell in the K space




1) (4p) Silicon has fully-filled valence bands and a band gap > 1eV. Briefly explain how can the intrinsic carriers, electron $n$ and hole $p$, be created in Si at a finite temperature.

At finite temperature T>0K



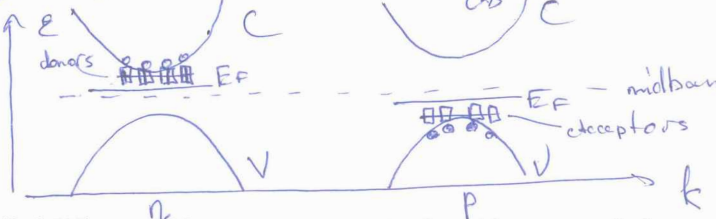

Occupacy = DOS × f(E)

Occupacy is defined as DOS · f(E). At T=0, f(E) is = 1 up to $E_F$ and = 0 after, which, multiplied by DOS, gives you fully filled states before $E_F$ and no allowed in conductance band. But as T>0, the f(E) is „blured" around $E_F$, which leads in DOS·f(E) empties some states in zones. You can consider that as at the finite T, some $e^-$ or $h^+$ statistically can have higher energy, so may leave their potential well.

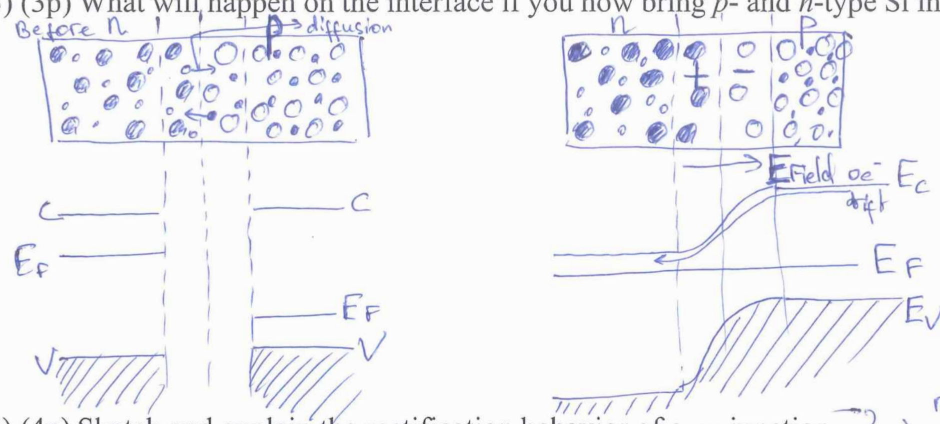
2) (4p) From the periodic table shown above, choose the elements for $p$- and $n$-type doping in Si, draw the schematic diagrams at the band edge (for $p$- and $n$-type). And identify the locations of the impurity bands in the Wigner-Seitz cell for $p$- and $n$-type dopings.

Please, regard to the picture of E(k) and periodic table. All 3-valent atoms can be p-dopings and all 5-valent — n-doping. The most common are n: $P^+$ $As^+$ and p: $B^-$.

Schematic:

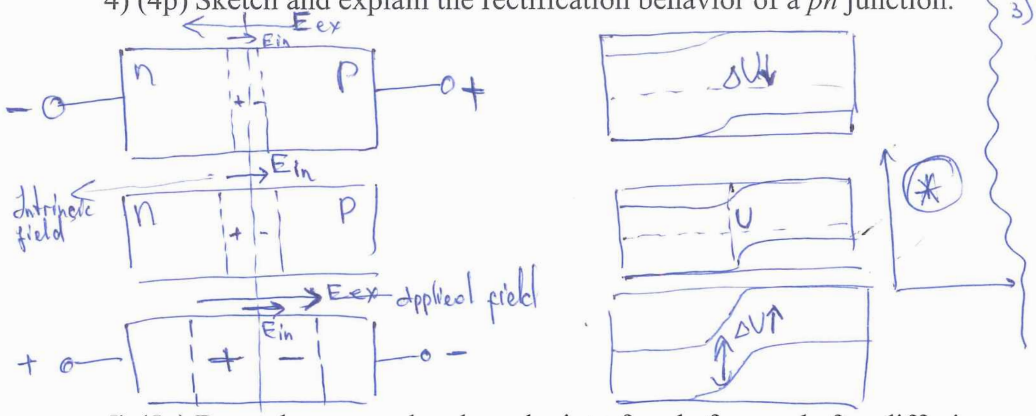



3) (3p) What will happen on the interface if you now bring $p$- and $n$-type Si in contact?

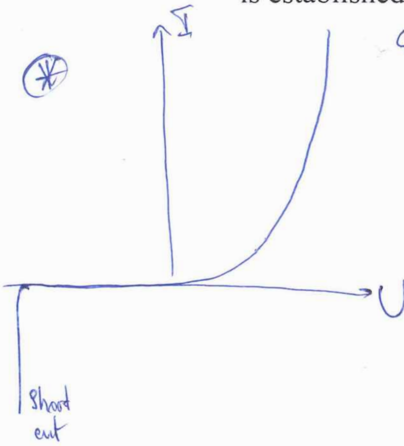



1) Once in contact → free $e^-$ and $h^+$ start moving to each other in the direction of $\nabla n$, so $e^-$ to p region and $h^+$ to n region.
2) As $e^-$ and $h^+$ left their ions and recombinated, the E field built up on the contact region.
3) As $E_c$ and $E_v$ bended, the E field helps non major carriers move in the direction of lowering potential — it's drift, and direction is opposite to diffusion.
4) Once they are compensated, the $\nabla$d equil. is set

4) (4p) Sketch and explain the rectification behavior of a $pn$ junction.



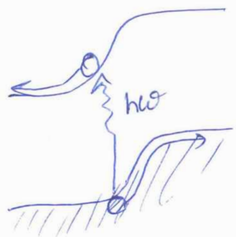

5) (5p) Draw the energy levels at the interface before and after diffusive equilibrium is established. Based on the energy diagram explain how a solar cell works.




4) Rectification: ∿∿∿ → ⌒⌒⌒ p-n junction will conduct only half of period of an alternating current.

As shown on diagrams, U applied directly and reverse either lower or enhancing potential barrier for carriers. It results to practical use of p-n junction as a rectifier, as it can conduct current when − to n and + to p and can not vice versa.

5)




Photon excites carriers on the interface creating an $e^-$-$h^+$ pair, then due to a contact's bands bending, carriers will move withing the band in order to min. their energy, so carriers will accum. on opp. sides of p-n element.

6) (4p) With very strong p doping, when dopant replaced 9% of Si, superconductivity was discovered at 0.35 K. What are the two hallmark physical properties to be expected for T < 0.35 K?

$R(T=0)=0$

$B_{in}(T=0)=0$

---------------------------------- End of Answersheet ----------------------------------