#3-1

Given a) CsCl $[100]$ direction

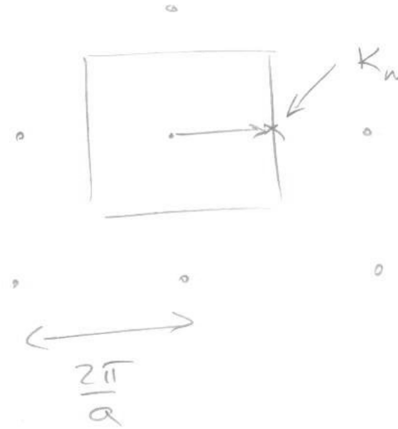
b) Ni $[111]$ — " —

Wanted: K_{max} $[\mathring{A}^{-1}]$

Solution: P. 81: CsCl $a = 4.12\ \mathring{A}$

CsCl: Simple cubic lattice with basis $\bar{0}$ and $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

Reciprocal lattice: S.C. with $\bar{b}_1 = \frac{2\pi}{a}\hat{x}$ etc.

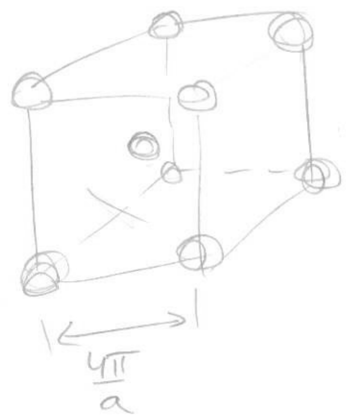


$K_{max}[100] = \frac{\pi}{a} = \frac{\pi}{4.12}\ \mathring{A}^{-1} =$

$= \underline{\underline{0.763\ \mathring{A}^{-1}}}$

b) Ni: fcc, $a = 3.52\ \mathring{A}$ (cover)

Reciprocal lattice: bcc with lattice param. $\frac{4\pi}{a}$



Nearest neighbor along $[111]$ is in center

$\Longrightarrow$ K_{max}-plane of 1:st B.Z. intersects at $\frac{1}{4}$ x space diagonal =

$= \frac{1}{4} \cdot \sqrt{3} \cdot \frac{4\pi}{a} = \frac{\sqrt{3}\,\pi}{a} =$

$= \frac{\sqrt{3} \cdot \pi}{3.52}\ \mathring{A}^{-1} = \underline{\underline{1.546\ \mathring{A}^{-1}}}$

#3-2

Given: Cu, $v_s = 4700$ m/s Cu: fcc, $a_{Cu} = 3.61$ Å

Model with interaction between nearest crystal-planes

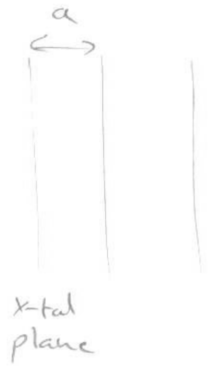
Wanted: ω_{max} for longitudinal lattice vib. in [100]-dir.

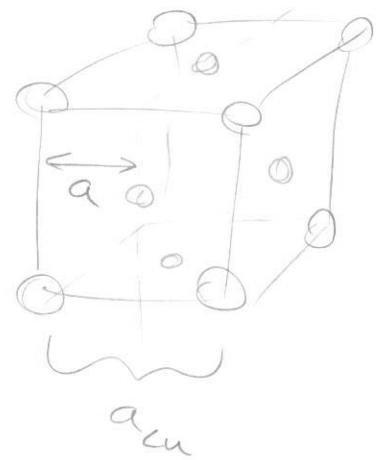
Solution: 1-dim. model with n.n. interaction:

$$\omega(K) = \underbrace{\sqrt{\frac{4C}{M}}}_{\omega_{max}} \left|\sin\frac{Ka}{2}\right|$$

$$v_s = \left.\frac{\partial\omega}{\partial K}\right|_{K\to 0} = \frac{a}{2}\cdot\sqrt{\frac{4C}{M}} = \frac{a}{2}\cdot\omega_{max}$$

What corresponds to a in this model?





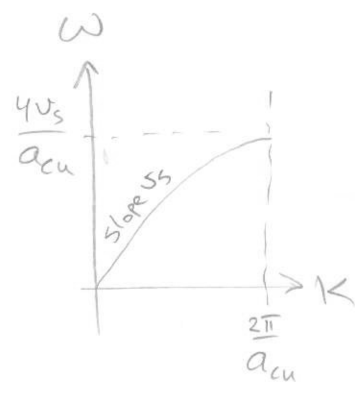
Nearest planes in [100]-direction

$$\Longleftrightarrow \quad a = \frac{a_{Cu}}{2} \quad \Longrightarrow \quad \omega_{max} = \frac{2v_s}{a} = \frac{4v_s}{a_{Cu}}$$

$$\omega_{max} = \frac{4\cdot 4700 \text{ m/s}}{3.61\cdot 10^{-10}\text{ m}} = \underline{\underline{5.2\cdot 10^{13}\ s^{-1}}}$$

$$K_{max}\cdot\frac{a}{2} = \frac{\pi}{2}$$

$$\Rightarrow K_{max} = \frac{\pi}{\left(\frac{a_{Cu}}{2}\right)} = \frac{2\pi}{a_{Cu}} = \underline{\underline{1.74\ \text{Å}^{-1}}}$$



$\boxed{\#3\text{-}3}$ Given:

Al, [100]-dir.

Wanted:

$v_g\,(\omega = 3\cdot 10^{13}\ \mathrm{rad/s})$

Solution: $v_g = \dfrac{\partial\omega}{\partial K}$; From fig: $\dfrac{\partial\omega}{\partial\left(\frac{K}{K_{max}}\right)} = \begin{cases} \dfrac{5.7}{0.65} & (L) \\ \dfrac{3.2}{1.0} & (T) \end{cases}$

$[10^{13}\ \mathrm{rad/s}]$

What is K_{max}?

Al: fcc, $a = 4.05$ Å

rec. lattice: bcc with lattice param. $\dfrac{4\pi}{a}$

$K_{max} = \{[100]\text{-direction, intersected halfway}\} =$

$= \dfrac{1}{2}\cdot\dfrac{4\pi}{a} = \dfrac{2\pi}{a}$

$10^{13}\cdot 10^{-10}$

$\Rightarrow v_g^L = \dfrac{5.7}{0.65}\cdot\dfrac{4.05}{2\pi}\cdot 10^3\ \mathrm{m/s} \approx 5600\ \mathrm{m/s}$

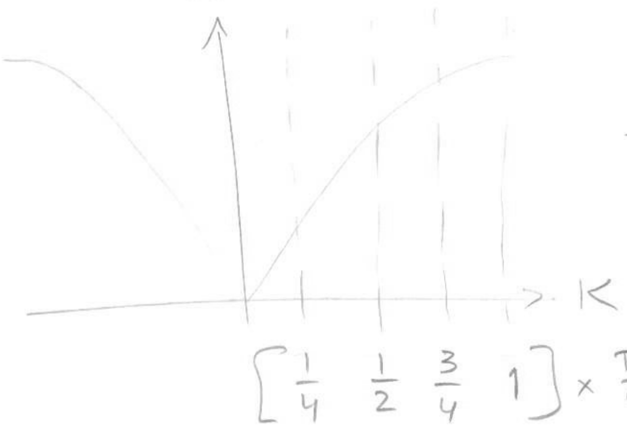
$v_g^T = \dfrac{3.2}{1.0}\cdot\dfrac{4.05}{2\pi}\cdot 10^3\ \mathrm{m/s} \approx 2100\ \mathrm{m/s}$

$$\boxed{v_g = \frac{\partial\omega}{\partial\left(\frac{K}{K_{max}}\right)}\cdot\frac{1}{K_{max}}}$$

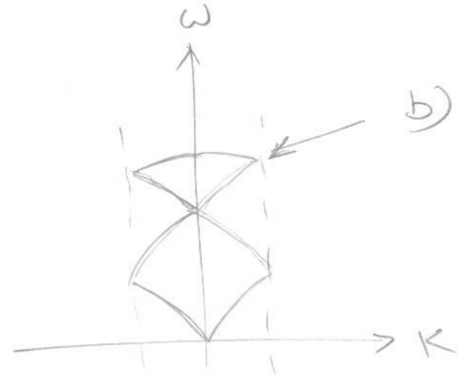
#3-4) Given: Start with monoatomic, one-dim. crystal

$$\omega = \omega_{max} \left| \sin \frac{Ka}{2} \right|$$

a) Construct $\omega(K)$ for 4 atoms/cell (unchanged physical)



$\Longrightarrow$



1 acoustic

3 optical branches

b) Given: ω_{max} (monoatomic)

Wanted: ω_{max} (4 at/cell, @ K_{max})

Solution: This corresponds to the point marked b)

which has a value of ω

corresponding to

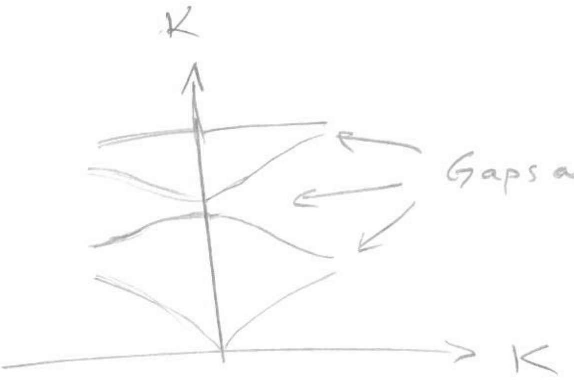
$$\omega = \omega_{max} \cdot \left| \sin \frac{\left(\frac{3\pi}{4a}\right) a}{2} \right| =$$

$$= \omega_{max} \cdot \sin\left(\frac{3\pi}{8}\right) =$$

$$= \underline{0.924 \cdot \omega_{max}}$$

c) Slightly different M's

$\Downarrow$



#3-5

Given: 1-dim, monoatomic lattice, lattice param. a

mass M

harmonic vib.

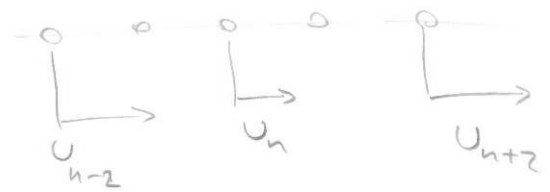
a) Atoms interact only if $d = x_1 - x_2 < d_{max}$

Show: This leads to linear dispersion, $\omega \propto K$

for long wavelengths ($\lambda \to \infty$)

i.e. $K \to 0$

Solution:



$$M \cdot \ddot{u}_n = C_1 \cdot (u_{n+1} - u_n) - C_1 (u_n - u_{n-1}) +$$

$$+ C_2 \cdot (u_{n+2} - u_n) - C_2 (u_n - u_{n-2}) + \dots$$

until distance for interaction too long

Ansatz: $u_n = A \cdot e^{i(Kna - \omega t)}$ $\quad (x = na)$

$$\ddot{u}_n = -\omega^2 u_n$$

$$u_{n+1} = e^{iKa} u_n \quad \text{etc.}$$

$$u_{n+2} = (e^{iKa})^2 u_n$$

$$-M\omega^2 u_n = -2u_n C_1 \overbrace{(\cos Ka - 1)}^{(2\sin^2 \frac{Ka}{2})} - 2u_n C_2 (\cos 2Ka - 1) - \dots$$

$$M\omega^2 = 2 \sum_{p=1}^{\text{range}} C_p \cdot [1 - \cos(pKa)]$$

$$\cos(pKa) \approx 1 - \frac{(pKa)^2}{2}$$

$K \to 0$

$p_{max} a = d_{max}$ finite

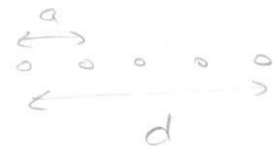
$$\Rightarrow \quad M\omega^2 = 2 \cdot \frac{(Ka)^2}{2} \sum_{p=1}^{\text{range}} C_p \cdot p^2$$

$$\omega = a \cdot K \cdot \sqrt{\frac{\sum_{p=1} C_p \cdot p^2}{M}}, \quad \text{i.e.,} \quad \omega \propto K$$

#3.5 b

Force constant

Given: $C \propto \frac{1}{d^2} \sim \frac{1}{p^2}$ where $p \cdot a = d$



$$\boxed{\frac{x}{2}\left(\pi - \frac{x}{2}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2}\left(1 - \cos nx\right)}$$

$0 \leq x \leq 2\pi$

Wanted: $\omega(K)$; $\lim_{K \to 0}$

Solution: From a) we have $M\omega^2 = 2 \sum_{p=1}^{\infty} C_p \left[1 - \cos(pKa)\right]$

Let $C_p = C_0 \cdot \frac{1}{p^2}$

$$M\omega^2 = 2C_0 \sum_{p=1}^{\infty} \frac{1}{p^2}\left[1 - \cos(pKa)\right] = 2C_0 \cdot \frac{Ka}{2}\left(\pi - \frac{Ka}{2}\right)$$

$$\omega = \sqrt{\frac{C_0}{M}} \cdot \left[Ka\left(\pi - \frac{Ka}{2}\right)\right]^{1/2}$$

$$K \to 0 \quad (\lambda \to \infty) \implies \underline{\underline{\omega = \sqrt{\frac{C_0}{M} \cdot a \cdot \pi} \cdot K^{1/2}}}$$

i.e. $\omega \propto \sqrt{K}$

c) Since experiments show

$\omega \propto K$ at low K

$\implies$ interatomic forces do not have infinite range

(Screening effects)

#4-1

Given Monoatomic, one-dim. crystal N atoms

Interaction only n.n., longitudinal

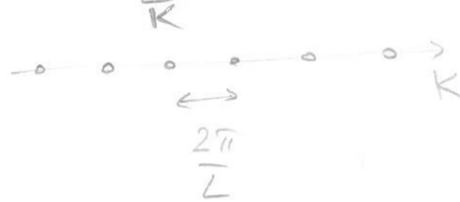
Show:

$$U = \int_0^{\omega_{max}} \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} \cdot \frac{2N}{\pi\sqrt{\omega_{max}^2 - \omega^2}}\, d\omega$$

Solution The model has

$$\omega = \underbrace{\sqrt{\frac{4C}{M}}}_{\omega_{max}} \left| \sin\frac{Ka}{2} \right|$$

$$\sum_K \rightarrow \frac{L}{2\pi}\int dK$$



$$U = \sum_K \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} =$$

$$= \frac{L}{2\pi}\int_0^{K_{max}} 2 \cdot \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1}\, dK =$$

pos and neg. K

$$\frac{d\omega}{dK} = \frac{a}{2} \cdot \omega_{max} \cdot \cos\frac{Ka}{2}$$

$$\sin^2 + \cos^2 = 1$$

$$\cos = \sqrt{1 - \sin^2} = \sqrt{1 - \left(\frac{\omega}{\omega_{max}}\right)^2}$$

$$\frac{d\omega}{dK} = \frac{a}{2} \cdot \sqrt{\omega_{max}^2 - \omega^2}$$

$$= \frac{N \cdot a}{\pi}\int_0^{\omega_{max}} \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} \cdot \frac{2}{a}\frac{d\omega}{\sqrt{\omega_{max}^2 - \omega^2}}$$

$$= \int_0^{\omega_{max}} \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} \cdot \frac{2N\, d\omega}{\pi\sqrt{\omega_{max}^2 - \omega^2}}$$

#4-2

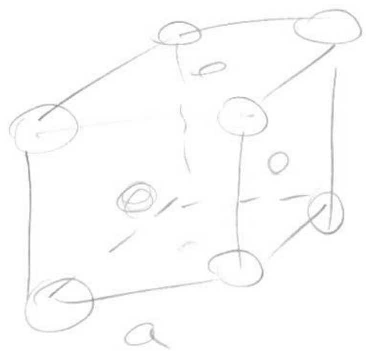
Given: $\omega_D \Longleftrightarrow \lambda = 2d$ where d = distance between nearest neighbors

Cu: fcc, $a = 3.6\ \text{Å}$

$v_s = 3560\ m/s$

Wanted: Θ_D

Solution: $K = \frac{2\pi}{\lambda} \Longrightarrow K_D = \frac{\pi}{d}$



Nearest neighbors: along surface diag.

$$d = \frac{1}{2}\sqrt{2}\,a = \frac{a}{\sqrt{2}}$$

$$\Longrightarrow K_D = \frac{\sqrt{2}\,\pi}{a}$$

$$\omega_D = v_s \cdot K_D = v_s \cdot \frac{\sqrt{2}\,\pi}{a}$$

$$\hbar\omega_D = k_B\Theta_D \Longrightarrow \boxed{\Theta_D = \frac{\hbar}{k_B} v_s \cdot \frac{\sqrt{2}\,\pi}{a}}$$

With numbers: $$\Theta_D = \frac{1.055\cdot 10^{-34}}{1.38\cdot 10^{-23}} \cdot 3560 \cdot \frac{\sqrt{2}\,\pi}{3.6\cdot 10^{-10}}\ K =$$

$$= \underline{\underline{336\ K}}$$

#4-3 **Given** (Ag)

T (K)	C_v (mJ/mol·K)
3.12	6.92
2.26	3.40
1.62	1.85
1.32	1.28

Wanted: Θ_D

Solution: $C_v \approx 234 \cdot \left(\frac{T}{\Theta_D}\right)^3 n k_B \iff C_v = 1941 \left(\frac{T}{\Theta_D}\right)^3$ J/mol·

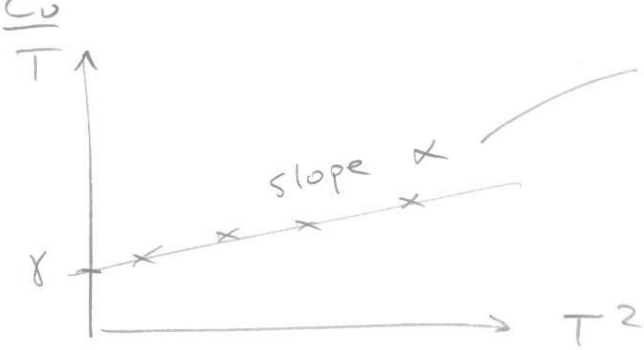
$R = 8.314$ J/mol·K

$R = \underbrace{N_A}_{6.022 \cdot 10^{23}} \cdot \underbrace{k_B}_{1.38 \cdot 10^{-23}}$

But: Electron contrib.

$$\boxed{C_v = \gamma T + \alpha T^3}$$

plot



$\alpha = \left(1.94 \cdot \frac{10^6}{\Theta_D^3}\right)$ mJ/mol·K

From graph: $\alpha = 0.154 = 1.94 \cdot \frac{10^6}{\Theta_D^3}$

$\Longrightarrow \Theta_D = \left(\frac{1.94}{\alpha}\right)^{1/3} \cdot 100 \text{ K} = \underline{\underline{233 \text{ K}}}$

#4-4 Given: 1-dim. crystal, length L

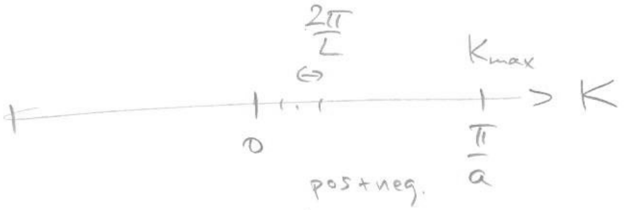
Debye model

Show: $C_v \propto T$ at low T

Solution Debye model: $\begin{cases} \omega = v_s \cdot |K| \\ N = \int_0^{\omega_D} D(\omega)\, d\omega \end{cases}$

$L = N \cdot a$

$\bar{a}_1 = a\hat{x} \quad \bar{b}_1 = \frac{2\pi}{a}\hat{x} \quad$ B.Z. border: $\frac{1}{2}\bar{b}_1 = \frac{\pi}{a}$



pos+neg.

$$D(\omega)d\omega = \frac{L}{2\pi} \cdot 2 \cdot dK = \frac{L}{2\pi} \cdot 2 \cdot \frac{d\omega}{v_s} \qquad \boxed{D(\omega) = \frac{L}{\pi v_s}}$$

$$N = \frac{L}{\pi v_s}\int_0^{\omega_D} d\omega = \frac{L \cdot \omega_D}{\pi v_s} \Rightarrow \boxed{\omega_D = \frac{\pi v_s}{a}}$$

$$\Theta_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar\pi v_s}{k_B a}$$

$$U = \int_0^{\infty} \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} D(\omega)\, d\omega =$$

$$= \int_0^{\omega_D} \frac{L}{\pi v_s} \frac{\hbar\omega\, d\omega}{e^{\hbar\omega/k_BT} - 1}$$

$$C_v = \frac{dU}{dT} = \int_0^{\omega_D} \frac{L}{\pi v_s} \frac{\hbar\omega}{(e^{\hbar\omega/k_BT} - 1)^2} e^{\hbar\omega/k_BT} \cdot \frac{\hbar\omega}{k_BT^2}\, d\omega =$$

$$= \left\{ x = \frac{\hbar\omega}{k_BT} \right\} = \frac{L k_B}{\pi v_s} \frac{k_B T}{\hbar} \int_0^{\Theta_D/T} \frac{x^2 e^x}{(e^x - 1)^2}\, dx$$

$$T \ll \Theta_D \Rightarrow \int_0^{\infty} \Rightarrow C_v \propto T$$

$\boxed{\#4\text{-}5}$ Given: $l_{el} \propto \dfrac{1}{n_{phonons}}$ number of phonons per volume

electron mean free path

Show: $\rho \propto T$ for $T >> \Theta_D$

Solution: $\sigma = \dfrac{ne^2\tau}{m} = \dfrac{ne^2 l_{el}}{m v_F} \Rightarrow \rho \propto \dfrac{1}{l_{el}} \propto n_{phonons}$

$$n_{phonons}(K) = \frac{1}{e^{\hbar\omega(K)/k_BT} - 1}$$

$$\hbar\omega << k_BT \Rightarrow n_{phonons}(K) = \frac{1}{1 + \frac{\hbar\omega}{k_BT} - 1} = \frac{k_BT}{\hbar\omega(K)}$$

$$\Rightarrow \rho \propto n_{phonons}$$

#4-6 **Given**

Inelastic scattering of photons

(visible light: Brillouin-scattering)

Photon velocity $\frac{c}{n}$

Phonon velocity v

Phonon energy << photon energy

Show $\Omega = \frac{2nv\omega}{c} \sin\left(\frac{\theta}{2}\right)$ — photon frequency

Ω: phonon frequency

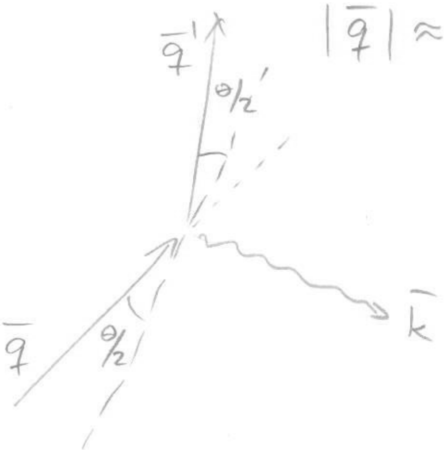
Solution

Energies: photon: $\hbar\omega = h\nu = \frac{h(c/n)}{\lambda} = p\cdot\frac{c}{n} = \hbar\cdot\underbrace{\frac{2\pi}{\lambda}}_{\bar{q}}\cdot\frac{c}{n}$

phonon: $\hbar\Omega << \hbar\omega$

Momentum: $\bar{q} = \frac{2\pi}{\lambda} = \frac{\omega\cdot n}{c}$

$\bar{k} = \frac{\Omega}{v}$



$|\bar{q}| \approx |\bar{q}'|$ (energies much larger than phonon energy)

Eq (Momentum):

$2|\bar{q}|\cdot\sin\left(\frac{\theta}{2}\right) = \bar{k}$

$2\cdot\frac{\omega n}{c}\cdot\sin\left(\frac{\theta}{2}\right) = \frac{\Omega}{v}$

$\Longrightarrow \boxed{\Omega = \frac{2nv\omega}{c}\cdot\sin\left(\frac{\theta}{2}\right)}$

#4-7 Given: Audible sound frequency 20-20 kHz

Cu: $v_s = 3560$ m/s

lattice param. $a = 3.61$ Å

Wanted: Explain why sound is propagating much faster than heat in Cu.

Solution

The wavelength of sound:

$$\underline{v_s = f \cdot \lambda} = \frac{\omega}{2\pi} \cdot \lambda \iff \omega = v_s \underbrace{\left(\frac{2\pi}{\lambda}\right)}_{K}$$

$$\lambda = \frac{v_s}{f} \sim \frac{3000 \text{ m/s}}{3000 \text{ s}^{-1}} \sim \underline{\underline{1 \text{ m}}}$$

$$K_{sound} = \frac{2\pi}{\lambda} \sim \underline{\underline{6 \text{ m}^{-1}}}$$

Maximum K: $K_{max} \sim \frac{\pi}{a} \sim \frac{3.14}{3.61 \cdot 10^{-10}} \text{ m}^{-1} \sim \underline{\underline{10^{10} \text{ m}^{-1}}}$

$K_{sound} << K_{max} \implies$ no Umklapp processes

$$\langle n \rangle = \frac{1}{e^{\hbar\omega/k_BT} - 1} \approx \frac{1}{\frac{\hbar\omega}{k_BT}} = \frac{k_BT}{\hbar\omega}$$

Thermal K: $\langle n \rangle = 1 \qquad k_BT = \hbar\omega = \hbar v_s K_T$

$$K_T = \frac{k_BT}{\hbar v_s} = \frac{0.025 \text{ eV}}{6.58 \cdot 10^{-16} \text{ eV}\cdot\text{s} \cdot 3560 \text{ m/s}} =$$

$$= 1.1 \cdot 10^{10} \text{ m}^{-1} \sim K_{max}$$

$\iff$ all K's available for thermal conduction at R.T.

Most K's larger than $\frac{G}{4} \implies$ lots of Umklapp

$\implies$ diffusive