F7 Värmekap. del 2 & Kristallbindning

Mån LV3

{ Kap. 5 i Kittel! }

Termisk ledning: $\kappa = \frac{1}{3} C \cdot V \cdot L$

- C = värmekap.
- V = fononhastighet
- L = medelfriväglängd

Lågt T → $\kappa \sim C \sim T^3$

Högt T → $\kappa \sim C \sim L \sim \frac{1}{T^x}$

Umklapp: dominerar termisk resistivitet vid höga temp.

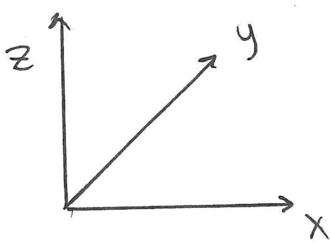
Einstein: N atomer i kristallen med samma frekvens

↳ Bra antagande vid högt T: $C = 3Nk_B$

↳ Ej rätt vid lågt T

→ Måste ta hänsyn till frekvensfördelningen! (tillstånds-täthet)

Tillståndstäthet i 3D



$N \times N \times N$ atomer (N^3)

$V = L^3$ (volym, ej hastighet)

$L = N \cdot a$

Periodiska RV → $\exp(i\bar{k}\bar{L}) = 1$

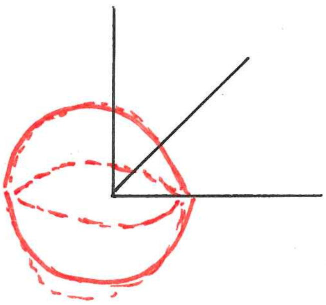
~~$\int \exp(i\bar{k}_x\bar{L}) = 1$~~

$$\left.\begin{aligned} &\exp(ik_xL) \\ &\exp(ik_yL) \\ &\exp(ik_zL) \end{aligned}\right\} = 1$$

$$\Rightarrow \left\{\begin{array}{l} k_x = \dfrac{2\pi}{L} n_x \\[2mm] k_y = \dfrac{2\pi}{L} n_y \\[2mm] k_z = \dfrac{2\pi}{L} n_z \end{array}\right. \qquad n_x; n_y; n_z = 0, \pm 1, \pm 2, \ldots$$

Tillståndstäthet i k-rummet: $N_k = \dfrac{1}{\left(\frac{2\pi}{L}\right)^3}$

$$D(\omega)d\omega = 3N(k)d^3k$$



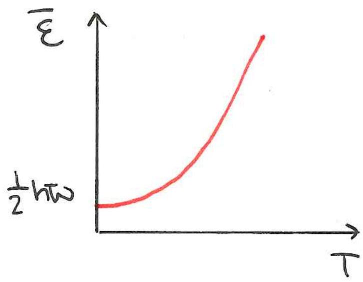
$$D(\omega)d\omega = 3\frac{V}{8\pi^3}d^3k$$

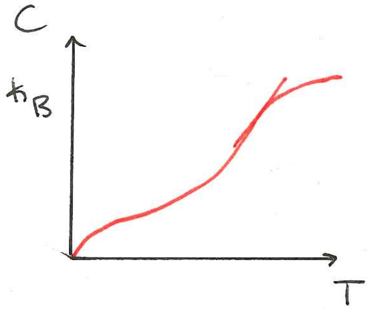
Volyms~~enhet~~element: $4\pi k^2 dk$

$$\to D(\omega)d\omega = \frac{3Vk^2}{2\pi^2}dk \to D(\omega) = \frac{3Vk^2}{2\pi^2}\left(\frac{dk}{d\omega}\right)$$

$$E = \int_0^\infty \left(\frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_BT}} - 1}\right) D(\omega)d\omega$$

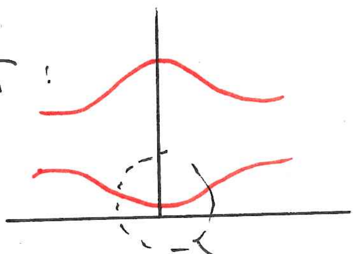
För en fonon:





Högt T: $C(T\ \text{hög}) = 3Nk_B$ $\left\{\begin{array}{l}2 \text{ transversella} \\ 1 \text{ longitudinell}\end{array}\right.$

Låg T:



$$\omega = v_s k \to k = \frac{\omega}{v_s} \to \boxed{\frac{dk}{d\omega} = \frac{1}{v_s}}$$

Debye: V_s samma för alla moder och gäller upp till en viss frekvens, ω_D (och vågtal, k_D)

$$D(\omega) = \frac{3Vk^2}{2\pi^2}\frac{dk}{d\omega} \rightarrow D(\omega) = \frac{3V\omega^2}{2\pi^2 V_s^3} \quad \{\text{enl. Debye}\}$$

Per definition är totala antalet moder 3N:

$$3N = \int_0^{\omega_D} D(\omega)\,d\omega = \int_0^{\omega_D} \frac{3V}{2\pi^2 V_s^3}\omega^2\,d\omega = \frac{3}{2\pi^2 V_s^3}\omega_D^3$$

$$\left\{\begin{array}{ll} \text{Debye-frekvens:} & \omega_D = \sqrt[3]{\dfrac{6N\pi^2 V_s^3}{V}} \\ \text{Debye-vågtal:} & k_D = \dfrac{\omega_D}{V_s} = \sqrt[3]{\dfrac{6N\pi^2}{V}} \\ \text{Debye-temperatur:} & \Theta_D = \dfrac{\hbar\omega_D}{k_D} \end{array}\right\}$$

$$\left\{ \omega = V_s k = a\sqrt{\frac{C}{m}}\,k \right\}$$

$$\left.\begin{array}{l} D(\omega) = \dfrac{3V}{2\pi^2 V_s^3}\omega^2 \\ \omega_D^3 = \dfrac{6N\pi^2 V_s^3}{V} \end{array}\right\} \rightarrow \begin{array}{l} \omega_D^3 \cancel{V}\cdot 3 = 6N\pi^2 V_s^3 \cdot 3 \\ \dfrac{3V}{\pi^2 V_s^3} = \dfrac{6N\cdot 3}{\omega_D^3} \\ \underbrace{\dfrac{3V}{2\pi^2 V_s^3}}_{D(\omega)} = \dfrac{9N}{\omega_D^3} \end{array}$$

$$\rightarrow D(\omega) = \frac{9N}{\omega_D^3}\omega^2$$

$$E = \int_0^\infty \left(\frac{1}{2}\hbar w + \frac{\hbar w}{\exp\left(\underbrace{\frac{\hbar w}{k_B T}}_{*}\right) - 1} \right) D(w)\, dw$$

$$= \frac{9N}{w_D^3} \int_0^\infty \left(\frac{1}{2}\hbar w + \frac{\hbar w}{\exp(*) - 1} \right. w^2\, dw$$

$$= \frac{9N\hbar w_D}{8}) + \frac{9N}{w_D^3} \int \frac{\hbar w}{\exp(*) - 1}\, dw$$

Debyes Nollpunktsenergi

$$C = \frac{dE}{dT} = \frac{9N}{w_D^3} \int \frac{\hbar w^3 \exp\left(\frac{\hbar w}{k_B T^2}\right)}{\left(\exp(*) - 1\right)^2}\, dw$$

$$\begin{cases} \Theta_D = \dfrac{\hbar w_D}{k_B} \\[2ex] x = \dfrac{\hbar w}{k_B T} \\[2ex] x_D = \dfrac{\hbar w_D}{k_B T} = \dfrac{\Theta_D}{T} \end{cases}$$

$$C = 9 N k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{x_D} \frac{x^4 e^x}{(e^x - 1)^2}\, dx$$

Låg T: $x_D \to \infty$, $C \to 9 N k_B \left(\frac{T}{\Theta_D}\right)^3 \frac{4\pi^4}{15}$

$$= \frac{12\pi^4}{5} N k_B \left(\frac{T}{\Theta_D}\right)^3$$

Debyes T^3-lag

Hög T: $x_D \to 0$, $C \to 9 N k_B \left(\frac{T}{\Theta_D}\right)^3 \cdot \frac{1}{3} \left(\frac{\Theta}{T}\right)^3 \to 3 N k_B$

Kristallbindning

Kan klassifiera material enligt bindningstyp! {4 huvudtyper}

Kohesive energi - mått på hur mycket energi för att spjälka upp en kristall i enskilda atomer

Jonkristaller - basen innehåller positiva och negativa joner!

α - Madelungs konstant, experimentellt bestämt

(kolla slides - massa information!)