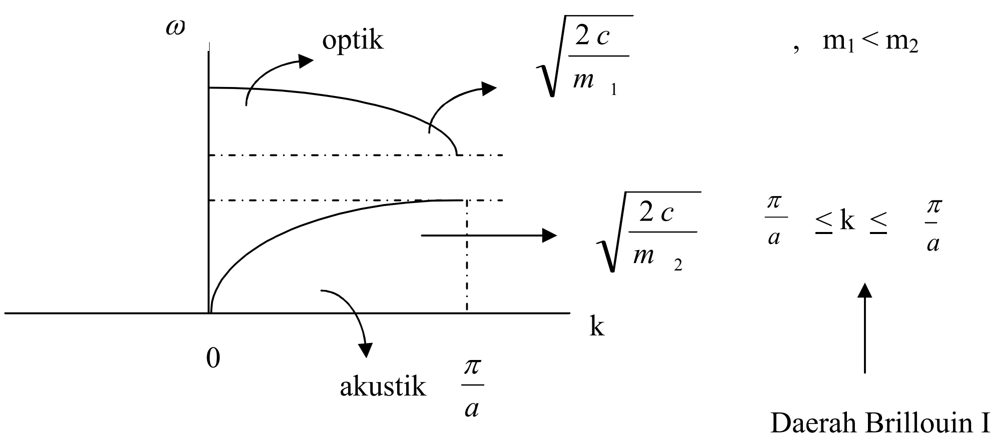
BAB V

THERMAL PROPERTIES (SIFAT TERMAL KRISTAL)

TIK: Untuk menentukan kapasitas panas jenis phonon pada temperatur tinggi dan temperatur rendah menurut model Einstein dan model Debye.

Di dalam Bab IV:

Jika dalam kristal terdapat phonon maka akan terjadi hubungan dispersi (diatomik) yang dinyatakan dengan grafik sebagai berikut:



Sehingga partikel phonon yang mempunyai frekuensi υ menurut kuantum planck

$E = h\upsilon = \hbar\omega$

Energi kristal untuk $k = k_1$

$$U_{k_1, P} = \sum_{p=1}^{3} \langle \eta_{k1,p} \rangle \hbar \omega k_1, p$$

→ Harga ini ditentukan oleh vektor panjang gelombang

→ Jenis polarisasinya

Artinya: setiap harga 1 k kita mempunyai 3 jenis polarisasi (1 longitudinal, 2 transversal)

Secara umum energi kristal untuk k

$$U_{k,P} = \sum_{p} \eta \hbar \omega_{kp}$$

Untuk seluruh nilai k , energi total kristal:

$$U_{Tot} = \sum_{k}^{p} U_{kp} = \sum_{k} \left(\sum_{p} U_{kp} \right)$$

$$U_{Tot} = \sum_{k} \left\{ \sum_{p} \langle \eta_{kp} \rangle \hbar \omega_{xp} \right\}$$

$\langle \eta_{kp} \rangle$ = probabilitas penempatan tingkat energi phonon

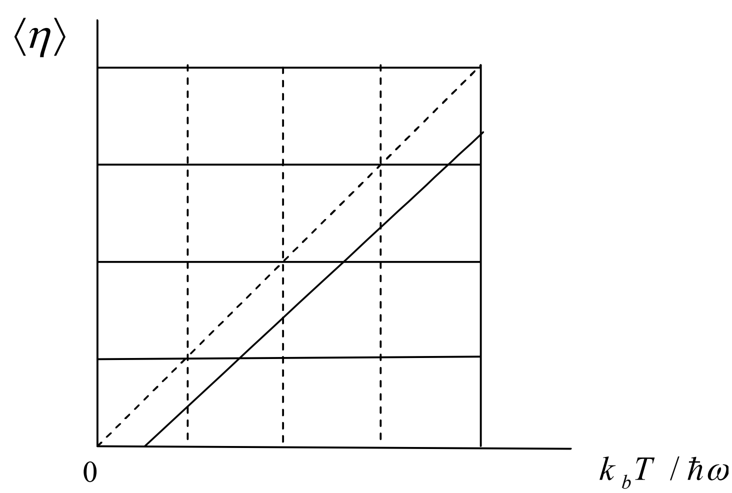
= distribusi planck = peluang pengisian = tingkat energi phonon yang bergantung suhu

$$= \langle \eta \rangle = \frac{1}{e^{\hbar \omega_{kp} / k_b T} - 1}$$

k_b = konstanta Boltzman

= 1,381 x 10^{-23} joule/K

Grafik fungsi distribusi planck



$$U_{Tot} = \sum_{kp} \frac{\hbar \omega_{kp}}{e^{\hbar \omega_{kp} / k_b T} - 1}$$

Untuk temperatur tinggi (T>>), $\frac{\hbar\omega}{k_b T}$ <<1

Ingat $e^{\pm X}$ ⟹ deret ⟹ $1 \pm X \pm X^2 \pm X^3 \pm \ldots$

Maka :

$$e^{\hbar \omega / k_b T} \Rightarrow \text{deret} \Rightarrow 1 + \frac{\hbar \omega}{k_b T} + \left(\frac{\hbar \omega}{k_b T}\right)^2 + \ldots$$

$$U = \sum_{kp} \frac{\hbar \omega_{kp}}{1 + \frac{\hbar \omega_{kp}}{k_b T} - 1}$$

$$U = \sum_{kp} k_b T$$

Sehingga menurut Einstein :

Atom-atom kristal dianggap bergetar satu sama lain di sekitar titik setimbangnya secara bebas. Getaran atomnya dianggap harmonik sederhana yang bebas sehingga mempunyai frekuensi sama ($\upsilon = \frac{\omega}{2\pi}$)

Sehingga di dalam zat padat jika terdapat sejumlah N atom maka ia akan mempunyai 3N osilator harmonik yang bergetar bebas dengan frekuensi (ω).

$$U = \sum_{kp} k_b T = 3N \; k_b T$$

$$c_v = \frac{\partial u}{\partial T} = \frac{d}{dT}\left[3Nk_b T\right] \Rightarrow c_v = 3Nk_b$$

$c_v = 3R$, R= Konstanta universal gas

Model Einstein untuk T >>

$c_v = 3N \; k_b T$ = 3R , sesuai dengan eksperimen dulang dan petit

Untuk T << → $\frac{\hbar \omega}{k_b T}$ >> 1

Bila $\omega_{kp} = \omega \Rightarrow$ model Einstein 3N

Jadi $U = \dfrac{3N\hbar\omega}{e^{\hbar\omega/k_bT} - 1}$

Jadi

$$c_v = \frac{\partial u}{\partial T} = \frac{\partial}{\partial T}\left[\frac{3N\hbar\omega}{e^{\hbar\omega/k_bT}}\right]$$

$$= 3N\hbar\omega\left(-\frac{1}{e^{\hbar\omega/k_bT} - 1}\right)^2\left(\frac{\hbar\omega e^{\hbar\omega/k_b\frac{T}{\hbar\omega}}}{k_bT^2\hbar\omega}\right)/k_bT$$

$$= \frac{3N\hbar\omega}{k_bT^2}\cdot\frac{e^{\hbar\omega/k_bT}}{\left(e^{\hbar\omega/k_bT} - 1\right)^2}$$

$$= \frac{3N\hbar^2\omega^2}{k_bT^2}\cdot\frac{e^{\hbar\omega/k_bT}}{e^{2\hbar\omega/k_bT} - 2e^{\hbar\omega/k_bT} + 1}$$

$$= \frac{3N\hbar^2\omega^2}{k_bT^2}\cdot\frac{1}{e^{\hbar\omega/k_bT-1}}$$

T $<< \Rightarrow \dfrac{\hbar\omega}{k_bT} >> 1 \Rightarrow$ *maka*

$$\boxed{c_v = \frac{3N\hbar^2\omega}{k_bT}.e^{-\hbar\omega/k_bT}}$$

MODEL DEBYE

- Atom-atom dianggap sebagai oscillator harmonis yang <u>tak bebas</u>.

> Gerakan atom-atom yang dipngaruhi oleh atom tetangga.

- Menyempurnakan Model Einstein Terutama : T <<

  Untuk : T << ⟶ υ << ⟶ beberapa pda cabang akuistik

RAPAT KEADAAN

$\{D(w)\}$ Didefinisikan : $\left\{\dfrac{Jumlah..Keadaan..(dN)}{\text{Rentang}..Energi..(dW)}\right\}$

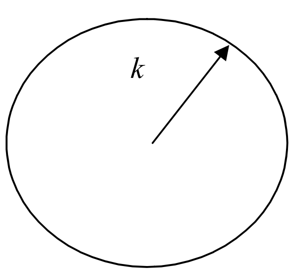
Maka jumlah keadaan : dN = D(w).dw

Energi Total :

$$U = \sum_k \left\{ \sum_p \frac{\hbar\omega_{kp}}{e^{\frac{\hbar\omega_{kp}}{k_b T}} - 1} \right\}$$

$$U = \sum_k \int \frac{\hbar\omega_{kp}}{e^{\frac{\hbar\omega_{kp}}{k_b T}} - 1} .D(\omega).d\omega$$

Volume untuk ruang : k



$$\text{N (number of modes)} = \frac{\frac{4\pi}{3}.k^3}{\left(\frac{2\pi}{L}\right)^3}$$

$\frac{4\pi}{3}.k^3$ → Volume bola jari-jari *k*

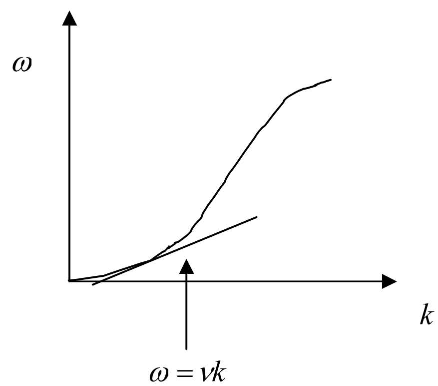
$\left(\frac{2\pi}{L}\right)^3$ → Volume sel primitif kubus

$$N = \frac{L^3k^3}{6\pi^2} \longrightarrow N = \frac{Vk^3}{6\pi^2}$$

$$D(k) = \frac{dN}{dk} = \frac{Vk^2}{2\pi^2}$$

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

$$V_g = \frac{d\omega}{dk}$$



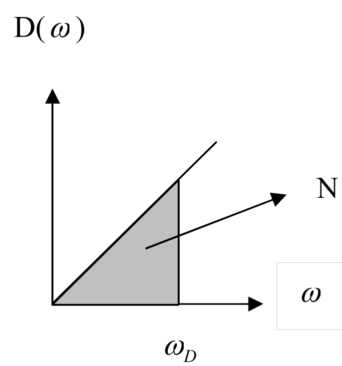
Debye

Contoh :

$$\omega = vk \longrightarrow \frac{dk}{d\omega} = \frac{1}{v}$$

- $D(\omega) = \frac{Vk^2}{2\pi}\frac{1}{v} = \frac{V\omega^2}{2\pi v}$
- $U = 3\int_0^{\omega_D} \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} \frac{V\omega^2}{2\pi v^3} d\omega$

$$N = \frac{Vk^3}{6\pi^2}$$



$\omega_D = \omega_{Debye}$

$\omega_D = vk_D$

$N(\omega) = N(Total)$

$$U = 3.\int_0^{\omega_D} \frac{\hbar\omega^3 V / 2\pi^2 v^2}{e^{\hbar\omega / k_B T} - 1}\, d\omega$$

Sehingga limit dari integral diatas didapat : ω_D

$$N(\omega) = N(total)$$

$$N = \frac{4/3\, \pi k_D^3}{\left(2\pi / L\right)^3} \longrightarrow \omega_D = v k_D$$

$$C_v = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T}\left\{ 3\int_0^{\omega_D} \frac{\hbar\omega^3 V / 2\pi^2 v^3}{e^{\hbar\omega / k_B T} - 1}\, d\omega \right\}$$

$$= \frac{3\hbar V}{2\pi^2} \int_0^{\omega_D} \frac{\omega^3}{1}\left[\frac{d}{dT}\left(\frac{1}{e^{\hbar\omega / k_b T} - 1}\right)\right] d\omega$$

$$C_V = \frac{3\hbar^2 V}{2\pi^2 v^3} \frac{1}{k_B T^2} \int_0^{\omega_D} \frac{\omega^4 . e^{\hbar\omega / k_B T}}{\left(e^{\hbar w / k_B T} - 1\right)^2} d\omega$$

Misalkan : x = $\frac{\hbar\omega}{k_B T} \rightarrow \frac{dx}{d\omega} = \frac{\hbar}{k_B T} \rightarrow d\omega = \frac{k_B T}{\hbar} dx$

$$C_V = \frac{3\pi^2 V}{2\pi^2 v^3 k_B T^2} \int_0^{\frac{\hbar\omega_D}{k_B T}} \frac{\left(k_B\right)^4 x^4 . e^x}{\left(e^x - 1\right)^2} \frac{k_B T}{\hbar} dx$$

Bila didefinisikan : $\theta_D = \frac{\hbar\omega_D}{k_B}$

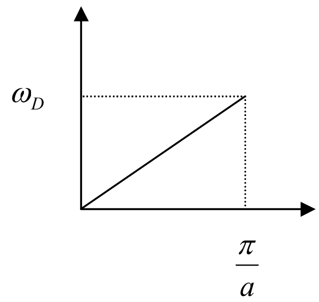
↑

Temperature debye

$$C_V = \frac{3V.k_B{}^4.T^3}{2\pi^2.\hbar^3.\nu^3} \int_0^{\theta_D/T} \frac{x^4.e^x}{\left(e^x-1\right)^2} dx$$

$$V = \frac{\in \pi^2 N \nu^3}{\omega_D{}^3}$$

Ini berasal dari :



$$N = \frac{V.k_D{}^3}{6\pi^2} = \frac{V.\left(\frac{\omega_D}{\nu}\right)^3}{6\pi^2.}$$

Sehingga :

$$C_V = 9Nk_B\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{e^x.x^4}{\left(e^x-1\right)^2} dx$$

Untuk T tinggi $\rightarrow T \rangle\rangle \theta_B \rightarrow x_D \rightarrow x_B \langle\langle 1$

Maka : $\frac{e^x.x^4}{\left(e^x-1\right)^2} = \frac{e^D.x^4}{\left(e^x-1\right)\left(1-e^{-x}\right)} = \frac{x^4}{2\left\{\frac{x^2}{2!}+\frac{x^4}{4!}+.....\right\}}$

Untuk daerah integrasi $0 \le x \le x_B$ dng $X_D << 1$

$$\frac{x^4}{2.\frac{x^2}{2!}} \approx x^2$$

Jadi : $C_V = 9.N.k_B.\frac{T^3}{\theta^3}\int_0^{x_D} x^2 dx$

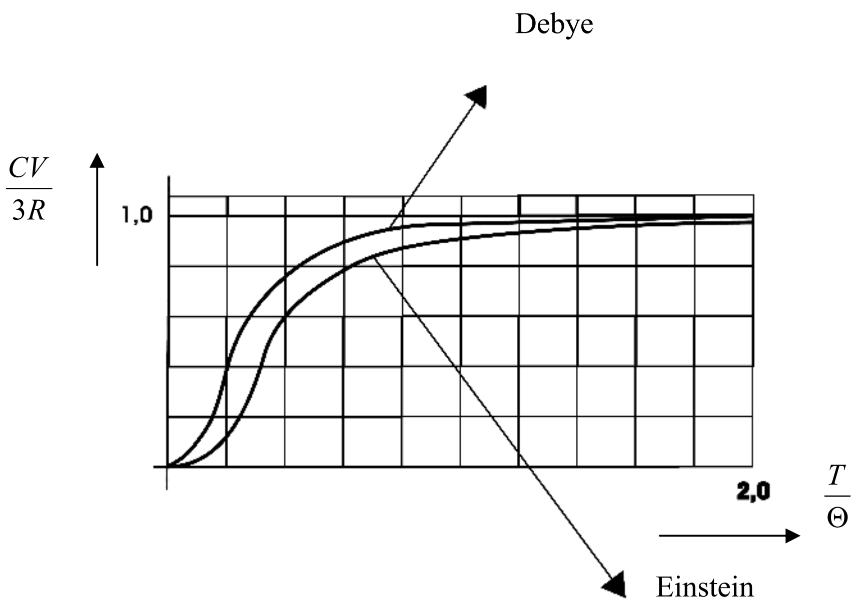
$= 9.N.\ k_B.\ \frac{T^3}{\theta^3}.\frac{1}{3}x^3 \rightarrow ingat : x_D = \frac{\theta}{T}$

$\theta = X.T$

$= 9^3.N.k_B.\frac{T^3}{x^3.T^3}.\frac{x^3}{9}$

$\therefore$ **Model debye : untuk suhu tinggi**

$C_V = 3.Nk_B = 3.R \approx$ sesuai exp.dulong & petit



Untuk T rendah $\Rightarrow$ T<< $\theta_D \rightarrow x_D$ >>1

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

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

Integral parsiel :

U= $x^4 \Rightarrow du = 4x^{3dx}$

dV= $\frac{e^x}{\left(e^x 1\right)^2}dx \Rightarrow \nu = \frac{-1}{\left(e^x-1\right)}$

$$\int UdV = UV - V\int dU.UV - \int VdU$$

$$C_V = 9Nk_B\left(\frac{T}{\theta}\right)^3\left\{\frac{-x^4}{e^x-1}+\int_e^4\frac{4x^3}{e^x-1}dx\right\}$$

$$\frac{-x^4}{e^x-1}\approx\frac{-\left(\frac{\theta}{T}\right)^4}{e^{\theta/T}-1}\Rightarrow T\approx 0=0$$

$$4\int_0\frac{x^3}{e^x-1}dx=4\{3!(4)\}$$

↓

Fungsi zeta reiman

$$=\frac{1}{1^4}+\frac{1}{2^4}+\frac{1}{3^4}\ldots\ldots\ldots\frac{\pi^4}{90}$$

$$C_V = 9.Nk_BT\left(\frac{T}{\theta}\right)^3.\left\{4.6.\frac{\pi^4}{90}\right\}$$

$$C_V = \frac{12}{15}\pi^4 \quad Nk_B\left(\frac{T}{\theta}\right)^3$$

$$C_V = 234 \quad \mathrm{N}\,k_B\left(\frac{T}{\theta}\right)^3$$

$$C_V = 234 \quad \frac{Nk_B}{9^3}T^3\ldots\ldots\ldots.Hk \quad T^3 deybe$$