Subgroup meeting 2010.12.07

introduction of thermal transport

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introduction of thermal transport

Phonon effect
- Lattice vibration
  - Debye model of lattice vibration
  - K space, Reciprocal lattice
  - Brillouin zone
  - Scattering mechanism
  - Boundary scattering
  - Phonon-phonon scattering
  - Normal Process
  - Umklapp process

Electron effect
- Debye temperature
- Bose-Einstein model
- Dulong-petit model
- The contribution of electron of heat capacity
- Heat capacity
Outline

• Dispersion relation (review)
• Specific heat (review)
• Different temperature ranges
• Low temperature range
• Debye temperature
- At lower energy (lower k)
- $K \alpha \ll \pi$ (near zero)
- The dispersion relation is regarded as linear

**Dispersion relation**

Electromagnetic wave
- $\omega/k = c$
- $c$: light speed
- $c$ is constant $\rightarrow$ linear dispersion relation
Dispersion relation

We get linear part of dispersion relation.
Group velocity \( v_g \) = 0 at \( k = \pi/a \)

Energy does not propagate in the medium (standing wave)
Dispersion relation

• Classical mechanism:
  Harmonic oscillator
  (conservative force and wave)

• We get dispersion relation by only classical assumption
There are three segments of the experiment curve of specific heat (Cv).
Specific heat

General form of specific heat

\[ C_v = \frac{\partial}{\partial T} \frac{1}{TV} \sum_s \int \frac{\hbar \omega_s(k)}{e^{\hbar \omega_s(k)/k_B T} - 1} \frac{4\pi k^2 L^3}{(2\pi)^3} \, dk \]

Quatum theory of Harmonic solid

- Bose-Einstein distribution function
- Stationary states of vibration
Different approximations of temperature ranges:

- Low temperature: Debye model
- Intermediate temperature: Debye & Einstein
- High temperature: → Dulong-Petit
Specific heat at Low temperature

Debye model

- The angular frequencies are diverse values.
- The maximum allowed value is cut-off frequency $\omega_D$
Debye model

Specific heat

\[ C_v = \frac{1}{V} \frac{\partial}{\partial T} \int_0^{\omega_D} D(\omega) \frac{\hbar \omega}{e^{\hbar \omega/k_BT} - 1} \, d\omega \]

\[ C_v = \frac{1}{V} 9nk_B \left( \frac{T}{\theta} \right)^3 \int_0^{\theta/T} x^4 e^x dx \frac{1}{(e^x - 1)^2} \]

where \( x = \frac{\hbar \omega}{k_BT} \)

- Density of states
- Energy per phonon
- Bose-Einstein distribution
- Cut-off frequency

\[ U = 9nk_B T \left( \frac{T}{\theta} \right)^3 \int_0^{x_D} x^3 \frac{dx}{e^x - 1} \]
Debye model

The spacing between constant frequency surface depends on (group velocity) $d\omega/dk$

For simple case that $v_p=v_g$

$\omega/k=\text{constant}=\text{sound velocity}$

We can get approximation $D(\omega)$ of Debye model (low temperature)

$$D(\omega) = \frac{V \omega^2}{2\pi^2 v^3}$$
Specific heat at Low temperature

Dispersion relation

- Ignored optical branches
- Replace acoustic branch with liner branches

\[ \omega = \frac{\hbar}{k_B T} \]
Specific heat at Low temperature

\[ C_v = \frac{\partial}{\partial T} \frac{1}{V} \sum_s \int \frac{\hbar \omega_s(k)}{e^{\hbar \omega_s(k)/k_B T} - 1} \frac{4\pi k^2 L^3}{(2\pi)^3} \, dk \]

When \( T \) is small

High frequencies result in large \( e^{\hbar \omega/k_B T} \)

The contributions of high frequencies for LOW temperature are negligible.
Specific heat at Low temperature

\[ C_v = \frac{\partial}{\partial T} \frac{1}{V} \sum_s \int \frac{\hbar \omega_s(k)}{e^{\hbar \omega_s(k)/k_B T} - 1} \frac{4\pi k^2 L^3}{(2\pi)^3} \, dk \]

\[ C_v = \frac{\partial}{\partial T} \sum_s \int_0^\infty \frac{\hbar c_s(k) k^3}{e^{\hbar c_s(k) k / k_B T} - 1} \frac{dk}{2\pi^2} \]

\[ \omega_s(k) = c_s(k) k \]

\[ \frac{1}{c_{ave}^3} = \frac{1}{3} \sum_s \int \frac{d\Omega}{4\pi} \times \frac{1}{c_s(k)^3} \]

\[ \sum_s = 3 \]

\[ x = \frac{\hbar \omega}{k_B T} \]

\[ \int_0^\infty \frac{x^3}{e^x - 1} \, dx = \frac{\pi^4}{15} \]
Specific heat at **Low temperature**

At very **low temperature**

Specific heat

\[ C_v \approx \frac{2\pi^2}{5} \frac{k_B(T)^3}{(\hbar c_{ave})^3} \]

Which is **Debye** \( T^3 \) **law**

Condition assumption:
- Only Acoustic modes are thermally excited
- For actual crystals Temperature may necessary to be below \( T=\theta/50 \)

\[ C_v \approx \frac{12\pi^4}{5} N k_B \left( \frac{T}{\theta} \right)^3 \]

\( \theta \) : Debye temperature
Debye temperature

Determine a cut-off frequency of specimen

\[ N = \left( \frac{L}{2\pi} \right)^3 \frac{4\pi k^3}{3} = \frac{V}{6\pi^2} (\omega v)^3 \]

\[ \omega_D^3 = 6\pi^2 v^3 N/V \]

\[ K_D = \left( \frac{6\pi^2 N}{V} \right)^{\frac{1}{3}} \]

\[ C_V = \frac{1}{V} \frac{\partial}{\partial T} \int_0^{\omega_D} D(\omega) \frac{\hbar \omega}{e^{\hbar \omega/k_B T} - 1} d\omega \]

Define Debye temperature \( \theta \) in terms of cut-off frequency

\[ \chi_D = \frac{\hbar \omega_D}{k_B T} \equiv \frac{\theta}{T} \]

\[ \theta = \frac{\hbar v}{k_B} \left( \frac{6\pi^2 N}{V} \right)^{\frac{1}{3}} \]
Debye temperature

\[ \theta = \frac{\hbar \nu}{k_B} \left( \frac{6\pi^2 N}{L^3} \right)^{\frac{1}{3}} \]

Compare boundary conditions:

Brillion Zone (atom spacing)

\[ K \leq \frac{\pi}{a} \]

Cut off frequency (atom packing)

\[ K \leq K_D = \left( \frac{6\pi^2 N}{V} \right)^{\frac{1}{3}} \]

For ideal simple cubic specimen

\[ \frac{\sqrt[3]{N}}{L} = \frac{n}{L} = \frac{1}{a} \quad K_D = \frac{(6\pi^2)^{\frac{1}{3}}}{a} \]

\( K_D \) are different with different kinds of lattice packing
Debye temperature

What are the factors that determine Debye temperature?

Theoretical:
\[ \theta = \frac{\hbar v}{k_B} \left( \frac{6\pi^2 N}{V} \right)^{\frac{1}{3}} \]

\( v(\rho,K,G) \): sound velocity in the specimen
\( N/V \): atom concentration (packing density)

Experimental:
The Debye temperature were determined by fitting the observed specific heats \( C_V \) formula at the point of \( \frac{1}{2} \) Dulong-Petit value \( (3Nk_B/2) \)

\[ C_V = \frac{1}{V} 9nk_B \left( \frac{T}{\theta} \right)^3 \int_0^{\theta/T} \frac{x^4 e^x dx}{(e^x - 1)^2} \]
### Debye temperature

\[ \theta \propto v \times \left( \frac{N}{V} \right)^{\frac{1}{3}} \]

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Future work

• Intermediate region
• High temperature region
• Electron Effect
Thanks for your attention