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Oct. 28, 2008

6.1 Quantitatively the melting point of a crystalline solid can be defined as the temperature $T_m$ at which the amplitude of simple harmonic vibrations of the individual atoms about their lattice sites is about 10% of the interatomic spacing a. Show that on this picture the frequency $\nu$ of the vibrations of a monatomic crystal (atomic weight M) satisfies $\nu \propto \frac{1}{a}\left(\frac{T_m}{M}\right)^{1/2}$

Vibrational energy p. 153 $E = \frac{1}{2} M \omega_E^2 (x_{max}^2 + y_{max}^2 + z_{max}^2)$

$x_{max} = y_{max} = z_{max} = \frac{1}{10} a, \quad \omega_E = 2\pi\nu$

Equipartion Theory: $E = kT_m$

$$kT_m = \frac{1}{2} M (2\pi\nu)^2 \left(\frac{1}{10} a\right)^2 3$$

$$\nu^2 = \frac{2kT_m}{3M(2\pi)^2}\left(\frac{10}{a}\right)^2$$

$$\nu^2 = \left(\frac{5k}{3\pi^2}\right)\frac{T_m}{Ma^2}$$

$$\nu^2 \propto \frac{T_m}{a^2 M}$$

$$\nu \propto \frac{1}{a}\left(\frac{T_m}{M}\right)^{1/2}$$

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Einstein temperatures of Al and Pb are 240K and 67K. Are these reasonable?

$\nu \propto \Theta_E \quad \frac{\nu_{Al}}{\nu_{Pb}} = \frac{240K}{67K} = 3.6 = \frac{a_{Pb}}{a_{Al}}\left(\frac{T_{mAl}}{T_{mPb}}\right)^{1/2}\left(\frac{M_{Pb}}{M_{Al}}\right)^{1/2}$

Pb interatomic distance > Al in. dist.

Al melting point > Pb melting point

Pb atomic mass > Al atomic mass

6.2 Calculate the entropy of the lattice vibrations of a monatomic crystal as described by the Einstein theory.

$$F = E - TS$$

$$S = \frac{E-F}{T} = \frac{3N\bar{E} - 3NF_1}{T}$$

(6.6) $F_1 = \frac{1}{2}\hbar\omega_E + \frac{1}{\beta}\ln[1-\exp(-\beta\hbar\omega_E)]$

(6.8) $E = 3N\bar{E} = 3N\left(\frac{1}{2}\hbar\omega_E + \frac{\hbar\omega_E}{\exp(\beta\hbar\omega_E)-1}\right)$ (6.7)

(6.10) $x \equiv \frac{\hbar\omega_E}{kT}$

$$S = \frac{3N\left(\frac{1}{2}\hbar\omega_E + \frac{\hbar\omega_E}{\exp(\beta\hbar\omega_E)-1}\right) - \left(\frac{1}{2}\hbar\omega_E - \frac{1}{\beta}\ln[1-\exp(-\beta\hbar\omega_E)]\right)3N}{T}$$

$$S = \cancel{\frac{\hbar\omega_E}{kT}\left(\frac{3Nk}{2} - \frac{3Nk}{2}\right)} + \frac{\hbar\omega_E}{kT}\left(\frac{3Nk}{\exp^{\hbar\omega_E/kT}-1}\right) - \frac{\cancel{kT}\ln[1-e^{-\hbar\omega_E/kT}]3N}{\cancel{T}}$$

$$S = 3Nk\left\{\left(\frac{x}{e^x-1}\right) - \ln(1-e^{-x})\right\}$$

Low temperature $x \gg 1$ $\quad S = 3Nk\left(\frac{x}{e^x} - \ln(1)\right) = \frac{3Nkx}{e^x}$

High temperature $x \ll 1$

$$S = 3Nk(x)$$

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6.3 $F = E - TS$

Eq. 6.6

$$F = -kT\ln Z_1 = \frac{1}{2}\hbar\omega_E + \frac{1}{\beta}\ln\left[1 - e^{-\beta\hbar\omega_E}\right]$$

6.23 $$f(\omega)d\omega = 9N\frac{\omega^2 d\omega}{\omega_D^3}$$

$$\Rightarrow F = \frac{9}{8}N\hbar\omega_D + \frac{9NkT}{x_D^3}\int_0^{x_D} dt\, t^2 \ln(1-e^{-t}) \qquad x_D = \frac{\Theta_D}{T} = \frac{\hbar\omega_D}{kT}$$

integrate by parts

$$F = \frac{9}{8}N\hbar\omega_D + 3NkT\ln(1-e^{-x_D}) - \frac{3NkT}{x_D^3}\int_0^{x_D}\frac{t^3 dt}{e^t - 1}$$

6.24b Debye Energy $$E = \frac{9}{8}Nk\Theta_D + \frac{9NkT}{x_D^3}\int_0^{x_D}\frac{x^3 dx}{e^x - 1}$$

$$\Rightarrow S = \frac{E - F}{T}$$

$$(T)S = \frac{9}{8}Nk\Theta_D + \frac{9NkT}{x_D^3}\int_0^{x_D}\frac{x^3 dx}{e^{x}-1} - \frac{9}{8}N\hbar\omega_D - 3NkT\ln(1-e^{-x_D})$$
$$+ \frac{3NkT}{x_D^3}\int_0^{x_D}\frac{t^3 dt}{e^t - 1}$$

$$S = \frac{12NkT}{T x_D^3}\int_0^{x_D}\frac{t^3 dt}{(e^t - 1)} - 3NkT\ln(1-e^{-x_D})$$

$$x_D \gg 1 \Rightarrow S = \frac{4}{5}\pi^4 Nk\left(\frac{T}{\Theta}\right)^3$$

$$x_D \ll 1 \Rightarrow S = 3NkT - 3Nk\ln\Theta_D + 4Nk$$

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6.4 $\nu^2 = 2\pi\sigma / \rho\lambda^3$ using $\int_0^\infty \frac{x^{4/3}}{e^x-1}dx = 1.68$

$$f(k)dk = \frac{Akdk}{2\pi}$$

$$f(\nu)d\nu = \frac{4\pi}{3}\left(\frac{\rho}{2\pi\sigma}\right)^{2/3} A\nu^{1/3}d\nu$$

$$E(T) = \int_0^{\nu_0} f(\nu)d\nu \left\{\frac{1}{2}h\nu + \frac{h\nu}{e^{\beta h\nu}-1}\right\}$$

$$\Rightarrow E(T) = E_0 + \frac{4\pi}{3}\left(\frac{\rho}{2\pi\sigma}\right)^{2/3} Ah\left(\frac{kT}{h}\right)^{7/3}\int_0^{x_0}\frac{x^{4/3}dx}{e^x-1}$$

with $x_0 >> 1$ $x_0 \to \infty$

$$E(T) = E_0 + 1.68\left(\frac{4\pi}{3}\right)\left(\frac{\rho}{2\pi\sigma}\right)^{2/3} A\frac{(kT)^{7/3}}{h^{4/3}}$$

estimate range of validity

$$nA = \int_0^{\nu_0} f(\nu)d\nu = \pi A\left(\frac{\rho}{2\pi\sigma}\right)^{2/3}\nu_0^{4/3}$$

cut-off temp $\Theta_0 = \frac{h\nu_0}{k}$ $n = (0.145 \cdot \frac{1}{4} \cdot 6 \cdot 10^{23})^{2/3}$

$\Theta_0 = 11.7K$ for $T << 12K$ and this formula holds