

FIG. 1.16. Specific heat of ^4He as a function of $T - T_\lambda$ in K. Notice that the shape of the specific heat curve is rather like the Greek letter λ , whence the origin of the term ' λ -transition'. The fact that the specific heat is only about ten times its 'normal' value even at temperatures only a few microdegrees from T_λ is correlated with the fact that the critical-point exponent is extremely small (in fact, α is probably zero, corresponding to a logarithmic divergence). The width of the small vertical line just above the origin indicates the portion of the diagram that is expanded in width in the curve directly to the right. After Buckingham and Fairbank (1965). [E. Stanley]

Simulations
of Jagla Model

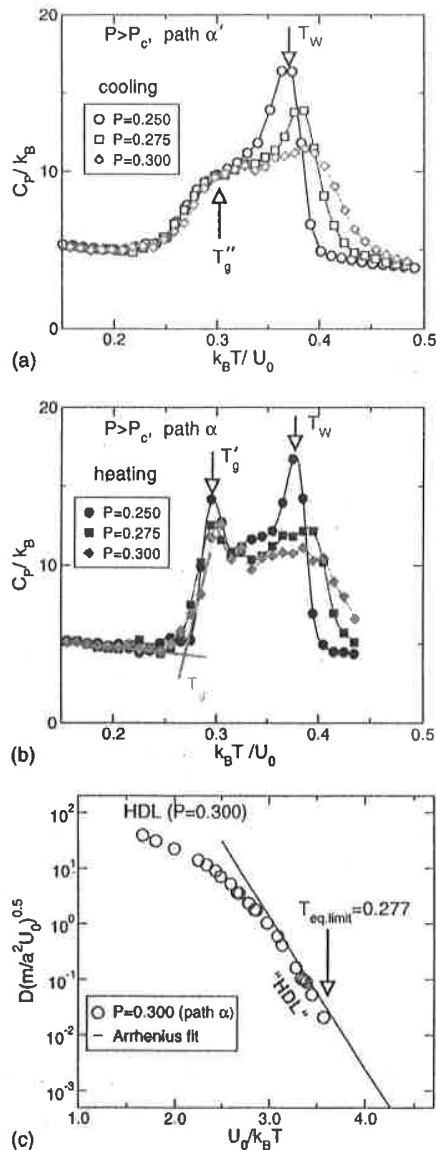


FIG. 4. (Color online) Contrast of C_p behavior near T_g and T_w and illustration of nonergodicity for the temperature dependence of the HDL specific heat C_p for $P > P_c$. (a) Cooling LDL along path α' and (b) heating along path α at different pressures $P > P_c$. Upon cooling, C_p shows a maximum at $T = T_w$ and a shoulder at $T_g'' \approx 0.3$, below which the liquid vitrifies to HDA. In contrast, upon heating HDA, C_p shows a peak at T_g' , characterizing the GT and corresponding to the shoulder found upon cooling in (a). The standard construction as in Fig. 3 gives $T_g \approx 0.27$. Further heating results in a second peak at the Widom line, $T = T_w$. While T_g is nearly constant at $P > P_c$, the Widom line temperature T_w shifts to higher values as P increases. Moreover, due to critical fluctuations as $P \rightarrow P_c$, the height of the Widom line peak is much more sensitive to P than that corresponding to the GT. We use a slow cooling rate of $q_1 = 1 \times 10^{-6} q_0$, since crystallization is not observed for $P > P_c$. In summary, parts (a) and (b) demonstrate that the GT peak is not sensitive to P but is sensitive to heating vs cooling, while the Widom line peak is sensitive to P but not to heating vs cooling. (c) Diffusion coefficient as a function of temperature in the liquid phase. The lowest temperature of the equilibrium liquid accessible in simulations is $T_{eq,limit} = 0.277$. This value is in agreement with the value $T_g = 0.27$ obtained from C_p in (b).

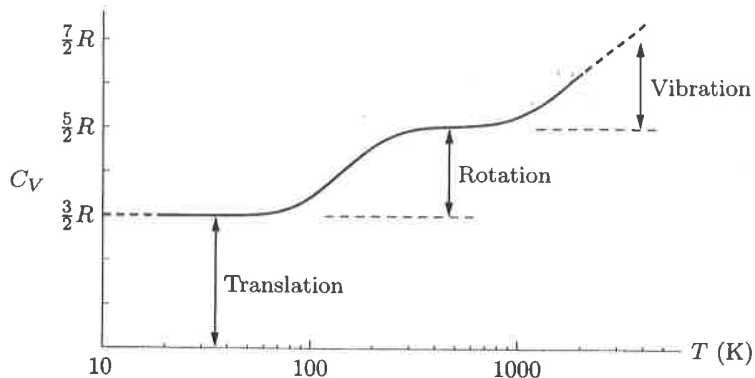


Figure 1.13. Heat capacity at constant volume of one mole of hydrogen (H_2) gas. Note that the temperature scale is logarithmic. Below about 100 K only the three translational degrees of freedom are active. Around room temperature the two rotational degrees of freedom are active as well. Above 1000 K the two vibrational degrees of freedom also become active. At atmospheric pressure, hydrogen liquefies at 20 K and begins to dissociate at about 2000 K. Data from Woolley et al. (1948).

QM needed

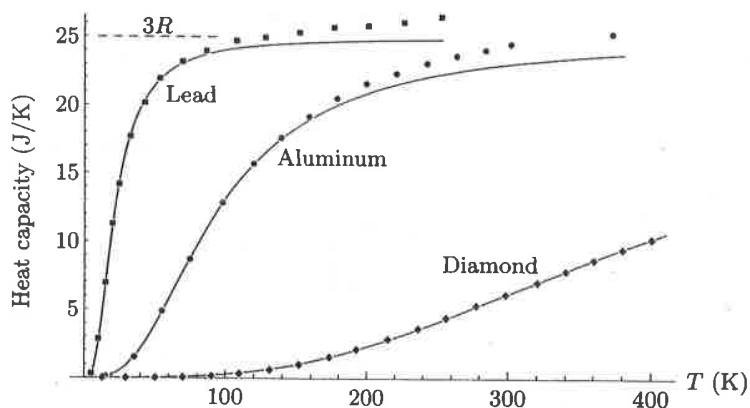


Figure 1.14. Measured heat capacities at constant pressure (data points) for one mole each of three different elemental solids. The solid curves show the heat capacity at constant *volume* predicted by the model used in Section 7.5, with the horizontal scale chosen to best fit the data for each substance. At sufficiently high temperatures, C_V for each material approaches the value $3R$ predicted by the equipartition theorem. The discrepancies between the data and the solid curves at high T are mostly due to the differences between C_P and C_V . At $T = 0$ all degrees of freedom are frozen out, so both C_P and C_V go to zero. Data from Y. S. Touloukian, ed., *Thermophysical Properties of Matter* (Plenum, New York, 1970).

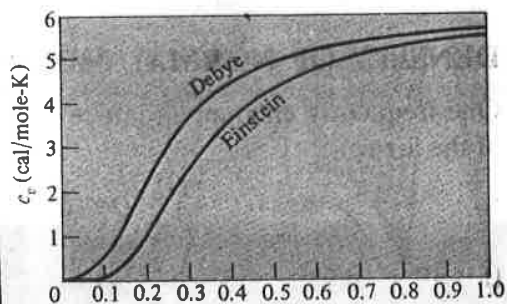


Fig. 23.5

T/θ [Ashcroft, Mermin]

$$= C_V + Nk = C_V + nR \quad (\text{ideal gas}). \quad (1.48)$$

mole of an ideal gas, the heat capacity at constant pressure by R , the gas constant. Oddly, the

Formation of Glasses from Liquids and Biopolymers

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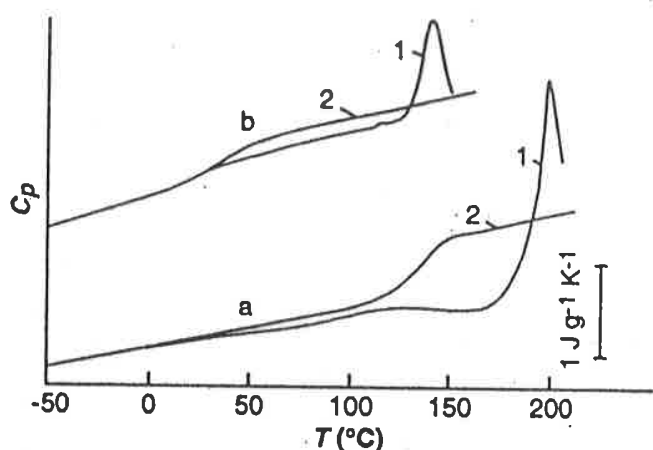


Fig. 9. Differential scanning calorimeter scans of the globular protein legumin both before and after denaturation, for different water contents (A) dry and (B) 10.4% by weight. Note the increase in calorimetric strengths of glass transitions after denaturation. The native state acts like a strong liquid. Comparison of the glass transition with a simple homopolypeptide, poly-L-asparagine is made in Fig. 10. [From (117b) by permission copyright Oxford University Press]

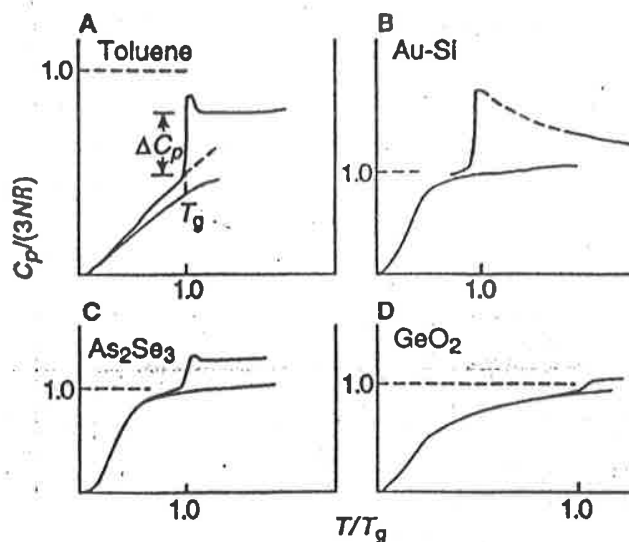


Fig. 2. Heat capacity forms for liquid and crystal phases of different substance. (A) Molecular systems like toluene where the glass transition occurs over a range where the crystal heat capacity is not classical; (B) metallic systems like Au-Si where crystal and glass reach the classical regime before the glass transition occurs; (C) covalent systems like As_2Se_3 where the jump in liquid heat capacity occurs on a classical background and ΔC_p remains large above T_g ; (D) open network systems like GeO_2 where ΔC_p is small and occurs on a classical background. The T_g is usually defined by the construction made at 10 K/min shown in (A) because this fixes T_g as the temperature where the average structural relaxation time is 100 s (10) for scanning at 10 K/s; N is the number of atoms per formula unit and R is the gas constant.

Experiments

BOSON PEAK

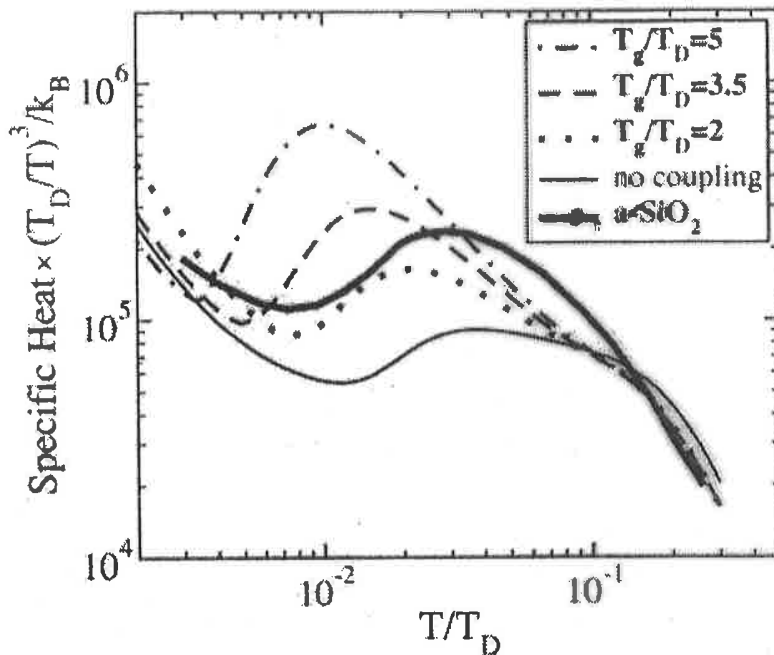


Fig. 2. The heat capacity per domain, which follows from the derived TLS + ripplon density of states, divided by T^3 . This includes the Debye contribution. The thin line neglects phonon coupling and has $T_g/T_D = 4$. The experimental curve for amorphous silica from ref. 20, originally given in J/gK^4 , is shown multiplied by $\hbar^3 \rho c_s^3 (6\pi^2)(\xi/a)^3 / k_B^4$, where we used $\omega_D = (c_s/a)(6\pi^2)^{1/3}$, $(\xi/a)^3 = 200$ (9), $\rho = 2.2$ g/cm³, $c_s = 4,100$ m/sec, and $T_D = 342$ K (3). By using the appropriate value of $k_B T_g / \hbar \omega_D = 4.4$ for a-SiO₂ would place the peak somewhat lower in temperature than observed.

V. Lubchenko & P.G. Wolynes, PNAS 100(4), 1515-1518 (2003)

Einstein oscillator in highly-random-packed bulk metallic glass

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Metallic glasses have often been regarded as ideal model systems of dense random packing with strong interaction among their components. Here we report direct evidence for the presence of the Einstein oscillator with an Einstein temperature θ_E of 74 K, which induces the boson peak at 4.9 meV in bulk metallic glass $Zr_{46.75}Ti_{8.25}Cu_{7.5}Ni_{10}Be_{27.5}$. The presence of an Einstein oscillator suggests the existence of the vibrations of loose atoms in an independent localized harmonic mode in the highly random packed metallic glasses. © 2005 American Institute of Physics. [DOI: 10.1063/1.1849420]

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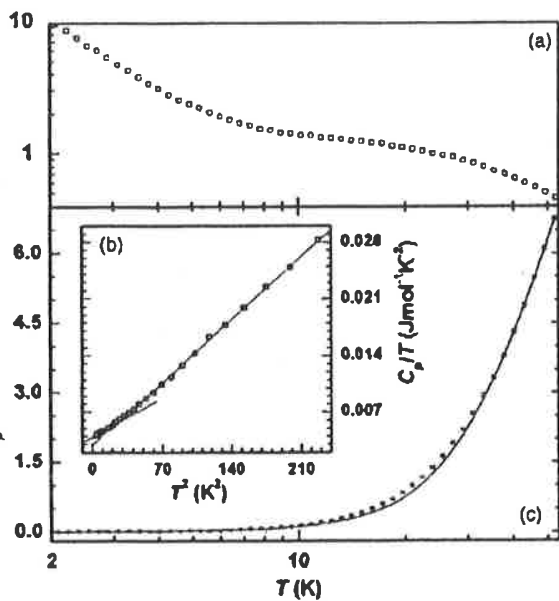


FIG. 1. The specific heat C_p of vit4 in the temperature range from 2 to 52 K. (a) Specific heat plotted as C_p/T^3 vs T . (b) The specific heat, shown as C_p/T^3 vs T . The solid lines are the results of the fitting specific heat between 2 and 52 K using the expression: $C_p/T = \gamma + \beta T^2$. (c) The specific heat is least-squares fitted by the Debye model.

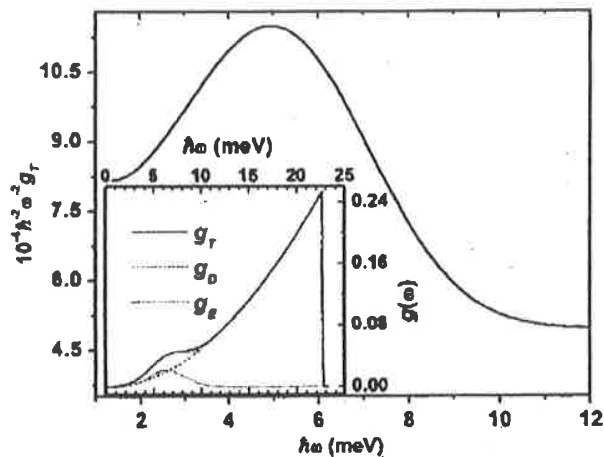


FIG. 3. The derived VDOS of vit4. The peak at about 4.9 meV is boson peak. The inset shows the total VDOS g_T (the solid line), and the VDOS contributed from the Debye g_D (the dashed line) and Einstein g_E (the dotted line) modes, respectively.

mode with $\theta_D=263$ K and $n_D=1.92$; C_E , and the dotted line in Fig. 2, is the contribution of the Einstein mode: $C_E = R(\theta_E/T)^2 e^{\theta_E/T} / (e^{\theta_E/T} - 1)^2$, with an Einstein temperature $\theta_E = 74$ K and the constant $n_E=0.10$ that stands for the Einstein oscillator strength per mole. The fact that one Einstein mode is needed to model the data indicates the presence of the

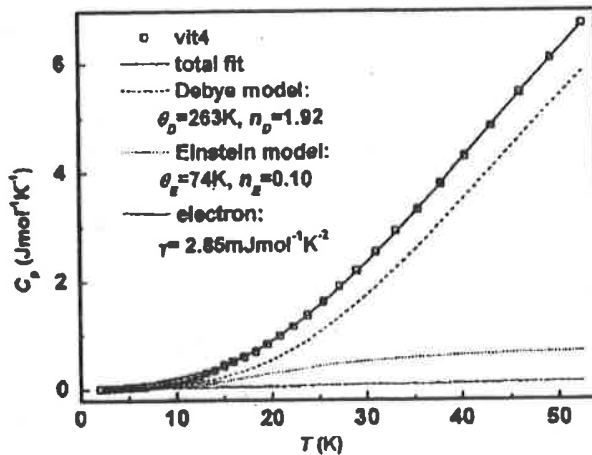


FIG. 2. The fitting results (the solid line) of the specific heat of vit4 between 2 and 52 K. The dashed and dotted lines represent contributions from the Debye mode and Einstein mode, respectively; the dash-dotted line is the contribution of electrons.

Problem 1.42

The specific heat capacity of Albertson's

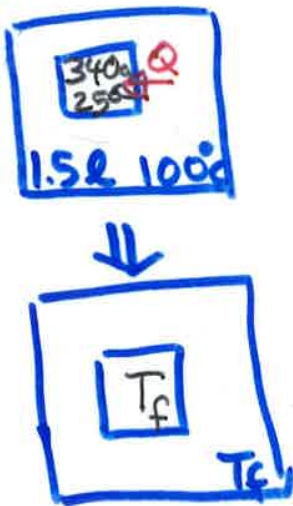
Rohini Tricolore is approximately $1.8 \text{ J/(g}^\circ\text{C)}$.

Suppose you toss 340 g of this pasta (at 25°C)

into 1.5 L of boiling water. $c_w = 4.186 \text{ J/(g}^\circ\text{C)}$ What effect

does this have on the temperature of water (before there is time for the stove to

provide more heat)? $|Q_{\text{out of water}}| = |Q_{\text{into pasta}}|$
 heat out of water heat into pasta



$$m_w c_w (T_w - T_f) = m_p c_p (T_f - T_p)$$

\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow
 1500 g $4.186 \text{ J/g}^\circ\text{C}$ 100°C 340 g $1.8 \text{ J/g}^\circ\text{C}$ 25°C

$T_f = \dots = 93.3^\circ\text{C}$ \rightarrow use bigger pot

Problem 1.51

Combustion of 1 mole of glucose

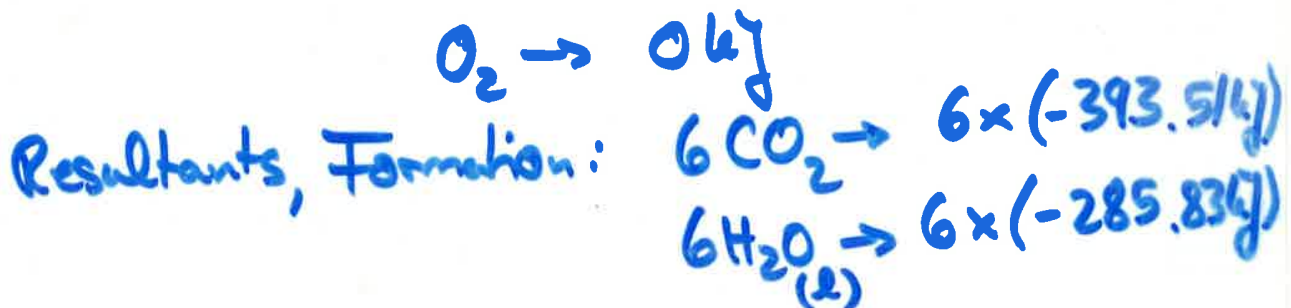
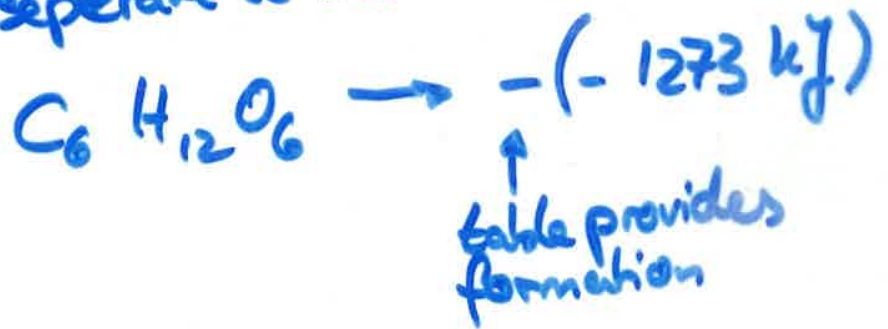


"(net) reaction that provides most of energy needs in our body"

$$\Delta H = ?$$

pages 404 and 405

Reactants: separate to individual elements



$$\boxed{\Delta H} = 1273 \text{ kJ} + 6 \times (-393.51 \text{ kJ}) + 6 \times (-285.83 \text{ kJ})$$
$$= \boxed{-2803 \text{ kJ}}$$