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1 History of Glass

Encyclopedia, 10.1 - 10.10

Figure 4 (a) Egypt (cosmetic jug, 18th dynasty, 24 × 30 cm; British Museum 22819); (b) Ur, Mesopotamia (flutted glass bottle, height 11.8 cm; BM 120659). *Source:* (a, b): © The Trustees of the British Museum.

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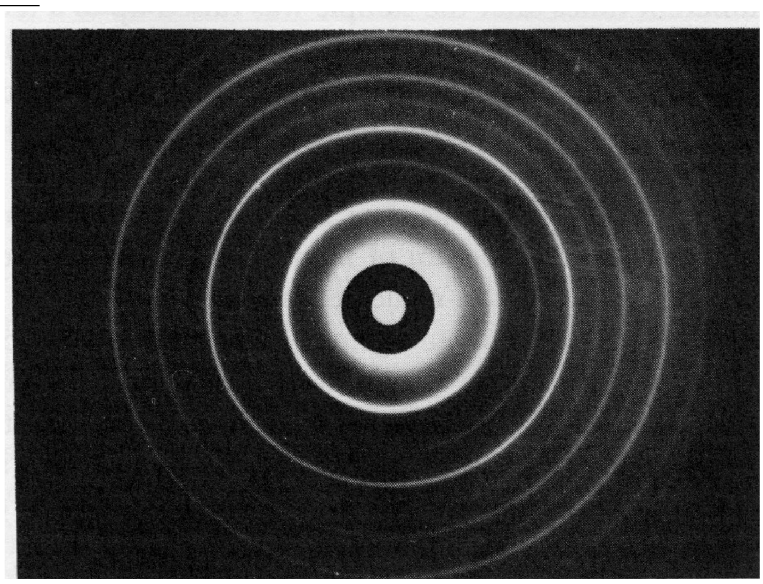
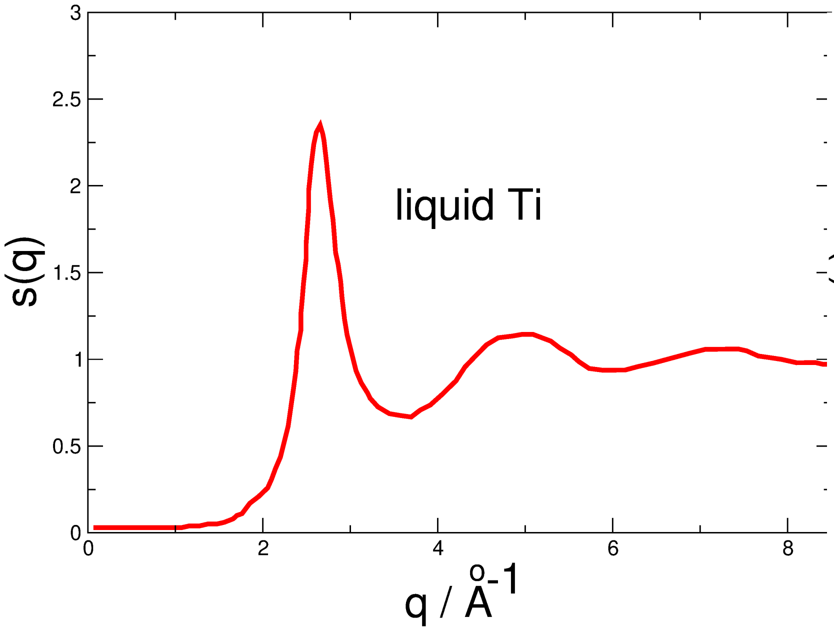
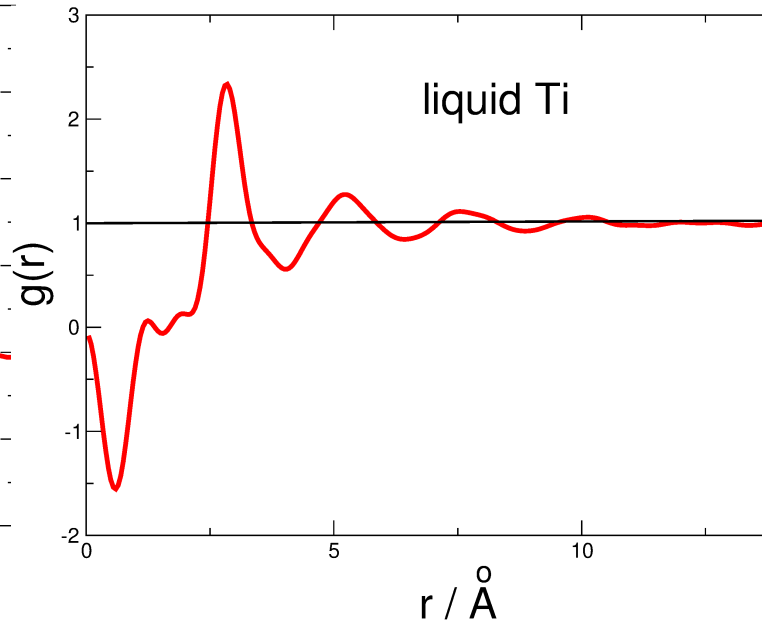
2 Hard-Sphere Percus-Yevick Theory for $S(q)$ and $g(r)$

Schirmacher, 2.8



X-ray image





$S(q)$ = Intensity from the middle outwards $g(r)$

$S(q)$ = X-Ray- and neutron-scattering structure factor [1, 2]

$$S(q) = 1 + \rho_0 \int_{-\infty}^{\infty} \mathrm{d}^3\mathbf{r} e^{i\mathbf{qr}} [g(r) - 1]$$
$$= 1 + 4\pi\rho_0 \int_0^{\infty} \mathrm{d}r r^2 \frac{\sin(qr)}{qr} [g(r) - 1]$$

Here $\rho_0 = N/V$ is the number density of the particles.

The radial distribution function $g(r)$ gives the statistics of distances r between the molecules

Direct Correlation function $c(r)$ (Ornstein, Zernike [2])

$$h(r) = g(r) - 1 = c(r) + \rho_0 \int \mathrm{d}^3\mathbf{r}' c(|\mathbf{r} - \mathbf{r}'|) c(r') + \cdots + \ldots \tag{1}$$

$$= c(r) + \rho_0 \int \mathrm{d}^3\mathbf{r}' h(|\mathbf{r} - \mathbf{r}'|) c(r') \tag{2}$$

$$= c(r) + \rho_0 [h \circ c](r)$$

$\Rightarrow$

$$\rho_0 h(q) = \left[S(q) - 1\right] = \rho_0 c(q) \left[1 + \rho_0 h(q)\right]$$

$\Rightarrow$

$$\rho_0 h(q) = \frac{\rho_0 c(q) \overbrace{}^{+1-1}}{1 - \rho_0 c(q)} = \underbrace{\frac{1}{1 - \rho_0 c(q)}}_{S(q)} - 1$$

$\Rightarrow$

$$S(q) = \frac{1}{1 - \rho_0 c(q)}$$

Percus-Yevick's [3] Closure relation in terms of the interatomic potential $\phi(r)$

$$c(r) = g(r) \left[1 - e^{\beta\phi(r)}\right] \tag{3}$$

Equations (1) and (2) constitute a set of integral equations

Hard-sphere (HS) potential

$$\phi_{HS}(r) = \begin{cases} \infty & r < d \\ 0 & r > d \ , \end{cases} \tag{4}$$

where d is the *hard-sphere diameter*. In this case the PY integral equation has been solved exactly by M. S. Wertheim [5] and E. Thiele [4] in 1963.

The solution is given in terms of the *packing fraction*

$$\eta = \frac{\text{volume filled with spheres}}{\text{total volume}} = \frac{\pi}{6} d^3 \rho_0 \tag{5}$$

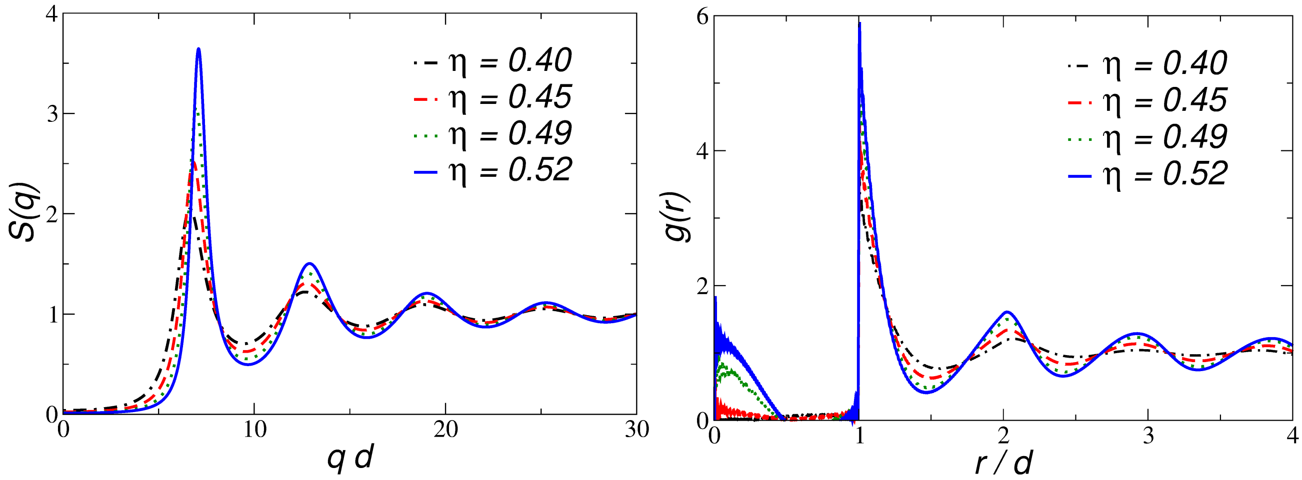
and the dimensionless variable $x = r/d$

$$c(r) = \begin{cases} \lambda_1 - 6\eta\lambda_2 x + \frac{1}{2}\eta\lambda_1 x^3 & x < 1 \\ \\ 0 & x > 1 \ , \end{cases} \tag{6}$$

with

$$\lambda_1 = (1 + 2\eta)^2/(1 - \eta)^4 \tag{7a}$$

$$\lambda_2 = (1 + \frac{1}{2}\eta)^2/(1 - \eta)^4 \tag{7b}$$



Hard-sphere Percus-Yevick structure factors $S(q)$ and pair correlation functions $g(r)$ for different packing fractions η

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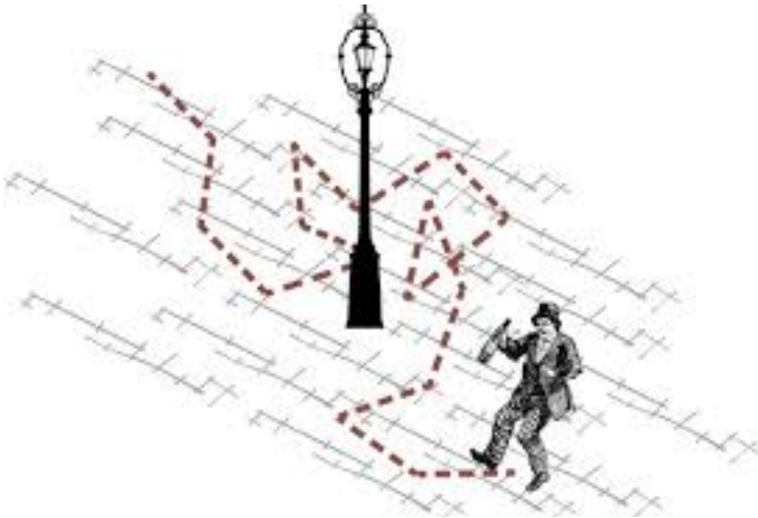
3 Structure of polymers

Schirmacher 4.3, 6.1

Polymer structure as a random walk:



1. Characterize the statistics of a random walk
2. Relation with a diffusion process
3. Derive thermodynamics of the polymer from the random walk statistics

4 Color of glass

Encyclopedia, 6.2

Figure 1 French stained glass from the thirteenth century (cf. Figure VI). (a) Notre-Dame of Chartres cathedral (1215–1240), Bay 5, James and Josuas, detail of The life of St. James the Greater (cf. Figure VI), Chartres. © Malnoury, Robert; Martin, J., Inventaire général, ADAGP. (b) Sainte Chapelle, Paris (1245–1250). © RMN (Musée de Cluny, Paris). (See electronic version for color figures)

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Georges Calas, Laurence Galoisy and Laurent Cormier

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Encyclopedia, 1.1 - 1.7

Figure 1 The initial melting step in the making of float glass: the 1-m deep bath of raw materials melted by the flames of a cross-fired furnace (Chapter 9.7). Pulls ranging from 500 to 1000 tons/ day and mean residence times of at least 24 hours. Electro-fused refractory materials made up of alumina-zirconia-silica in contact with the melt, and of alumina and alumina-silica elsewhere (cf. Chapter 9.8). *Source:* Photo courtesy Simonpietro Di Pierro, Saint-Gobain Research Paris.

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6 Mechanical Properties

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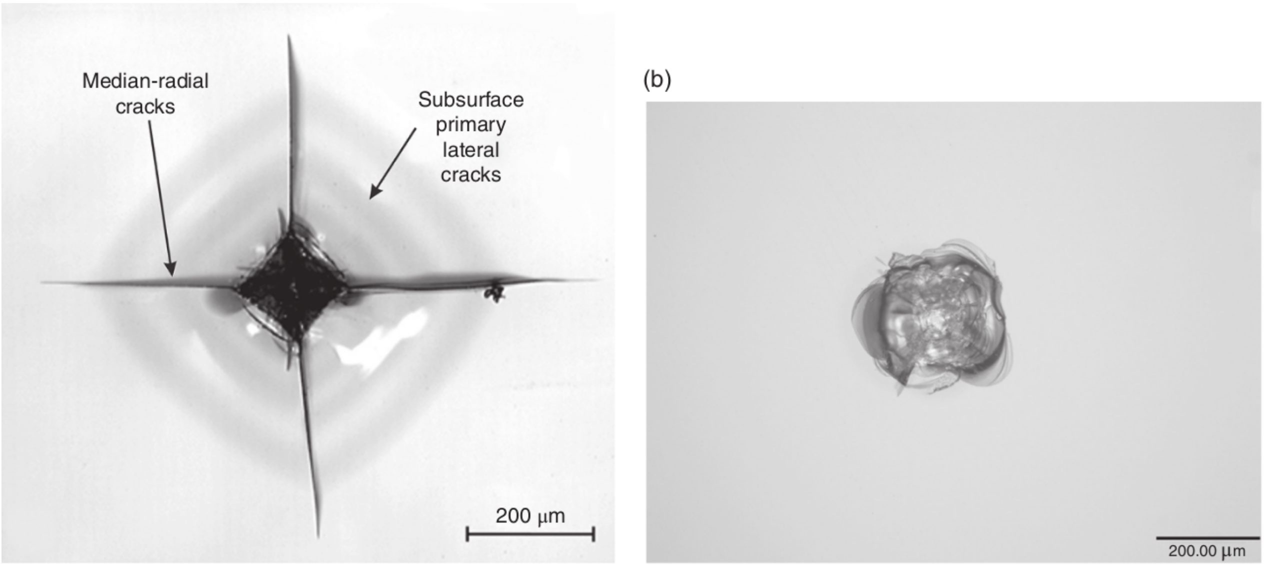

Figure 5 Contrast between Vicker's indentations on "normal" and "anomalous" glasses. (a) Soda-lime-silica glass showing the centrally deformed region, cross-shaped median-radial cracks as well as primary subsurface lateral cracks, which are visible as interference fringes; (b) fused silica.

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7 Optical Properties

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Atkins, Topic 18 C

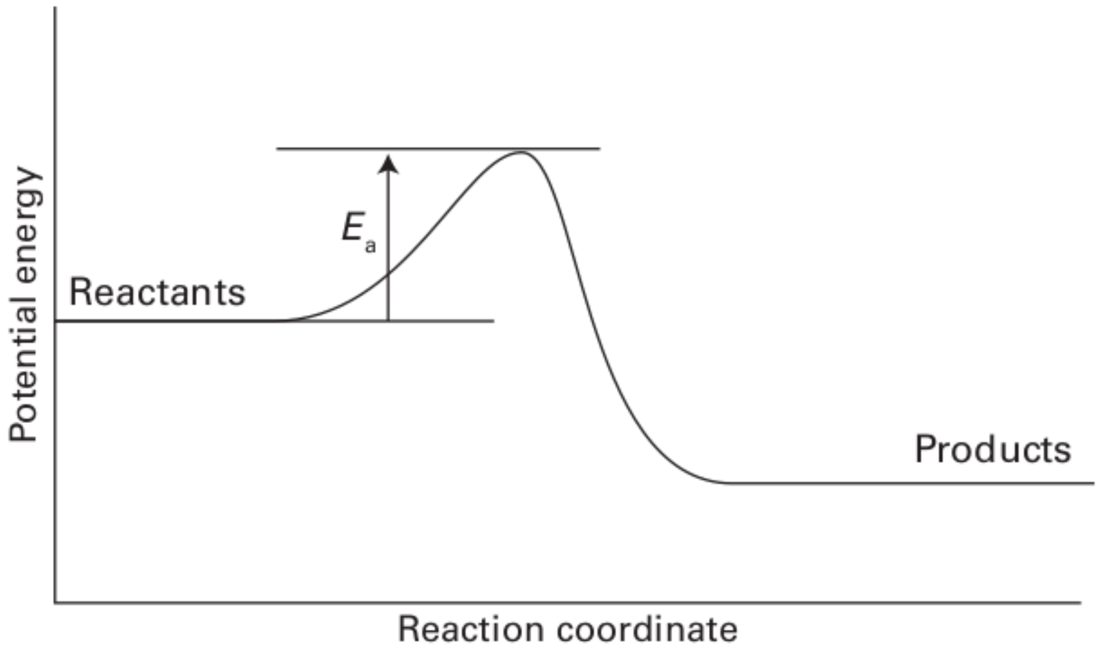


Figure 18C.1 A potential energy profile for an exothermic reaction. The height of the barrier between the reactants and products is the activation energy of the reaction.

18C.1 The Eyring equation

(a) The formulation of the equation

(b) The rate of decay of the activated complex

(c) The concentration of the activated complex

(d) The rate constant

9 Coherent-Potential Approximation

Schirmacher, 4.4

Random walk with fluctuating walk rates W_{ij}:

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\mathbf{r}_n, t) = \sum_{\substack{\ell \\ \mathrm{n.N.}}} W_{n\ell} \left[P(\mathbf{r}_\ell, t) - P(\mathbf{r}_n, t) \right]$$

If we set the left side of Eq. (4.43) equal to zero, we obtain the steady-state condition

$$\sum_{\substack{\ell \\ \mathrm{n.N.}}} W_{n\ell} \left[P(x_\ell) - P(x_n) \right] = 0 \, ,$$

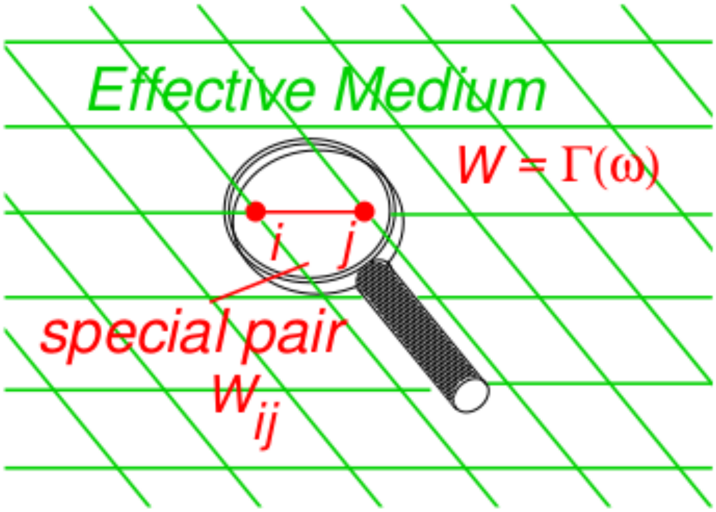
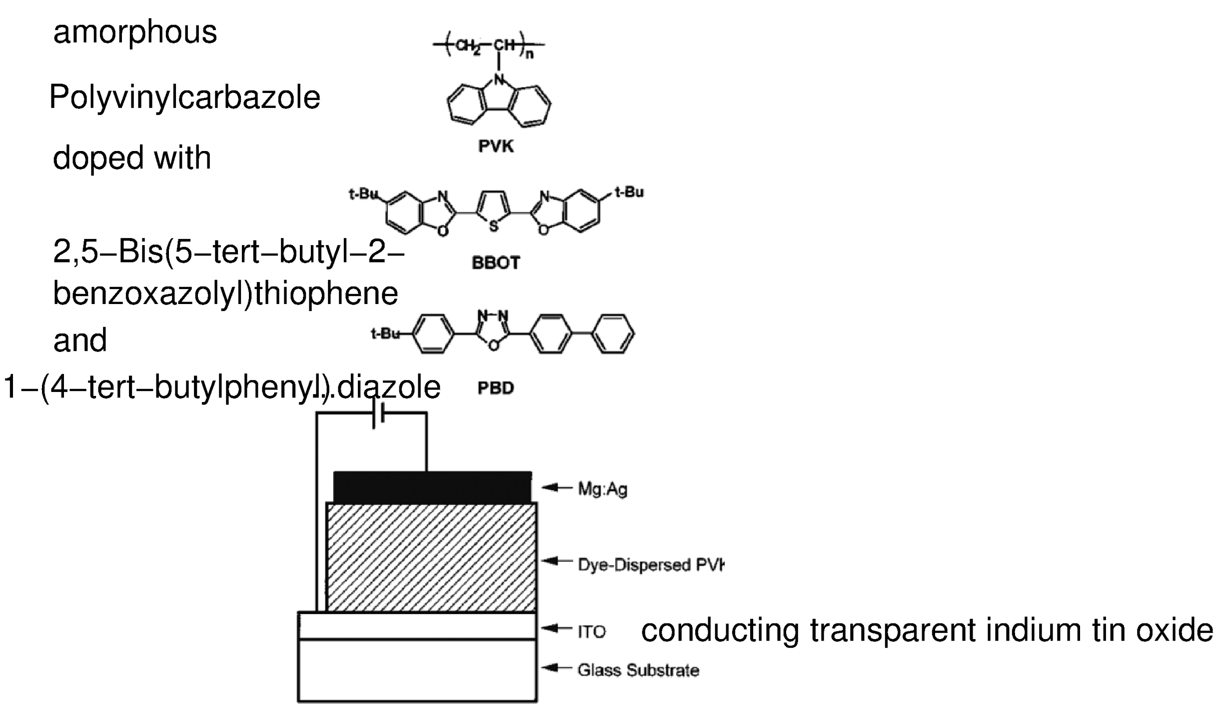


FIG. 4.4: Effective-Medium procedure for the 2-site coherent-potential approximation (CPA)

1. Derivation on a cubic lattice
2. Modification for a topological disordered system
3. calculating the AC conductivity

Encyclopedia, 6.10



Device structure and materials used in the first polymer-based white OLED reported by Kido, Shionoya, and Nagai (1995). BBOT and PBD are electron-transporting materials that are added to the hole-transporting PVK matrix to improve carrier balance. From Kido, Shionoya, and Nagai, 1995.

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11 Amorphous Ice

Encyclopedia, 3.14

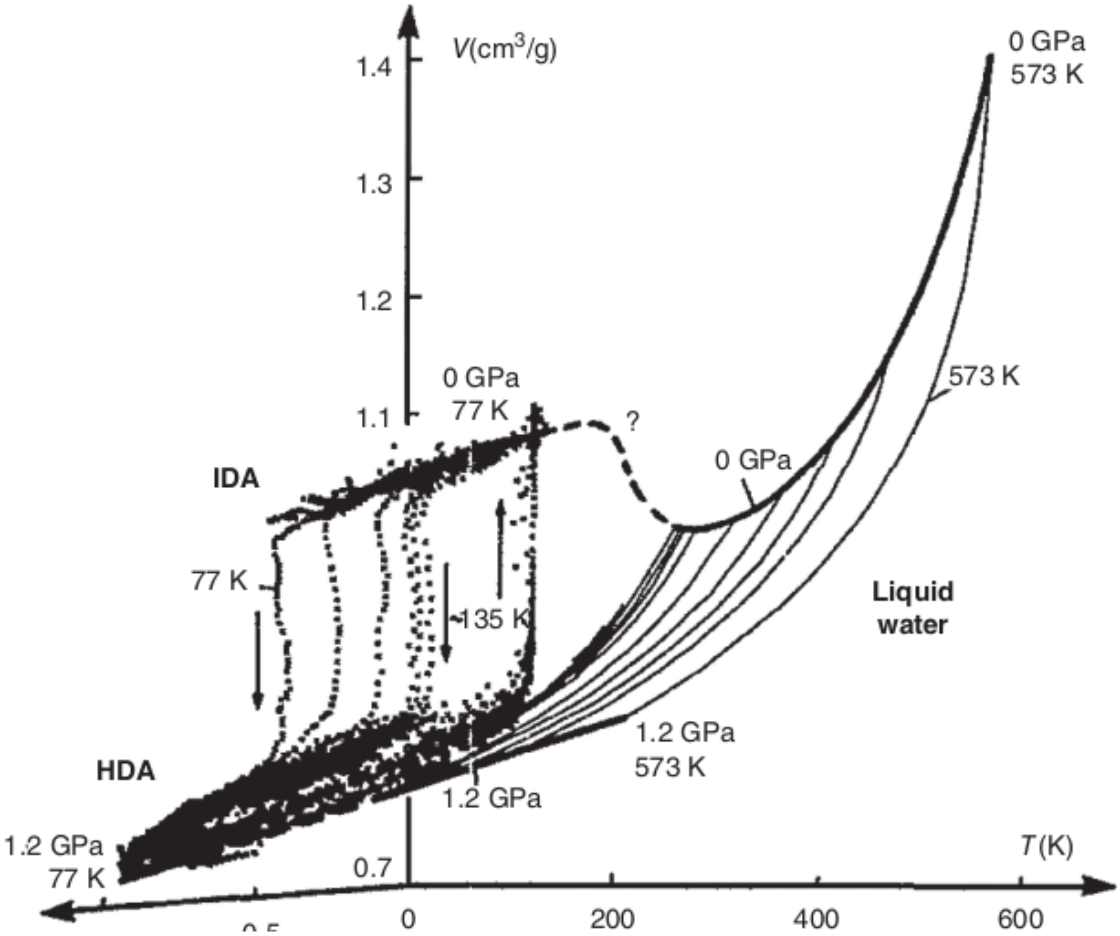

Figure 7 Volume changes as a function of pressure and temperature for the transition between the high- and low-density amorphous ices under nominal pressure of 0.55, 0.45, 0.38, and 0.32 GPa at 77, 100, 121, and 135 K respectively. Liquid water under 1.2 GPa at zero pressure also represented versus temperature. Connection between LDA and liquid state at zero pressure (e.g. liquid 1) occurring at 227 K. *Source:* Reproduced with permission from [7], © AIP Publishing.

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