Equation of State

First, density, ρ (g/cm³) is essentially the reciprocal of volume V (cm³) times molecular weight, M:

 $\rho = M/V$

Effect of Temperature: Expansivity

The thermal expansivity, α , is

$$\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_{H}$$

Integration gives the total effect on volume with changing temperature

$$\int_{T_o}^T \alpha(T) dT = \ln(V(T)/V_o) \equiv \Phi$$

Holland and Powell [1998] advocated a relationship between expansivity and temperature T(K), defined by a single constant a° for each mineral:

$$\alpha(T) = a^{\circ}(1 - 10\sqrt{T})$$

which gives

$$\partial \alpha / \partial T = 5a^o / T^{3/2}$$

and

$$\Phi = \ln(V(T)/V_o) = \int_{T_o}^T \alpha(T)dT = a^o \left\{ (T - T_o) - 20(\sqrt{T} - \sqrt{T_o}) \right\}$$

where V(T) is the molar volume at temperature, V_o is the molar volume at STP, and $T_o = 298$ K.

The density at elevated temperature $\rho(T)$ is related to the density at STP ρ_o by:

$$\rho(T) = \rho_o e^{-\Phi}$$

Effect of Pressure: Bulk Modulus

The isothermal compressibility, β_T , describes how volume changes as a function of pressure:

$$\beta_T = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T$$

The isothermal bulk modulus, K_T , (the reciprocal of the compressibility) is usually used instead:

$$\frac{1}{K_T} = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T$$

Moduli at High Temperature

The isothermal bulk modulus at elevated temperature $K_T(T)$ is related to the isothermal bulk modulus at STP K_{To} by:

$$K_T(T) = K_{To} e^{-\delta_T \Phi}$$

where δ_T is the second Grüneisen parameter:

$$\delta_T = \left(\frac{\partial \ln K_T}{\partial \ln \rho}\right)_P = \left(\frac{1}{K_T \alpha}\right) \left(\frac{\partial K_T}{\partial T}\right)_P$$

The shear modulus at elevated temperature $\mu(T)$ follows in similar fashion from the shear modulus at STP μ_{To} :

$$\mu_T(T) = \mu_{T_o} e^{-\Gamma \Phi}$$

where

$$\Gamma = \left(\frac{\partial \ln \mu}{\partial \ln \rho}\right)_P = -\left(\frac{1}{\mu\alpha}\right)\left(\frac{\partial \mu}{\partial T}\right)_P$$

Moduli at High Pressure

The relationship between strain ε and volume or density is

$$\left(\frac{V_o}{V}\right) = \left(\frac{\rho}{\rho_o}\right) = (1 - 2\varepsilon)^{3/2} = (1 + 2f)^{3/2}$$

where

 $f=-\varepsilon$

is the compression. The compression can be calculated recursively from

$$P/K_T = 3f(1+2f)^{5/2} \left\{ 1 - 2\xi f + f^2/6[4\xi(4-3K') + 5(3K'-5)] \right\}$$

where

$$\zeta = 0.75(4 - K')$$

and

$$K' = (dK_T / dP)_T$$

typically evaluated at T_o . The density at elevated pressure $\rho(P)$ is then

$$\rho(P) = \rho_o (1+2f)^{3/2}$$

Properties at High Temperature and Pressure

The bulk modulus at elevated pressure and temperature $K_T(T,P)$ is

$$K_T(T,P) = K_T(T) \Big\{ 1 - (5 - 3K') f^2 (3K' - 7)(3K' - 5) \Big\} (1 + 2f)^{5/2}$$

The expansivity at elevated pressure and temperature $\alpha(T,P)$ is

$$\alpha(T,P) = \alpha(T) [\rho(P)/\rho_o]^{-\delta_T}$$

The isentropic or adiabatic bulk modulus K_s is

$$K_S = K_T(T, P) [1 + T\gamma_{th} \alpha(T, P)]$$

where γ_{th} is the first Grüneisen parameter:

$$\gamma_{th} = \frac{VK_T\alpha}{C_V}$$

The shear modulus at elevated pressure and temperature $\mu(T,P)$ is

$$\mu(T,P) = \mu(T)(1+2f)^{5/2} \left\{ 1 - f \left[5 - 3\mu' K_T(T) / \mu(T) \right] + 0.5f^2 \left[9(K'-4)\mu' K_T(T) / \mu(T) + 35 \right] \right\}$$

The density at elevated pressure and temperature $\rho(P,T)$ is

$$\rho(T,P) = [\rho(P)/\rho_o]\rho(T)$$

From this it is possible to calculate the P-wave velocity V_P , shear wave velocity V_S , and Poisson's ratio v:

$$V_P = \sqrt{K_S + 4/3\mu/\rho}$$
$$V_S = \sqrt{\mu/\rho}$$
$$v = (3K_S - 2\mu)/(6K_S + 2\mu)$$

Physical Properties of Rocks

The physical property Ψ of a mineral aggregate can be calculated from the physical property Ψ_i of *n* constituent minerals using a a Reuss average (uniform stress):

$$\Psi_R = \sum_{i=1}^n [v_i \Psi_i]$$

a Voigt average (uniform strain):

$$\Psi_V = 1 / \sum_{i=1}^n [v_i / \Psi_i]$$

or a Voigt-Reuss-Hill average:

$$\Psi_{VRH} = \left\{ \Psi_{V+} \Psi_{R} \right\} / 2 = \left\{ \sum_{i=1}^{n} \Psi_{i} \nu_{i} + 1 / \sum_{i=1}^{n} [\nu_{i} / \Psi_{i}] \right\} / 2$$

where v_i is the volume proportion of each mineral. Because mass in aggregates is a simple sum of component masses, only Ψ_v is used in calculating ρ for aggregates.

Holland, T.J.B., and R. Powell, An internally consistent thermodynamic data set for phases of petrological interest, *Journal of Metamorphic Geology*, *16*, 309-343, 1998.