Elastic and thermal properties formulas

- Tetragonal shear modulus

$$C' = \frac{C_{11} - C_{12}}{2}$$

- Cauchy pressure

$$C_p = (C_{12} - C_{44})$$

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- The Kelixman parameter

$$\xi = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}}$$

- Pugh’s ratio

$$k = \frac{G}{B}$$

- Machinability

$$\mu_m = \frac{B}{C_{44}}$$

- Elastic Anisotropy,
  - $A_1 = \frac{4C_{44}}{C_{11} + C_{33} - 2C_{13}}$
  - $A_2 = \frac{4C_{55}}{C_{22} + C_{33} - 2C_{23}}$
  - $A_3 = A_1 . A_2$
- Universal log-Euclidean index,
  - $A_L = \sqrt{\left[\ln\left(\frac{B^v}{B^R}\right)\right]^2 + 5\left[\ln\left(\frac{C_{44}^V}{C_{44}^R}\right)\right]^2}$
  - $C_{44}^V = C_{44}^R + \frac{3}{5}\left\{\frac{(C_{11} - C_{12} - 2C_{44})^2}{3(C_{11} - C_{12}) + 4C_{44}}\right\}$
  - $C_{44}^R = \frac{5}{3}\left\{\frac{C_{44}(C_{11} - C_{12})}{3(C_{11} - C_{12}) + 4C_{44}}\right\}$

- Universal anisotropy index,

$$A^U = 5\left(\frac{G^v}{G^R}\right) + \left(\frac{B^v}{B^R}\right) - 6 \geq 0$$

- Universal Anisotropy in compressibility,

$$A^B = \frac{B_V + B_R}{B_V - B_R}$$

- Anisotropy in shear,

$$A^G \vee A^C = \frac{G^v - G^R}{2G^H}$$

- Equivalent Zener Anisotropy,

$$A^{eq} = \left(1 + \frac{5}{12}A^U\right) + \sqrt{\left(1 + \frac{5}{12}A^U\right)^2 - 1}$$

- Uniaxial bulk modulus along a, b and c – axis,
  - $B_a = a\frac{dp}{da} = \frac{\Lambda}{1+\alpha+\beta}$
  - $B_b = a\frac{dp}{db} = \frac{B_a}{\alpha}$
  - $B_c = a\frac{dp}{dc} = \frac{B_a}{\beta}$
  - $\Lambda = C_{11} + 2C_{12}\alpha + C_{22}\alpha^2 + 2C_{13}\beta + C_{33}\beta^2 + 2C_{33}\alpha\beta$
  - $\alpha = \frac{(C_{11} - C_{12})(C_{33} - C_{13}) - (C_{23} - C_{13})(C_{11} - C_{13})}{(C_{33} - C_{13})(C_{22} - C_{12}) - (C_{13} - C_{23})(C_{12} - C_{23})}$
  - $\beta = \frac{(C_{22} - C_{12})(C_{11} - C_{13}) - (C_{11} - C_{12})(C_{23} - C_{12})}{(C_{22} - C_{12})(C_{33} - C_{13}) - (C_{12} - C_{23})(C_{13} - C_{23})}$
  - $B_{relax} = \frac{\Lambda}{(1+\alpha+\beta)^2}$
- Anisotropics of bulk modulus along a-axis and c-axis,
  - $\{\}^A B_a = \frac{B_a}{B_c}$
  - $\{\}^A B_c = \frac{B_c}{B_b}$
- Linear compressibility along a-axis and c-axis,
  - $\beta_a = \frac{C_{33} - C_{13}}{(C_{11}+C_{12})C_{33} - 2(C_{13})^2}$
  - $\beta_c = \frac{C_{11} + C_{12} - 2C_{13}}{(C_{11}+C_{12})C_{33} - 2(C_{13})^2}$
  - Ratio of linear compressibility,

$$\alpha = \frac{\beta_C}{\beta_a}$$

- Transverse velocity,

$$v_t = \sqrt{\frac{G}{\rho}}$$

- Longitudinal velocity,

$$v_l = \left[\frac{3B + 4G}{3\rho}\right]^{\frac{1}{2}}$$

- Average velocity,

$$v_a = \left[\frac{1}{3} \left(\frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]$$

- Density of compound,

$$\rho = \frac{z \frac{m}{N_a}}{V_0}$$

- Acoustic impedance,

$$z = \sqrt{\rho G}$$

- Radiation factor on intensity of sound,

$$I = \sqrt{\frac{G}{\rho^3}}$$

- The Gruneisen parameter (where, σ = Poisson's ratio),

$$\gamma = \frac{3(1+\sigma)}{2(2-3\sigma)}$$

- Debye temperature,
  - $\theta_D = \frac{h}{K_B} \left(\frac{3n}{4\pi V_0} \right)^{\frac{1}{3}} v_a$
  - Or, $\theta_D = \frac{h}{K_B} \left[\left(\frac{3n}{4\pi} \right) \frac{N_A \rho}{M} \right]^{\frac{1}{3}} v_a$
- Melting temperature,

$$T_m = 354\,k + \frac{4.5\,k}{3\,Gpa} \left(2C_{11} + C_{33} \right) \pm 300\,k$$

- Thermal expansion coefficient
  - $\alpha = \frac{1.6 \times 10^{-3}}{G}$
  - $\alpha = \frac{0.02}{T_m}$
- Heat capacity of a material per unit volume
  - $\rho_{C_p} = 3 K_B N$, where N = no. of atoms per unit volume
- Minimum thermal Conductivity
  - $K_{min}^{clarke} = K_B V_a \left(V_{atomic} \right)^{\frac{-2}{3}}$
  - $K_{min}^{cahill} = \frac{K_B}{2.18} n^{\frac{2}{3}} \left(v_l + 2 v_t \right)$

    where n = atoms per unit volume.
- Lattice thermal conductivity
  - $k_{ph} = A(\gamma) \frac{M_{av} \theta_D^3 \delta}{\gamma^2 n^{\frac{2}{3}} T}$
  - $A(\gamma) = \frac{5.72 \times 10^7 \times 0.849}{2 \left[1 - \frac{0.514}{\gamma} + \frac{0.224}{\gamma^2} \right]}$
  - $\delta = \left(\frac{V_0}{N} \right)^{\frac{1}{3}}$
  - $M_{av} = \frac{Mass\ of\ compound}{No\ of\ atoms}$
  - $n = no\ of\ atoms\ per\ unit\ cell$

- $T = 300\,k$

- $H_{macro} = 2\left\{\left[\left(\frac{G}{B}\right)^2 G\right]^{0.585}\right\} - 3$
- $H_{micro} = \frac{(1-2\sigma)}{6(1+\sigma)}$
- $(H_V)_{Tian} = 0.92 * \left(\frac{G}{B}\right)^{1.137} G^{0.708}$
- $(H_V)_{Mazhnik} = 0.096 * X(\sigma) * Y$
- $X(\sigma) = \frac{1 - 8.5\sigma + 19.5\sigma^2}{1 - 7.6\sigma + 12.2\sigma^2 + 19.6\sigma^3}$

- Wave length of dominant phonon at T,
  - $\lambda_{dom} = \frac{12.566 \times v_a}{T} \times 10^{-12}$