

The Parameters used for MgO

EoS	V_o [cm ³]	K_o [GPa]	α_o [$\times 10^{-5} K^{-1}$]	a	b [$\times 10^{-3}$]	c [$\times 10^{-7}$]	d [$\times 10^{-10}$]	f	g [$\times 10^{-9}$]
Garai	11.142	165.15	2.957	1.721	-2.249	-2.0903	4.4	10.3	6.903

The Equation of State used here is:

$$V = nV_o e^{\frac{-p}{ap+bp^2+K_o} + (\alpha_o + cp+dp^2)T + \left(1 + \frac{cp+dp^2}{\alpha_o}\right)^f gT^2} \quad (1)$$

where, a is a linear, b is a quadratic term for the pressure dependence of the bulk modulus, c is a linear and d is a quadratic term for the pressure dependence of the volume coefficient of thermal expansion and f and g are parameters describing the temperature dependence of the volume coefficient of thermal expansion. The theoretical explanations for Eq. (1) and the physics of the parameters are discussed in detail [1]. The equation has an analytical solution for the temperature

$$T = \frac{-(\alpha_o + cp + dp^2) \pm \sqrt{(\alpha_o + cp + dp^2)^2 + 4g \left(1 + \frac{cp + dp^2}{\alpha_o}\right)^f \left[\ln\left(\frac{V}{V_o}\right) + \frac{p}{ap + bp^2 + K_o}\right]}}{2g \left(1 + \frac{cp + dp^2}{\alpha_o}\right)^f} \quad (2)$$

The pressure is determined by repeated substitutions as:

$$p = \lim_{n \rightarrow \infty} f^n(p) \quad (3)$$

where

$$f^n(p) = (K_o + ap_{n-1} + bp_{n-1}^2) \left[(\alpha_o + cp_{n-1} + dp_{n-1}^2) T + \left(1 + \frac{cp_{n-1} + dp_{n-1}^2}{\alpha_o}\right)^f gT^2 - \ln\left(\frac{V}{V_o}\right) \right] \quad (4)$$

$$n \in \mathbb{N}^* \quad \text{and} \quad p_0 = 0$$

The convergence of Equation (4) depends on pressure. For the maximum pressure used in this study (up to 140 GPa) $n = 15$ is sufficient. The maximum convergence error $[\varepsilon]$ for the investigated data set is 0.05 GPa where

$$\varepsilon \geq |f^{15}(p) - f^{14}(p)|. \quad (5)$$

Reference: [1] J. Garai, J. Applied Phys., 102 (2007) 123506.