EoS

The Equation of State used here is:

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

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

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

The pressure is determined by repeated substitutions as:

$$p = \lim_{n\to\infty} f^n(p) \tag{3}$$

where

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

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

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

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

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