MoB_2 BAJO PRESIÓN

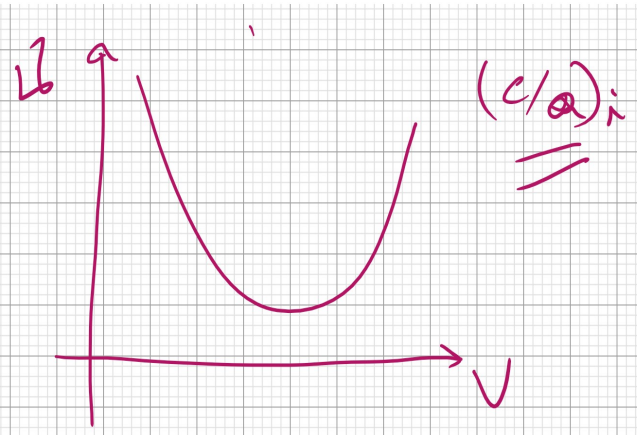
Birch-Murnagham EOS[5]

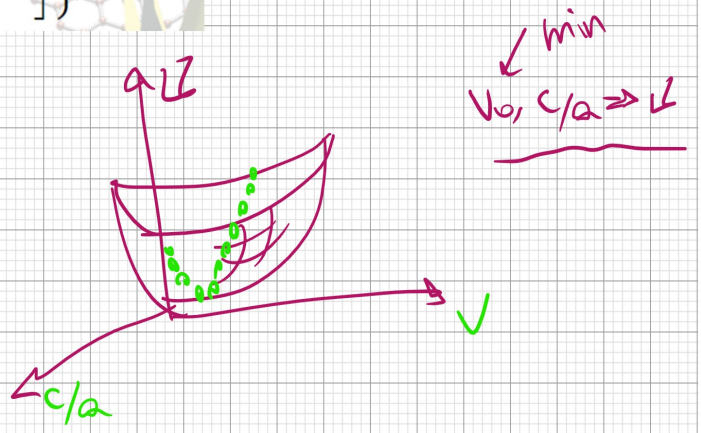
$$E(V) = E_0 + \frac{9B_0V_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 B' + \ldots\right.$$
$$\left. \ldots + \left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\},$$

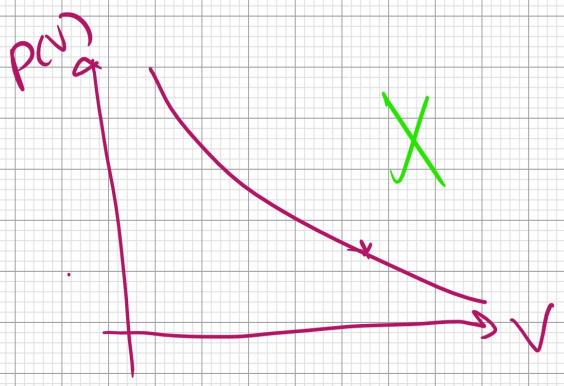
$$P(V) = \frac{3B_0}{2}\left[\left(\frac{V_0}{V}\right)^{7/3} - \left(\frac{V_0}{V}\right)^{5/3}\right] \times \ldots$$
$$\ldots \times \left\{1 + \frac{3}{4}(B' - 4)\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]\right\}.$$

$\nearrow P(V) = -\left.\frac{\partial E(V)}{\partial V}\right|_T$

$B_0 = -V\left.\frac{\partial P}{\partial V}\right|_T = V\left.\frac{\partial^2 E(V)}{\partial V^2}\right|_T$







Tasks

i) Invertir la ecuación $P(V) \Rightarrow V(P)$ ← analítico !!

$P(V): V \to P \Rightarrow V(P)$ $P \to V$ ⇐ 0 → 120GPa (1GPa) ← step

ii) (c/a) a ??? p

$c/a(V) = c/a(V_0) + \alpha(1 - V/V_0) + \beta(1 - V/V_0)^2$