

# Mineral Physics I

## Chapter 4. Equation of State

### Section 2. Birch-Murnaghan EOS

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# Finite strain theory

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## q Finite strain

Ø It deals with large compression, which cannot be approximated by the infinite strain

ü The compression in Eq. (4.1.8)  $P = K_{T0} \ln \left( \frac{V_0}{V} \right)$  is already large, though.

## q Eulerian finite strain

1. Compression is expressed by a state NOT before BUT **after compression** as a reference.

ü Compression is described not by  $V/V_0$  but by  $V_0/V$

§ When  $V$  goes to 0  $\Rightarrow P$  goes to  $\infty$   $\leftarrow$  easily expressed using  $\frac{V_0}{V} \rightarrow \infty$

2. Discussion starts from **change in squared length** by compression.



# Eulerian finite strain -1

q A cube with edge lengths of  $L_0$  in an unstrained state

$$\emptyset \text{ Volume: } V_0 = L_0^3 \quad (4.2.1)$$

q Uniformly compressed to edge lengths of  $L$

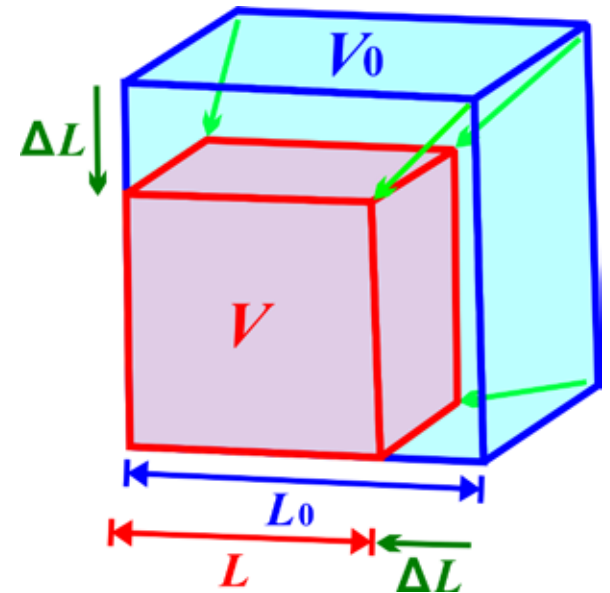
$$\emptyset \text{ Volume; } V = L^3 \quad (4.2.2)$$

q Shortening (displacement)  $\Delta L < 0$

$$\emptyset L = L_0 + \Delta L \quad (4.2.3)$$

q Change in squared edge length

$$\emptyset L_0^2 - L^2 = (L - \Delta L)^2 - L^2 = \Delta L^2 - 2L\Delta L \quad (4.2.4)$$



# Eulerian finite strain -2

q The shortening should be proportional to the edge length

$$\emptyset \Delta L = cL \quad (4.2.5)$$

q Eq. (4.2.4) is substituted to Eq. (4.2.5)

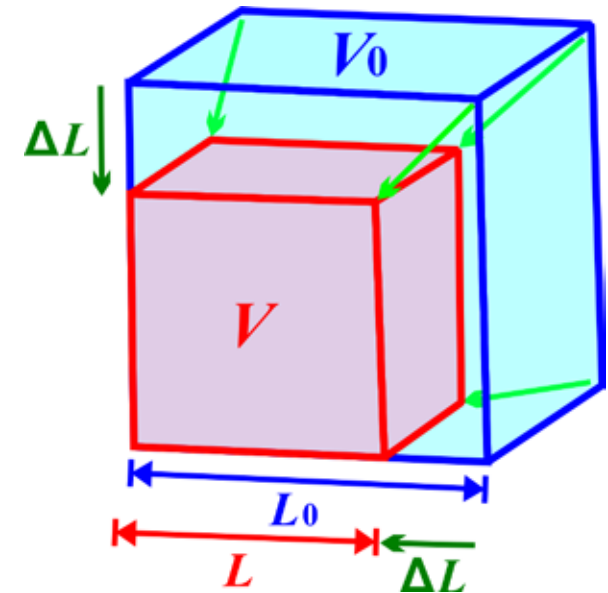
$$\begin{aligned} \emptyset L_0^2 - L^2 &= \Delta L^2 - 2L\Delta L = (cL)^2 - 2LcL \\ &= (c^2 - 2c)L^2 \end{aligned} \quad (4.2.6)$$

q Define the Eulerian finite strain as:

$$\emptyset f \equiv \frac{1}{2}c^2 - c \quad (4.2.7)$$

q Using this definition, Eq. (4.2.6) becomes

$$\emptyset L_0^2 - L^2 = 2fL^2$$



## Eulerian finite strain -3

$$\emptyset L_0^2 - L^2 = 2fL^2$$

$$\emptyset L_0^2 = (1 + 2f)L^2$$

$$\emptyset L_0^2/L^2 = (1 + 2f)$$

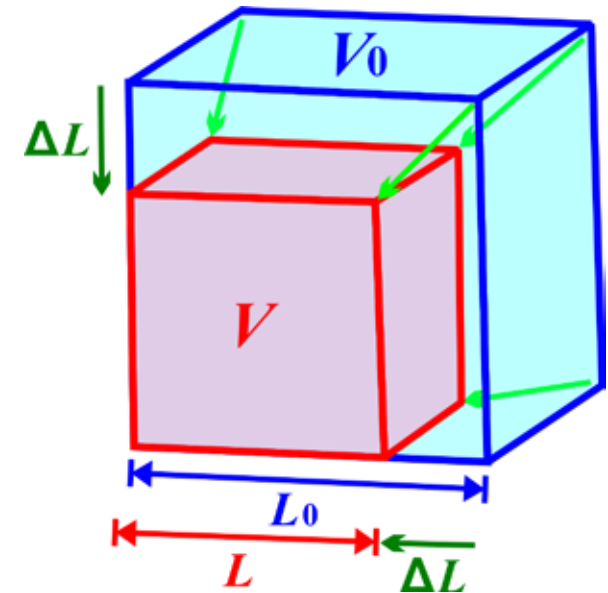
$$\emptyset L_0/L = (1 + 2f)^{1/2}$$

$$\emptyset V_0/V = L_0^3/L^3 = (1 + 2f)^{3/2}$$

$$\emptyset (V_0/V)^{2/3} = 1 + 2f$$

$$\emptyset f = \frac{1}{2} [(V_0/V)^{2/3} - 1] \quad (4.2.8)$$

ü The Eulerian finite strain is expressed by the volume compression



# 2<sup>nd</sup>-order Birch-Murnaghan EOS

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-1

q  $P$  is  $V$  derivative of  $F$  at constant  $T$

$$\emptyset P = -(\partial F / \partial V)_T \quad (4.1.1)$$

q  $F$  is assumed to increase proportionally to the squared  $f$  with  $V$  decrease

$$\emptyset \Delta F \cong a f^2 \quad (4.2.9)$$

ü  $a$ : constant

q  $V$  derivative of  $F$  is expressed by

$$\emptyset (\partial F / \partial V)_T = \{\partial(a f^2) / \partial V\}_T = 2 a f (\partial f / \partial V)_T$$

$$\emptyset P = -2 a f (\partial f / \partial V)_T \quad (4.2.10)$$

q As is shown later:

$$\emptyset a = (9/2) K_{T_0} V_0 \quad (4.2.11)$$



## 2<sup>nd</sup>-order Birch-Murnaghan EOS

-2

q The  $V$  derivative of  $f$  is:

$$\emptyset f = \frac{1}{2} \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] \quad (4.2.8)$$

$$\emptyset \left( \frac{\partial f}{\partial V} \right)_T = \frac{1}{2} V_0^{\frac{2}{3}} \frac{\partial}{\partial V} \left( V^{-\frac{2}{3}} \right)_T = -\frac{1}{3} V_0^{\frac{2}{3}} V^{-\frac{5}{3}} = -\frac{1}{3V_0} \left( \frac{V_0}{V} \right)^{\frac{5}{3}} \quad (4.2.12)$$

q The 2<sup>nd</sup>-order Birch-Murnaghan EOS:

$$\emptyset P = -2af \left( \frac{\partial f}{\partial V} \right)_T = -2 \left( \frac{9}{2} K_{T_0} V_0 \right) \times \frac{1}{2} \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] \times \left\{ -\frac{1}{3V_0} \left( \frac{V_0}{V} \right)^{\frac{5}{3}} \right\} \quad (4.2.10)$$

$$\emptyset P = \frac{3}{2} K_{T_0} \left[ \left( \frac{V_0}{V} \right)^{\frac{7}{3}} - \left( \frac{V_0}{V} \right)^{\frac{5}{3}} \right] \quad (4.2.13)$$



# Derivation of $a = \frac{9}{2} K_{T0} V_0$ -1

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q  $V$  derivative of  $f$  at  $P = 0$

$$\emptyset \left( \frac{\partial f}{\partial V} \right)_T = - \left( \frac{1}{3V_0} \right) \left( \frac{V_0}{V} \right)^{\frac{5}{3}} \quad (4.2.12)$$

$$\emptyset \left( \frac{\partial f}{\partial V} \right)_{T,P=0} = - \frac{1}{3V_0} \quad (4.2.14)$$

$$\ddot{u} V = V_0 \text{ at } P = 0$$

q  $V$  derivative of  $P$  at  $P = 0$

$\emptyset$  Definition of the isothermal bulk modulus:  $K_T = -V \left( \frac{\partial P}{\partial V} \right)_T$

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

$$\emptyset \left( \frac{\partial P}{\partial V} \right)_{T,P=0} = - \frac{K_{T0}}{V_0} \quad (4.2.15)$$





# Derivation of $a = \frac{9}{2} K_{T_0} V_0$ -2

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q  $V$  derivative of  $P$  is expressed by  $V$  derivative of  $f$  at  $P = 0$  from Eq. (4.2.10)

$$\emptyset P = -2af \left( \frac{\partial f}{\partial V} \right)_T \quad (4.2.10)$$

$$\emptyset \left( \frac{\partial P}{\partial V} \right)_T = \left[ \frac{\partial}{\partial V} \left\{ -2af \left( \frac{\partial f}{\partial V} \right)_T \right\} \right]_T = -2a \left[ \left( \frac{\partial f}{\partial V} \right)_T^2 + f \left( \frac{\partial^2 f}{\partial V^2} \right)_T \right] \quad (4.2.15)$$

$$\emptyset \left( \frac{\partial P}{\partial V} \right)_{T,P=0} = -2a \left( \frac{\partial f}{\partial V} \right)_{T,P=0}^2 \quad (4.2.16)$$

$$\ddot{u} f = 0 \text{ at } P = 0$$

q By substituting (4.2.14) and (4.2.15) into (4.2.16), we have;

$$\emptyset -\frac{K_{T_0}}{V_0} = -2a \left( -\frac{1}{3V_0} \right)^2$$
$$\emptyset a = \frac{9}{2} K_{T_0} V_0 \quad (4.2.11)$$



# 3<sup>rd</sup>-order Birch-Murnaghan EOS -1

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q The concept of the 3rd-order Birch-Murnaghan EOS: almost identical to that of the 2nd-order

q Difference: change in  $F$  is expanded not to the 2nd-order but to the 3rd-order of  $f$

$$\emptyset \Delta F \cong af^2 + bf^3 \quad (4.2.17)$$

q  $P$ :  $V$  derivative of  $F$ :

$$\emptyset P = - \left( \frac{\partial F}{\partial V} \right)_T$$

$$\emptyset \left( \frac{\partial F}{\partial V} \right)_T = \left\{ \frac{\partial}{\partial V} (af^2 + bf^3) \right\}_T = (2af + 3bf^2) \left( \frac{\partial f}{\partial V} \right)_T = 2af \left( 1 + \frac{3b}{2a} f \right) \left( \frac{\partial f}{\partial V} \right)_T$$

$$\emptyset P = -2af \left( 1 + \frac{3b}{2a} f \right) \left( \frac{\partial f}{\partial V} \right)_T \quad (4.2.18)$$



# 3<sup>rd</sup>-order Birch-Murnaghan EOS

-2

qAs shown in the next page

$$\emptyset \frac{3b}{2a} = \frac{3}{2}(K'_{T,0} - 4) \quad (4.2.19)$$

qBy substituting (4.2.8), (4.2.11), (4.2.12) and (4.2.19) into (4.2.18)  $P = -2af \left(1 + \frac{3b}{2a}f\right) \left(\frac{\partial f}{\partial V}\right)_T$ , we obtain the 3<sup>rd</sup>-order Birch-Murnaghan EOS:

$$\emptyset P = -2 \left(\frac{9}{2}K_{T_0}V_0\right) \times \frac{1}{2} \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right] \times \left\{1 + \frac{3}{2}(K'_{T_0} - 4) \frac{1}{2} \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]\right\} \times \left\{-\frac{1}{3V_0} \left(\frac{V_0}{V}\right)^{\frac{5}{3}}\right\}$$

$$\emptyset P = \frac{3}{2}K_{T_0} \left[\left(\frac{V_0}{V}\right)^{\frac{7}{3}} - \left(\frac{V_0}{V}\right)^{\frac{5}{3}}\right] \times \left\{1 + \frac{3}{4}(K'_{T_0} - 4) \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]\right\} \quad (4.2.20)$$

ü The 3<sup>rd</sup>-order BM-EOS becomes identical to the 2<sup>nd</sup>-order BM-EOS when

$$K'_{T_0} = 4$$



# Derivation of $\frac{3b}{2a} = \frac{3}{2} (K'_{T_0} - 4)$ -1

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q For simplicity,  $m = \frac{3b}{2a}$

q Eq. (4.2.18)  $P = -2af \left(1 + \frac{3b}{2a}f\right) \left(\frac{\partial f}{\partial V}\right)_T$  becomes

$$\emptyset P = -2af(1 + mf) \left(\frac{\partial f}{\partial V}\right)_T \quad (4.2.21)$$

q Differentiating (4.2.21) by  $V$ :

$$\begin{aligned} \emptyset \left(\frac{\partial P}{\partial V}\right)_T &= \left[\frac{\partial}{\partial V} \left\{-2af \left(\frac{\partial f}{\partial V}\right)_T (1 + mf)\right\}\right]_T \\ &= -2a \left[ \left(\frac{\partial f}{\partial V}\right)_T^2 + 2mf \left(\frac{\partial f}{\partial V}\right)_T + f \left(\frac{\partial^2 f}{\partial V^2}\right)_T + mf^2 \left(\frac{\partial^2 f}{\partial V^2}\right)_T \right] \end{aligned} \quad (4.2.22)$$



# Derivation of $\frac{3b}{2a} = \frac{3}{2} (K'_{T_0} - 4)$ -2

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q Eq. (4.2.22) is once again differentiated by  $V$ :

$$\emptyset \left( \frac{\partial^2 P}{\partial V^2} \right)_T = -2a \left[ \frac{\partial}{\partial V} \left\{ \left( \frac{\partial f}{\partial V} \right)_T^2 + 2mf \left( \frac{\partial f}{\partial V} \right)_T + f \left( \frac{\partial^2 f}{\partial V^2} \right)_T + mf^2 \left( \frac{\partial^2 f}{\partial V^2} \right)_T \right\} \right]_T$$

$$\left( \frac{\partial^2 P}{\partial V^2} \right)_T = -2a \left[ 3 \left( \frac{\partial f}{\partial V} \right)_T \left( \frac{\partial^2 f}{\partial V^2} \right)_T + 2m \left( \frac{\partial f}{\partial V} \right)_T^3 + 6mf \left( \frac{\partial f}{\partial V} \right)_T \left( \frac{\partial^2 f}{\partial V^2} \right)_T + f \left( \frac{\partial^3 f}{\partial V^3} \right)_T + \right]$$



# Derivation of $\frac{3b}{2a} = \frac{3}{2} (K'_{T_0} - 4)$ -3

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q 2<sup>nd</sup>  $V$  derivative of  $f$

$$\emptyset \left( \frac{\partial^2 f}{\partial V^2} \right)_T = \left( \frac{\partial}{\partial V} \left\{ -\frac{1}{3} V_0^{\frac{2}{3}} V^{-\frac{5}{3}} \right\} \right)_T = \frac{5}{9V_0^2} \left( \frac{V_0}{V} \right)^{\frac{8}{3}} \quad \text{à} \quad \left( \frac{\partial^2 f}{\partial V^2} \right)_{T,P=0} = \frac{5}{9V_0^2} \quad (4.2.25)$$

ü  $V_0/V = 1$  at  $P = 0$

q  $K_T'$  and 2<sup>nd</sup>  $V$  derivative of  $P$

$$\emptyset K_T' = \left( \frac{\partial K_T}{\partial P} \right)_T = \left( \frac{\partial K_T}{\partial V} \right)_T \left( \frac{\partial V}{\partial P} \right)_T = \left( \frac{\partial \{-V(\partial P/\partial V)_T\}}{\partial V} \right)_T \frac{-V}{-V(\partial P/\partial V)_T} = \frac{V^2(\partial^2 P/\partial V^2)_T}{K_T} - 1$$

$$\emptyset \left( \frac{\partial^2 P}{\partial V^2} \right)_T = \frac{K_T}{V^2} (K_T' + 1)$$

$$\emptyset \left( \frac{\partial^2 P}{\partial V^2} \right)_{T,P=0} = \frac{K_{T_0}}{V_0^2} (K'_{T_0} + 1) \quad (4.2.26)$$



# Derivation of $\frac{3b}{2a} = \frac{3}{2} (K'_{T_0} - 4)$ -4

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q By substituting (4.2.11)  $a = \frac{9}{2} K_{T_0} V_0$ , (4.2.15)  $\left(\frac{\partial f}{\partial V}\right)_{T,P=0} = -\frac{1}{3} V_0$ , (4.2.23)

$$\left(\frac{\partial^2 f}{\partial V^2}\right)_{T,P=0} = \frac{5}{9V_0^2}, \quad (4.2.24) \quad \left(\frac{\partial^2 P}{\partial V^2}\right)_{T,P=0} = \frac{K_{T_0}}{V_0^2} (K'_{T_0} + 1) \text{ into (4.2.26) } \left(\frac{\partial^2 P}{\partial V^2}\right)_{T,P=0} =$$

$$- 2a \left[ 3 \left(\frac{\partial f}{\partial V}\right)_{T,P=0} \left(\frac{\partial^2 f}{\partial V^2}\right)_{T,P=0} + 2m \left(\frac{\partial f}{\partial V}\right)_{T,P=0}^3 \right]$$

$$\emptyset \frac{K_{T_0}}{V_0^2} (K'_{T_0} + 1) = -2 \left(\frac{9}{2} K_{T_0} V_0\right) \left[ 3 \left(-\frac{1}{3V_0}\right) \frac{5}{9V_0^2} + 2m \left(-\frac{1}{3V_0}\right)^3 \right]$$

$$\emptyset \frac{K_{T_0}}{V_0^2} (K'_{T_0} + 1) = \frac{2}{27V_0^3} \frac{9}{2} K_{T_0} V_0 (2m + 15) \quad (4.2.27)$$

q By simplifying (4.2.27)

$$\emptyset m = \frac{3b}{2a} = \frac{3}{2} (K'_{T_0} - 4) \quad (4.2.19)$$



# 4<sup>th</sup>-order Birch-Murnaghan EOS

-1

q The concept of the 4<sup>th</sup>-order Birch-Murnaghan EOS: almost identical to that of the 2<sup>nd</sup>- and 3<sup>rd</sup>-orders

q Change in  $F$  is expanded to the 4<sup>th</sup>-order of  $f$

$$\emptyset \Delta F \cong a_2 f^2 + a_3 f^3 + a_4 f^4 \quad (4.2.28)$$

q  $P$ :  $V$  derivative of  $F$ :

$$\emptyset P = - \left( \frac{\partial F}{\partial V} \right)_T$$

$$\begin{aligned} \emptyset \left( \frac{\partial F}{\partial V} \right)_T &= \left\{ \frac{\partial}{\partial V} (a_2 f^2 + a_3 f^3 + a_4 f^4) \right\}_T = (2a_2 f + 3a_3 f^2 + 4a_4 f^3) \left( \frac{\partial f}{\partial V} \right)_T \\ &= 2af \left( 1 + \frac{3a_3}{2a_2} f + \frac{2a_4}{a_2} f^2 \right) \left( \frac{\partial f}{\partial V} \right)_T \end{aligned} \quad (4.2.29)$$





# 4<sup>th</sup>-order Birch-Murnaghan EOS

-2

q As shown in the next page

$$\emptyset \frac{2a_4}{a_2} = \frac{9K'_{T_0}{}^2 - 63K'_{T_0} + 9K_{T_0}K''_{T_0} + 143}{6} \quad (4.2.30)$$

ü  $K''_{T_0}$ : the second pressure derivative of  $K_{T_0}$

q Similarly to the 3<sup>rd</sup>-order Birch-Murnaghan EOS, we have 4<sup>th</sup>-order EOS:

$$\begin{aligned} \emptyset P &= -2 \left( \frac{9}{2} K_{T_0} V_0 \right) \times \frac{1}{2} \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] \times \left\{ -\frac{1}{3V_0} \left( \frac{V_0}{V} \right)^{\frac{5}{3}} \right\} \\ &\times \left\{ 1 + \frac{3}{2} (K'_{T_0} - 4) \frac{1}{2} \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] + \frac{9K'_{T_0}{}^2 - 63K'_{T_0} + 9K_{T_0}K''_{T_0} + 143}{6} \left\{ \frac{1}{2} \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] \right\}^2 \right\} \\ \emptyset P &= \frac{3}{2} K_{T_0} \left[ \left( \frac{V_0}{V} \right)^{\frac{7}{3}} - \left( \frac{V_0}{V} \right)^{\frac{5}{3}} \right] \times \left\{ 1 + \frac{3}{4} (K'_{T_0} - 4) \left[ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] + \frac{9K'_{T_0}{}^2 - 63K'_{T_0} + 9K_{T_0}K''_{T_0} + 143}{24} \left\{ \left( \frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right\}^2 \right\} \end{aligned} \quad (4.2.31)$$



# Derivation of $\frac{2a_4}{a_2} = \frac{9K'_{T_0}{}^2 - 63K'_{T_0} + 9K_{T_0}K''_{T_0} + 143}{6}$ -1

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q For simplicity,  $m_2 = 2a_4/a_2$

q Eq. (4.2.18)

$$\begin{aligned} \emptyset P &= -(2a_2f + 3a_3f^2 + a_4f^3) \left(\frac{\partial f}{\partial V}\right)_T \\ &= -2a_2f(1 + m_1f + m_2f^2) \left(\frac{\partial f}{\partial V}\right)_T \end{aligned} \quad (4.2.31)$$

q Differentiating (4.2.31) by  $V$ :

$$\emptyset \left(\frac{\partial P}{\partial V}\right)_T = -2a_2 \left\{ (1 + 2m_1f + 3m_2f^2) \left(\frac{\partial f}{\partial V}\right)_T^2 + (f + m_1f^2 + m_2f^3) \left(\frac{\partial^2 f}{\partial V^2}\right)_T \right\} \quad (4.2.32)$$



$$\text{Derivation of } \frac{2a_4}{a_2} = \frac{9K'_{T_0}{}^2 - 63K'_{T_0} + 9K_{T_0}K''_{T_0} + 143}{6} \quad -2$$


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q Eq. (4.2.32) is once again differentiated by  $V$ :

$$\emptyset \left( \frac{\partial^2 P}{\partial V^2} \right)_T = -2a_2 \left\{ \begin{array}{l} (2m_1 + 6m_2 f) \left( \frac{\partial f}{\partial V} \right)_T^3 \\ + 3 \left( 1 + 2m_1(2m_1 + 6m_2 f) \left( \frac{\partial f}{\partial V} \right)_T^3 + 3m_2 f^2 \right) \left( \frac{\partial f}{\partial V} \right)_T \left( \frac{\partial^2 f}{\partial V^2} \right)_T \\ + (f + m_1 f^2 + m_2 f^3) \left( \frac{\partial^3 f}{\partial V^3} \right)_T \end{array} \right\} \quad (4.2.33)$$

q Eq. (4.2.33) is once again differentiated by  $V$ :

$$\emptyset \left( \frac{\partial^3 P}{\partial V^3} \right)_T = -2a_2 \left\{ \begin{array}{l} 6m_2 \left( \frac{\partial f}{\partial V} \right)_T^4 + 6(2m_1 + 6m_2 f) \left( \frac{\partial f}{\partial V} \right)_T^2 \left( \frac{\partial^2 f}{\partial V^2} \right)_T \\ + 3(1 + 2m_1 f + 3m_2 f^2) \left( \frac{\partial^2 f}{\partial V^2} \right)_T^2 + 4(1 + 2m_1 f + 3m_2 f^2) \left( \frac{\partial f}{\partial V} \right)_T \left( \frac{\partial^3 f}{\partial V^3} \right)_T \\ + (f + m_1 f^2 + m_2 f^3) \left( \frac{\partial^4 f}{\partial V^4} \right)_T \end{array} \right\} \quad (4.2.34)$$



$$\text{Derivation of } \frac{2a_4}{a_2} = \frac{9K'_{T_0}{}^2 - 63K'_{T_0} + 9K_{T_0}K''_{T_0} + 143}{6} \quad -3$$

q At  $P = 0$ ,  $V_0/V = 1$ ,  $f = 0$ :

$$q \left( \frac{\partial^3 P}{\partial V^3} \right)_T = -2a_2 \left\{ \begin{aligned} &6m_2 \left( \frac{\partial f}{\partial V} \right)_T^4 + 6(2m_1 + 6m_2 f) \left( \frac{\partial f}{\partial V} \right)_T^2 \left( \frac{\partial^2 f}{\partial V^2} \right)_T \\ &+ 3(1 + 2m_1 f + 3m_2 f^2) \left( \frac{\partial^2 f}{\partial V^2} \right)_T^2 + 4(1 + 2m_1 f + 3m_2 f^2) \left( \frac{\partial f}{\partial V} \right)_T \left( \frac{\partial^3 f}{\partial V^3} \right)_T \\ &+ (f + m_1 f^2 + m_2 f^3) \left( \frac{\partial^4 f}{\partial V^4} \right)_T \end{aligned} \right\}$$

$$q \left( \frac{\partial^3 P}{\partial V^3} \right)_{T,0} = -2a_2 \left\{ 6m_2 \left( \frac{\partial f}{\partial V} \right)_{T,0}^4 + 12m_1 \left( \frac{\partial f}{\partial V} \right)_{T,0}^2 \left( \frac{\partial^2 f}{\partial V^2} \right)_{T,0} + 3 \left( \frac{\partial^2 f}{\partial V^2} \right)_{T,0}^2 + \right.$$

(4.2.35)



$$\text{Derivation of } \frac{2a_4}{a_2} = \frac{9K'_{T_0}{}^2 - 63K'_{T_0} + 9K_{T_0}K''_{T_0} + 143}{6} \quad - 4$$


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q 3<sup>rd</sup>  $V$  derivative of  $f$

$$\emptyset f = \frac{1}{2} \left\{ \left( \frac{V_0}{V} \right)^{2/3} - 1 \right\}$$

$$\emptyset \left( \frac{\partial f}{\partial V} \right)_T = \partial / \partial V \left[ (1/2) \left\{ \left( \frac{V_0}{V} \right)^{2/3} - 1 \right\} \right] = - \left( \frac{1}{3V_0} \right) \left( \frac{V_0}{V} \right)^{5/3}$$

$$\emptyset \left( \frac{\partial^2 f}{\partial V^2} \right)_T = \left( \partial / \partial V \left\{ - \left( \frac{1}{3V_0} \right) \left( \frac{V_0}{V} \right)^{5/3} \right\} \right)_T = \left( \frac{5}{9V_0^2} \right) \left( \frac{V_0}{V} \right)^{8/3}$$

$$\emptyset \left( \frac{\partial^3 f}{\partial V^3} \right)_T = \left( \partial / \partial V \left\{ \left( \frac{5}{9V_0^2} \right) \left( \frac{V_0}{V} \right)^{8/3} \right\} \right)_T = \left( - \frac{40}{27V_0^3} \right) \left( \frac{V_0}{V} \right)^{11/3} \quad (4.2.36)$$

q at  $P = 0$ ,  $V_0/V = 1$

$$\ddot{u} \left( \frac{\partial^3 f}{\partial V^3} \right)_{T,0} = - \frac{40}{27V_0^3} \quad (4.2.37)$$



$$\text{Derivation of } \frac{2a_4}{a_2} = \frac{9K_{T_0}'^2 - 63K_{T_0}' + 9K_{T_0}K_{T_0}'' + 143}{6} \quad -5$$

q 3<sup>rd</sup>-V derivative of P expressed by  $K_T$ ,  $K_T'$  and  $K_T''$

$$\emptyset \left( \frac{\partial P}{\partial V} \right)_T = -\frac{K_T}{V}, \quad \left( \frac{\partial^2 P}{\partial V^2} \right)_T = \frac{\partial}{\partial V} \left\{ -\frac{K_T}{V} \right\} = \frac{K_T}{V^2} (K_T' + 1)$$

$$\emptyset \left( \frac{\partial^3 P}{\partial V^3} \right)_T = \frac{\partial}{\partial V} \left\{ \frac{K_T}{V^2} (K_T' + 1) \right\}_T = \left\{ \frac{\partial P}{\partial V} \frac{\partial K_T}{\partial P} \right\} \frac{(K_T' + 1)}{V^2} - 2 \frac{K_T}{V^3} (K_T' + 1) + \frac{K_T}{V^2} \frac{\partial P}{\partial V} \frac{\partial K_T'}{\partial P}$$

$$\emptyset \left( \frac{\partial^3 P}{\partial V^3} \right)_T = - \left( -V \frac{\partial P}{\partial V} \right) K_T' \frac{(K_T' + 1)}{V^3} - 2 \frac{K_T}{V^3} (K_T' + 1) - \frac{K_T}{V^3} \left( -V \frac{\partial P}{\partial V} \right) K_T''$$

$$\emptyset \left( \frac{\partial^3 P}{\partial V^3} \right)_T = -\frac{K_T}{V^3} (K_T'^2 + 3K_T' + 2 + K_T K_T'')$$

q At zero pressure,

$$\emptyset \left( \frac{\partial^3 P}{\partial V^3} \right)_{T,0} = -\frac{K_{T,0}}{V_0^3} (K_{T,0}'^2 + 3K_{T,0}' + K_{T,0}K_{T,0}'' + 2) \quad (4.2.38)$$

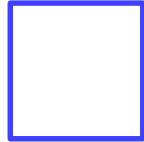
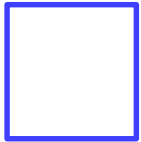
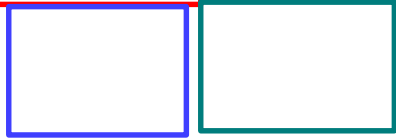


Derivation of  $\frac{2a_4}{a_2} = \frac{9K'_{T_0}{}^2 - 63K'_{T_0} + 9K_{T_0}K''_{T_0} + 143}{6}$  - 6

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q Eq. (4.2.35) becomes

$$\emptyset \left( \frac{\partial^3 P}{\partial V^3} \right)_{T,0} = -2a_2 \left\{ 6m_2 \left( \frac{\partial f}{\partial V} \right)_T^4 + 12m_1 \left( \frac{\partial f}{\partial V} \right)_{T,0}^2 \left( \frac{\partial^2 f}{\partial V^2} \right)_{T,0} + 3 \left( \frac{\partial^2 f}{\partial V^2} \right)_{T,0}^2 + \right.$$



The 3<sup>rd</sup>-order EOS is not obtained by  $K''_{T,0} = 0$ .



# Publications

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## English version

### A Simple Derivation of the Birch–Murnaghan Equations of State (EOSs) and Comparison with EOSs Derived from Other Definitions of Finite Strain

by  Tomoo Katsura<sup>1,2,\*</sup>  and  Yoshinori Tange<sup>3</sup> 

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## Japanese version

解説

### バーチ・マーンハン状態方程式の平易な導出と、他の状態方程式との比較

A Plain Derivation of Birch-Murnaghan Equations of State, and Comparison with Other Equations of State

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丹下 慶範<sup>3</sup>

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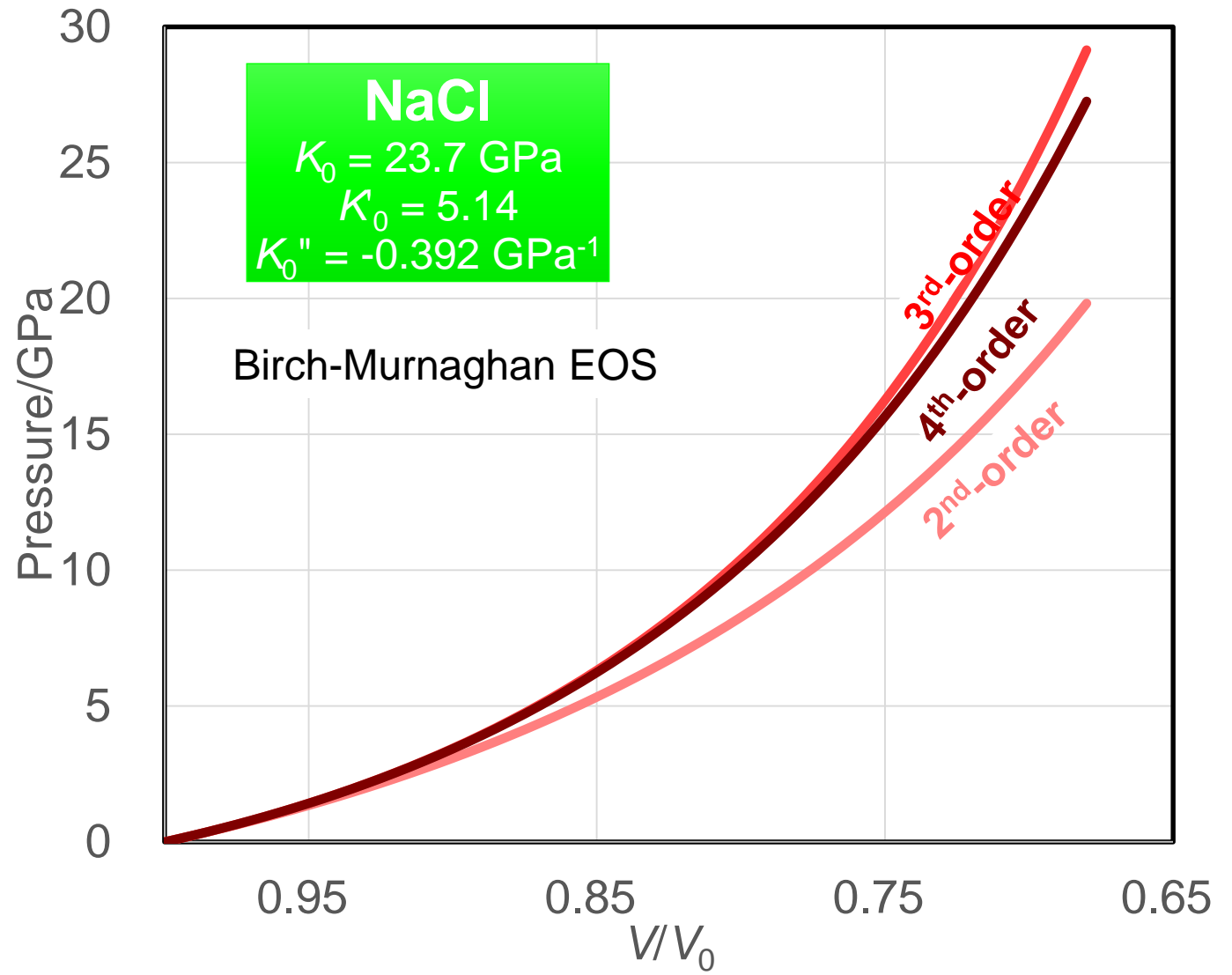
# Compression of NaCl based on BM-EOS

Very low  $K_0 = 23.7$  GPa

$K_0$  larger than 4 (5.14)

negative  $K_0''$

Relatively low pressure values even at high compression



# Compression of MgO based on BM-EOS

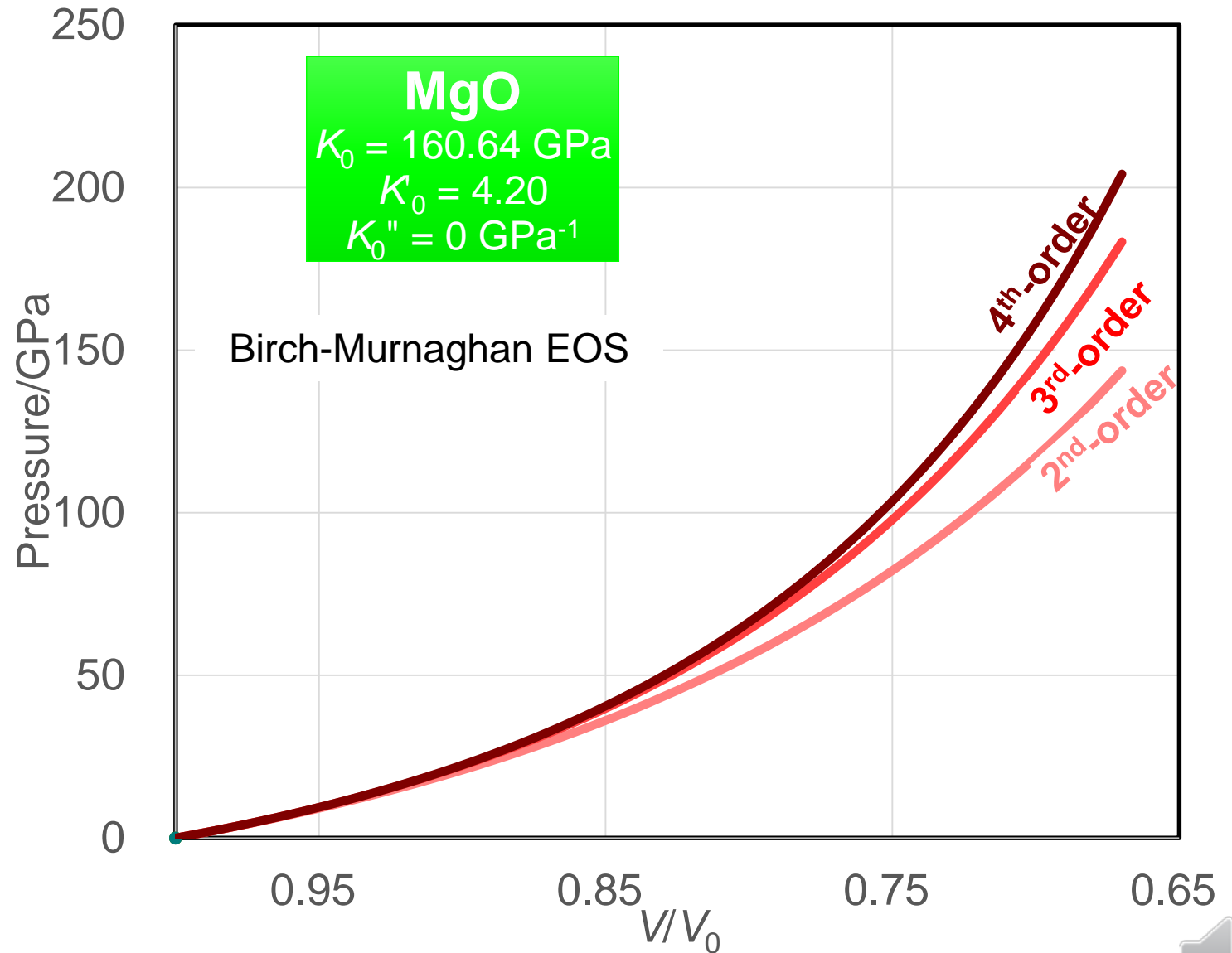
Relatively high  $K_0 = 160$  GPa

$K_0$  slightly larger than 4 (4.20)

No  $K_0''$  data

$K_0''=0$  does not mean that 4<sup>th</sup> EOS becomes 3<sup>rd</sup> EOS

Relatively high pressure values by large compression



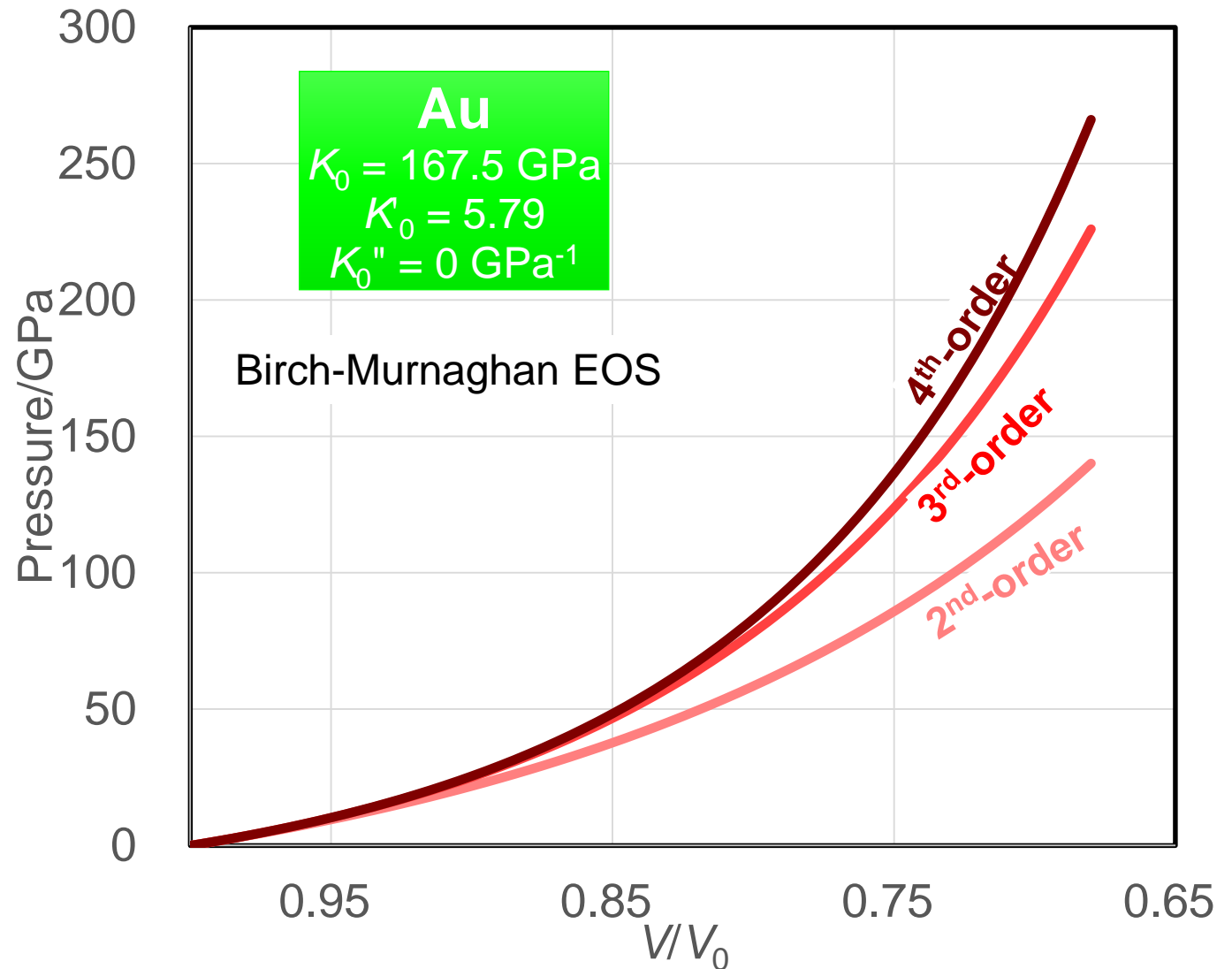
# Compression of Au based on BM-EOS

Relatively high  $K_0 = 168$  GPa

$K_0$  larger than 4 (5.8)

No  $K_0''$  data

Relatively high pressure values by large compression



Mineral Physics I  
Chapter 4. Equation of state  
Section 2. Birch-Murnaghan equation of state

End

