Ultrasonic measurements of polycrystalline MgO and standard-free pressure calibration at high pressures and high temperatures

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**Acknowledgment to Auke Barnhoon and Ian Jackson for supplying MgO sample used here
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Problem in determining P-V-T equation of state (EoS)

Determination of P-V-T EoS by high-pressure X-ray diffraction study **uses pressure** calculated from previously reported EoS

→The P-V-T relation depends on previous pressure scale.

In order to determine correct pressure from P-V-T EoS, we need to establish P-V-T EoS **without pressure scale.**

Birch-Murnaghan equation of state

$$P = 3K_{T0}(1+2\varepsilon)^{5/2}\varepsilon(1+3(K'_{T0}-4)\varepsilon/2)$$

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

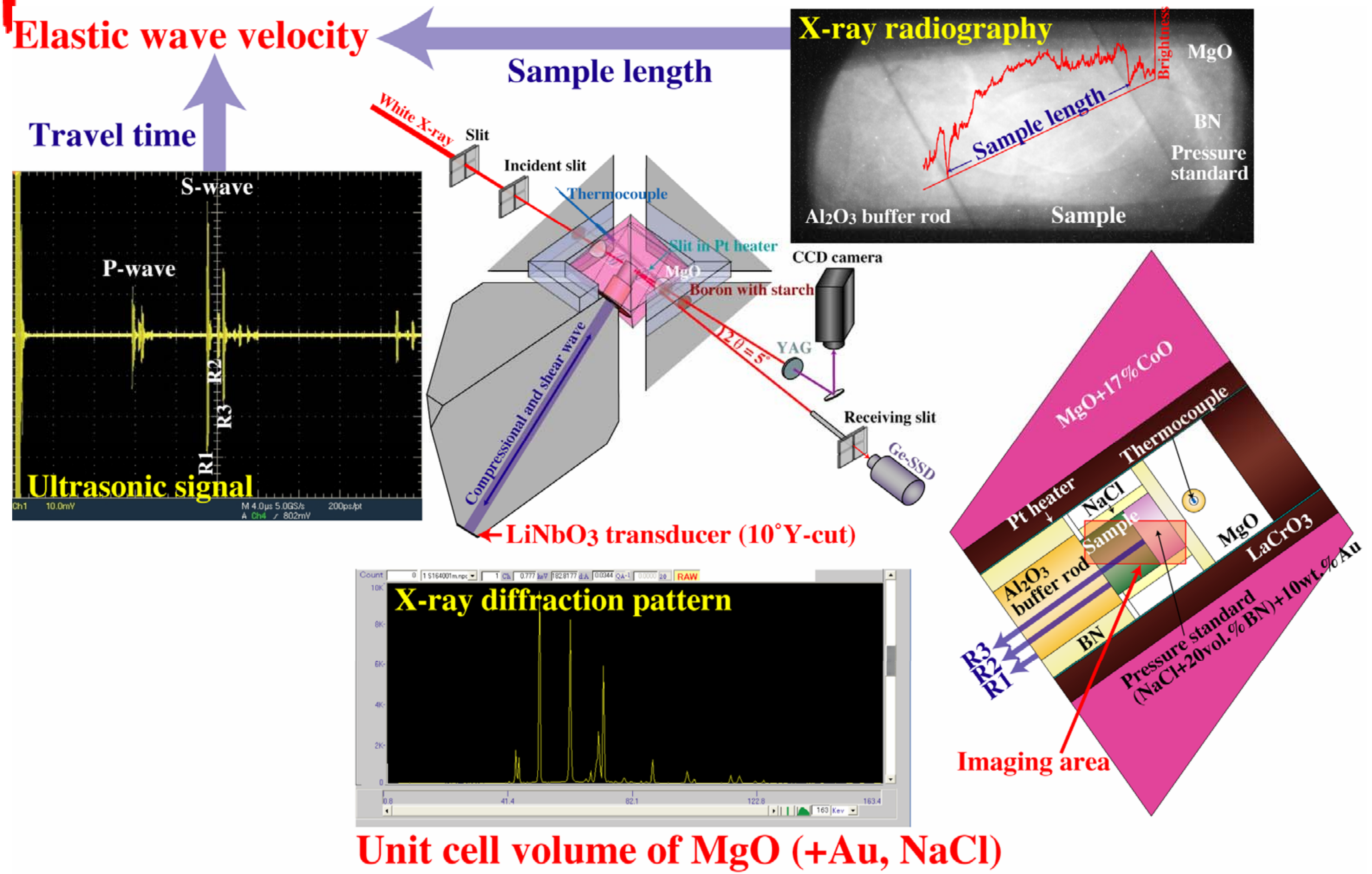
Elastic wave velocity measurement + X-ray diffraction experiment
→Ks, unit cell volume without pressure scale
→Standard-free P-V-T EoS

Standard-free pressure calibration from elastic wave velocity measurement

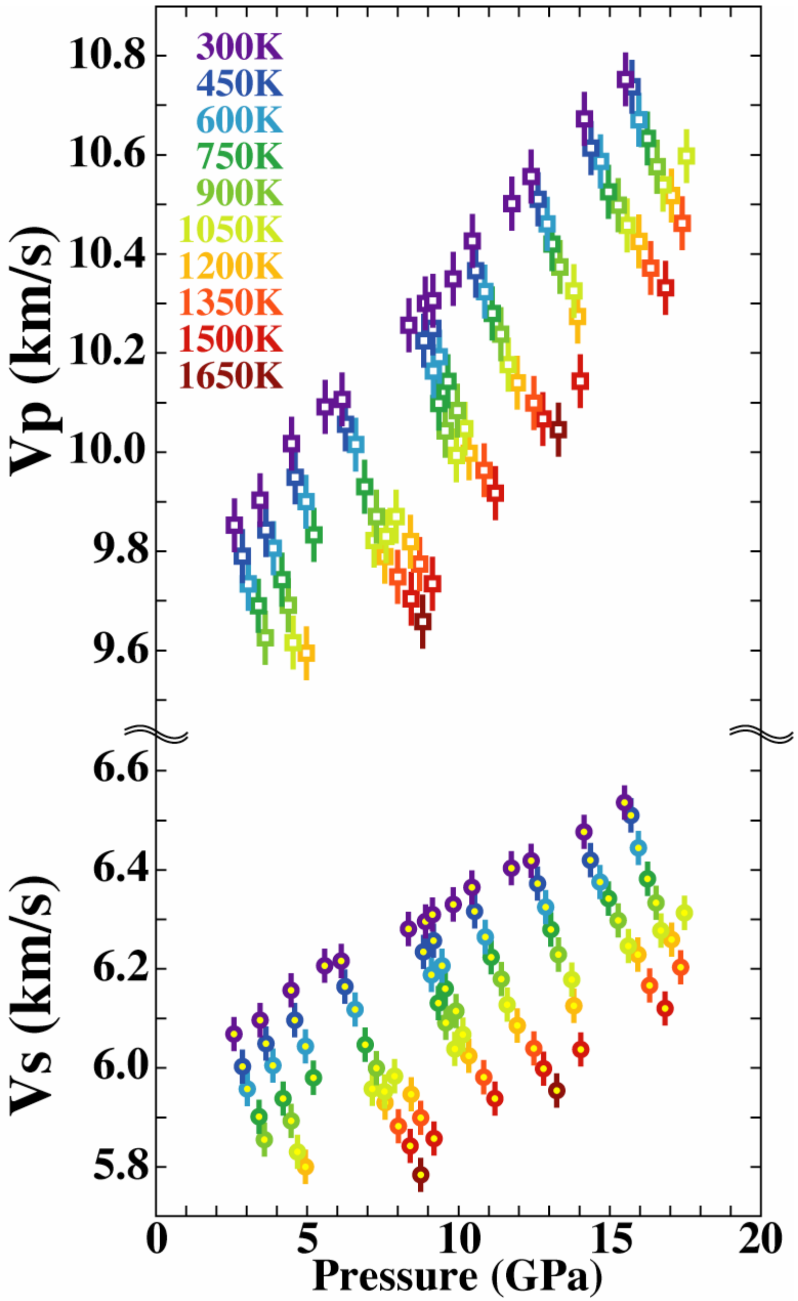
	Method	Pressure	Temperature	Sample
Zha et al. (2000)	Brillouin scattering	55 GPa	**300 K**	**MgO**
Mueller et al. (2003)	Ultrasonic	~8 GPa	**300 K**	NaCl
Li et al. (2005)	Ultrasonic	20 GPa	**300 K**	Ferropericlase
				Wadsleyite
Li et al. (2006)	Ultrasonic	11 GPa	**300 K**	**MgO**
This study	**Ultrasonic**	**18 GPa**	**1650 K**	**MgO**

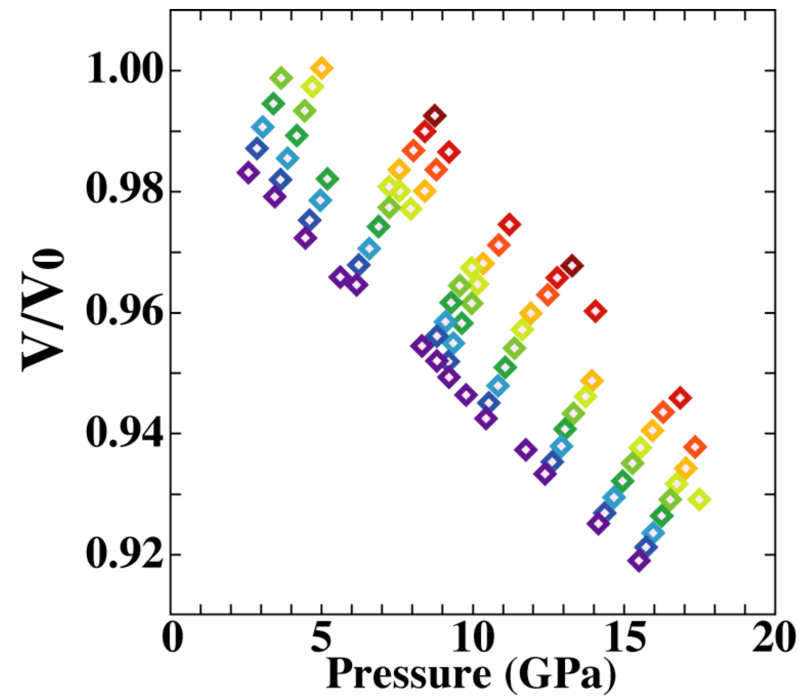
No standard-free pressure calibration has been carried out at high temperatures.

Elastic wave velocity measurement at BL04B1, SPring-8



Experimental results





The pressures are temporally calculated from the EoS of Anderson et al. (1989)

Determination of isothermal bulk modulus without pressure

$$K_S = \rho(Vp^2 - 4Vs^2/3)$$

$$K_T = K_S/(1+\alpha\gamma T)$$

$$K_T = K_{T0}(1+2\varepsilon)^{5/2}(1+(3K'_T-5)\varepsilon) \qquad \varepsilon = \{(V_0/V)^{2/3}-1\}/2$$

$$K_S/(1+\alpha\gamma T) = 3K_{T(0,T)}(1+2\varepsilon)^{5/2}\varepsilon(1+3(K'_{T(T)}-4)\varepsilon/2)$$

$$K_{T(0,T)} = K_{T0} + \partial K_T/\partial T \times T$$

$$K'_{T(T)} = K'_{T0} + \partial^2 K_T/\partial PT \times T$$

Fixed parameters

α_0 : **Dubrovinsky and Saxena (1997)**

γ_0, q_0, q_1 : **Speziale et al. (2001)**

Determined parameters

$$K_{T0},\ K'_{T0},\ \partial K_T/\partial T,\ \partial^2 K_T/\partial PT$$

K_{T0} and K'_{T0} of MgO

	K_{T0}	K'_{T0}
Ultrasonic		
This study	**160.6 (5)**	**4.30 (6)**
Li et al. (2006)	161.3	4.24
Brillouin scattering		
Zha et al. (2000)	160.2 (7)	4.03 (3)
P-V relation		
Speziale et al. (2001)	160.2 (fix)	3.99 (1)
MD simulation		
Matsui et al. (2000)	161	4.1
Shock wave		
Vassilou &Ahrens (1981)	162.7 (fix)	4.27 (24)

High-temperature third-order Birch-Murnaghan EoS

$$P = 3K_{T(0,T)}(1+2\varepsilon)^{5/2}\varepsilon(1+3(K'_{T(T)}-4)\varepsilon/2)$$

$$\frac{V_0}{V} = \frac{V_{(0,T)}/V_{(0,300)}}{V_{(P,T)}/V_{(0,300)}} = \frac{\exp\left(\int_{300}^{T}\alpha_0 dT\right)}{V_{(P,T)}/V_{(0,300)}}$$

$$\alpha_0 = 2.6025\times10^{-5} + 1.3535\times10^{-8}\times T + 6.5687\times10^{-3}\times T^{-2} - 1.8281\times T^{-3}$$

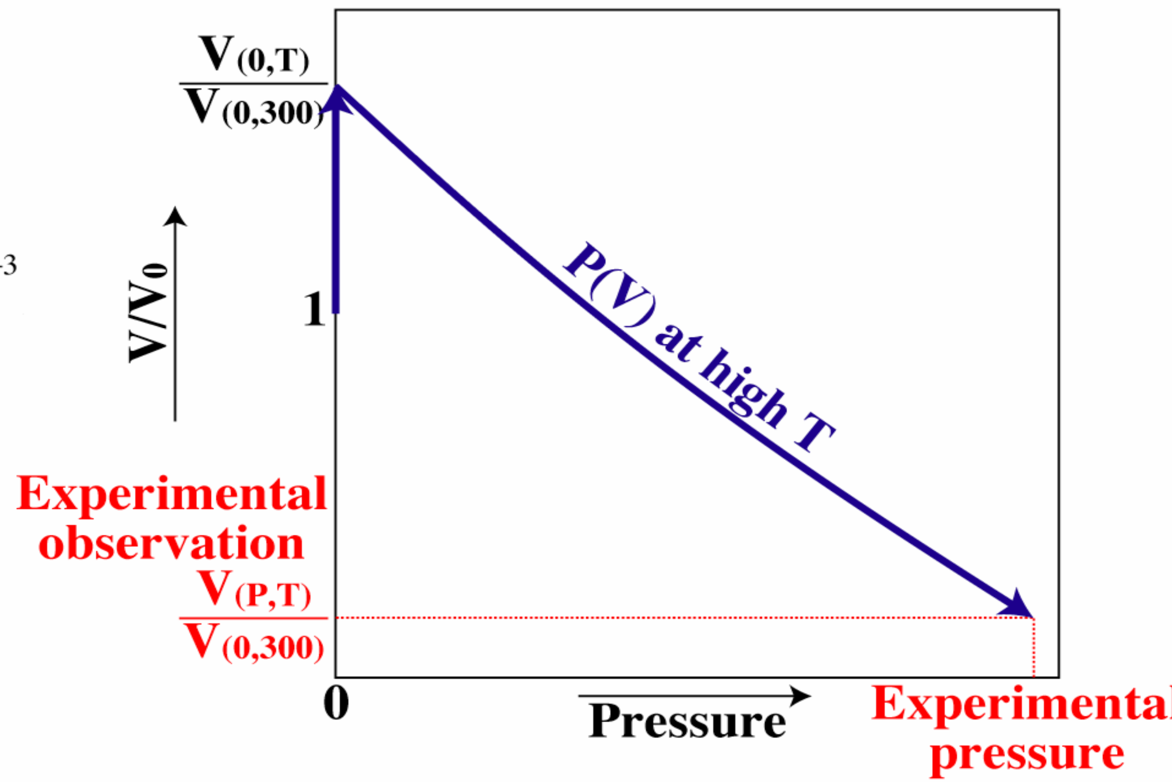
Dubrovinsky and Saxena (1997)

$$K_{T0} = 160.6(5)$$

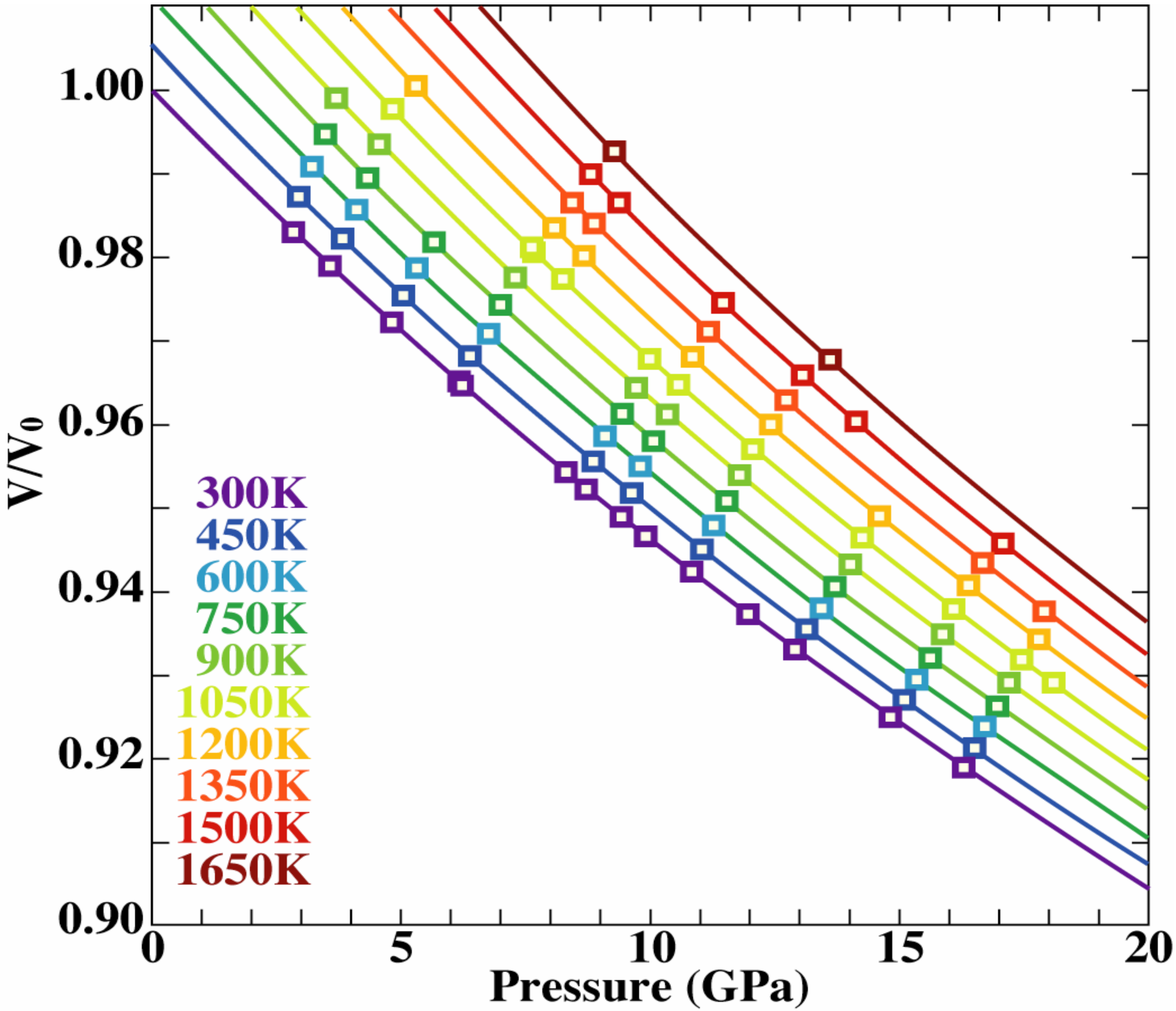
$$K'_{T0} = 4.30(6)$$

$$\partial K_T/\partial T = -0.0309(8)$$

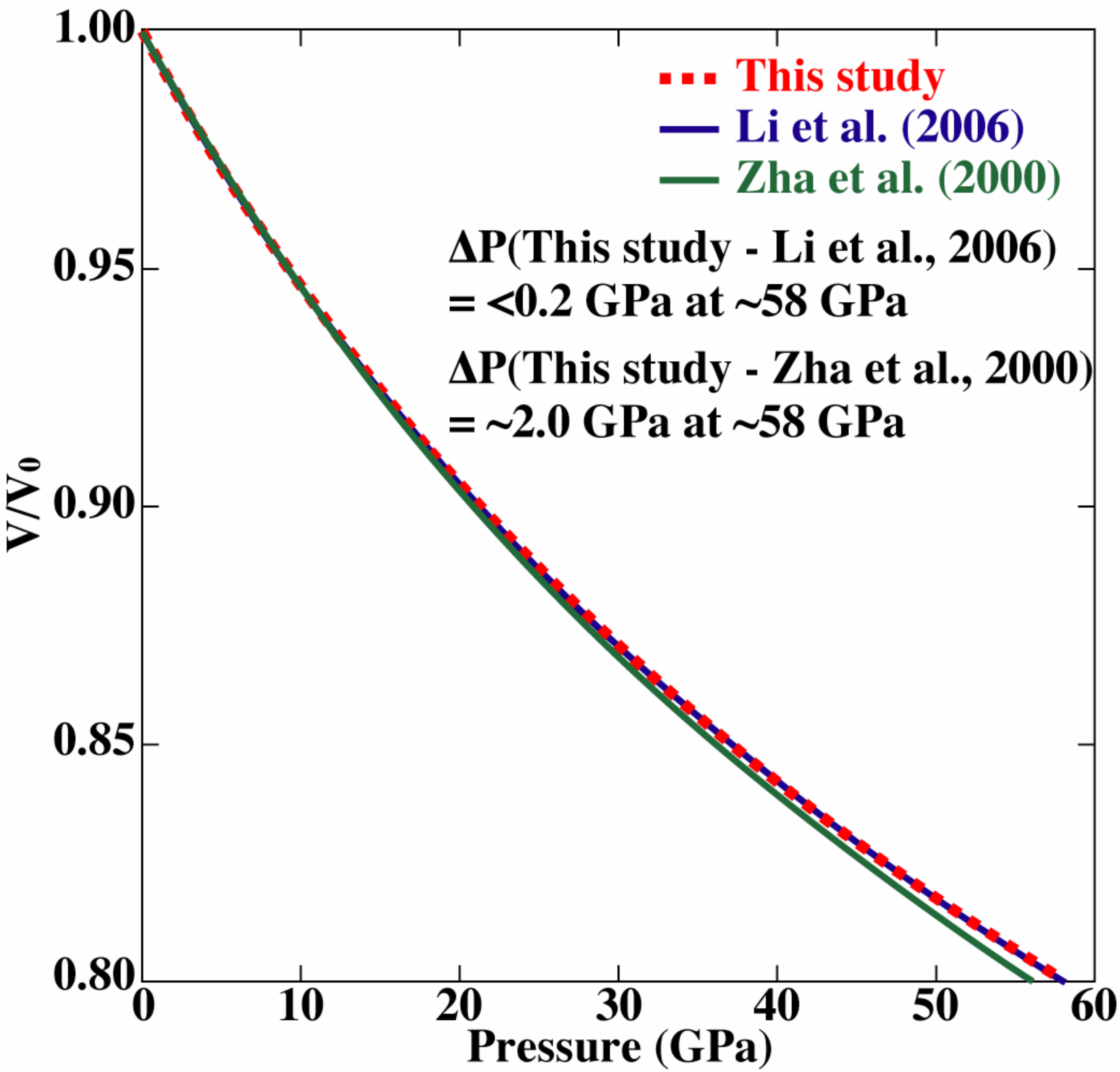
$$\partial^2 K_T/\partial PT = 0.00032(9)$$



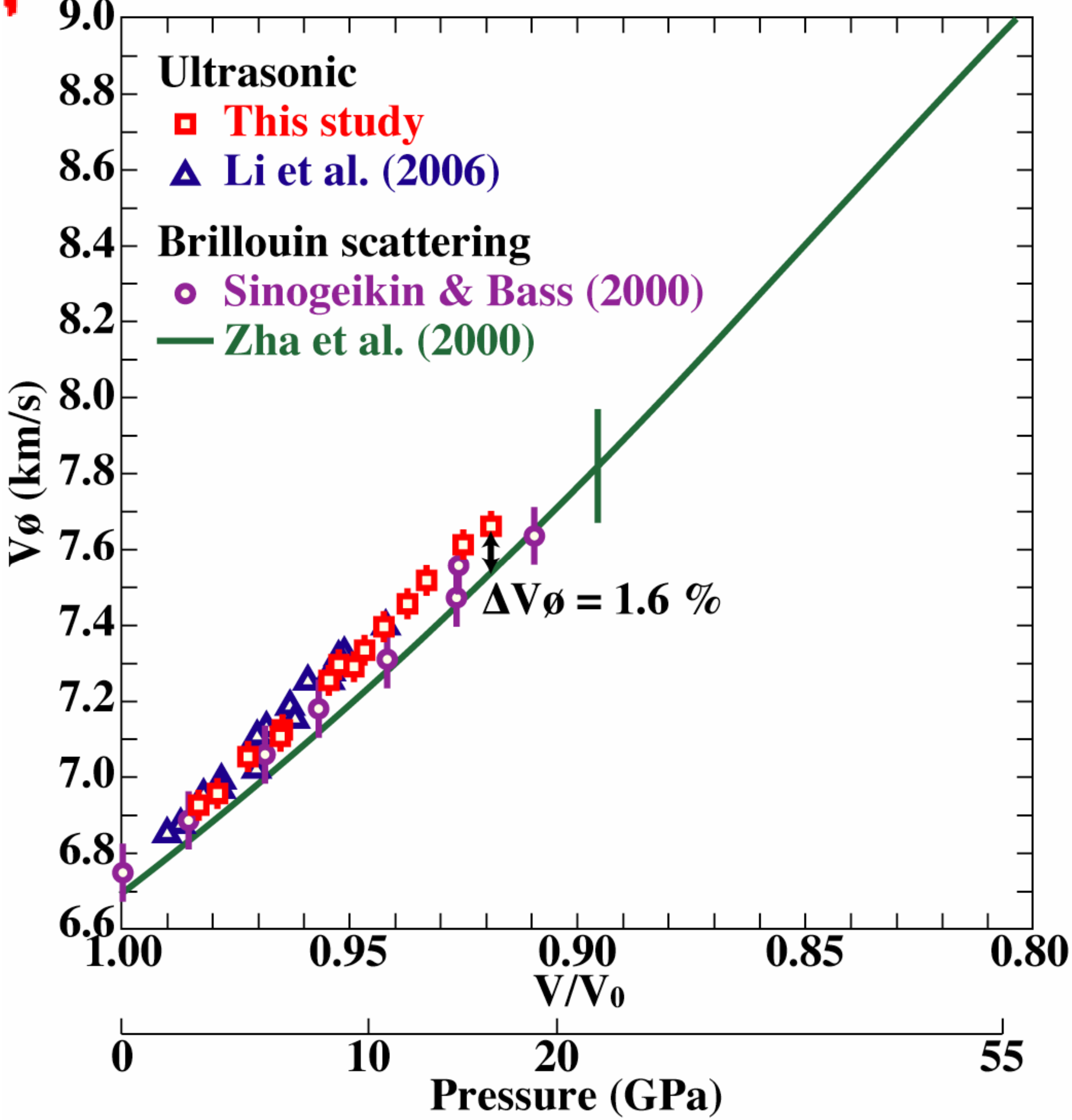
Standard-free P-V-T relation of MgO



Standard-free P-V relations of MgO at 300K



Bulk sound velocity (Vø) from ultrasonic measurement and Brillouin scattering



Zha et al. (2000)

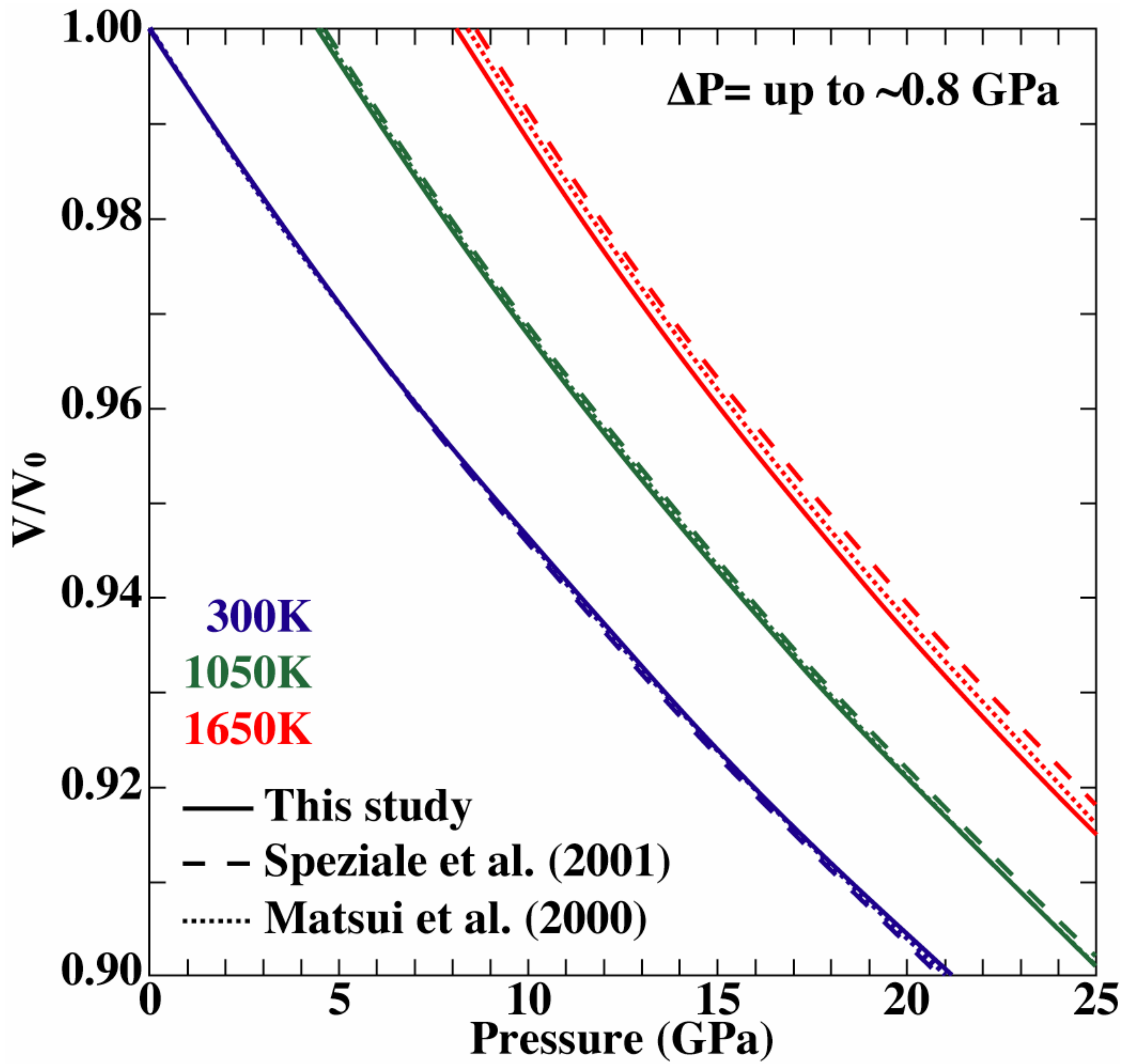
$V\text{ø}=6.69+0.057\text{x}P-0.0027\text{x}P^2$

$$P = 3\times K_{T0}(1+2\varepsilon)^{5/2}\varepsilon(1+3(K'_{T0}-4)\varepsilon/2)$$

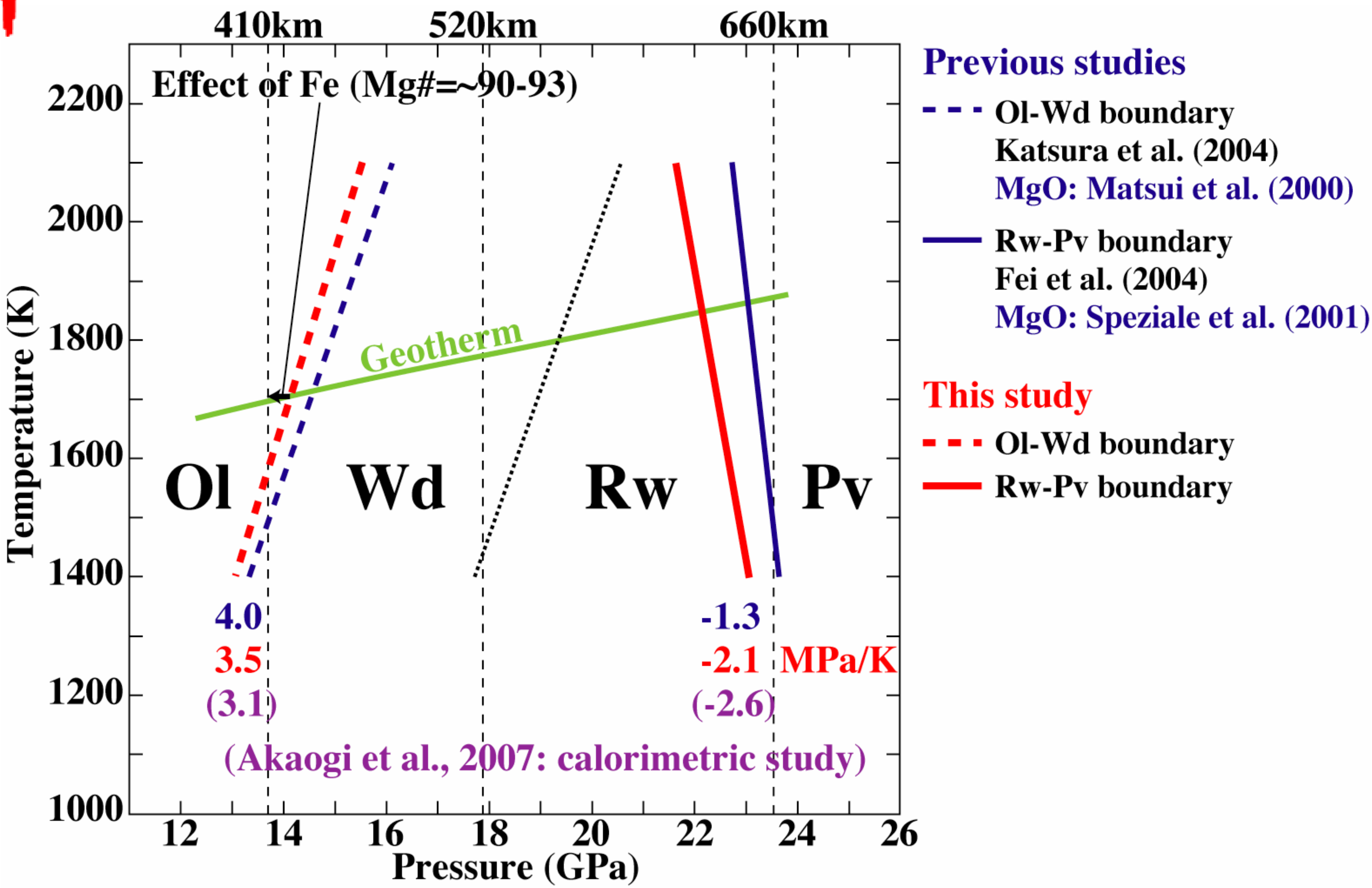
$$K_{T0} = 160.2$$

$$K'_{T0} = 4.03$$

P-V-T relations of MgO (This study vs Previous studies)



Phase transition of Mg_2SiO_4 at the mantle transition zone



Conclusion

We determined standard-free P-V-T equation of state of MgO, and recalculated phase boundary of Mg_2SiO_4 under the P-T condition of the mantle transition zone.

Recalculated phase boundary of Mg_2SiO_4 show

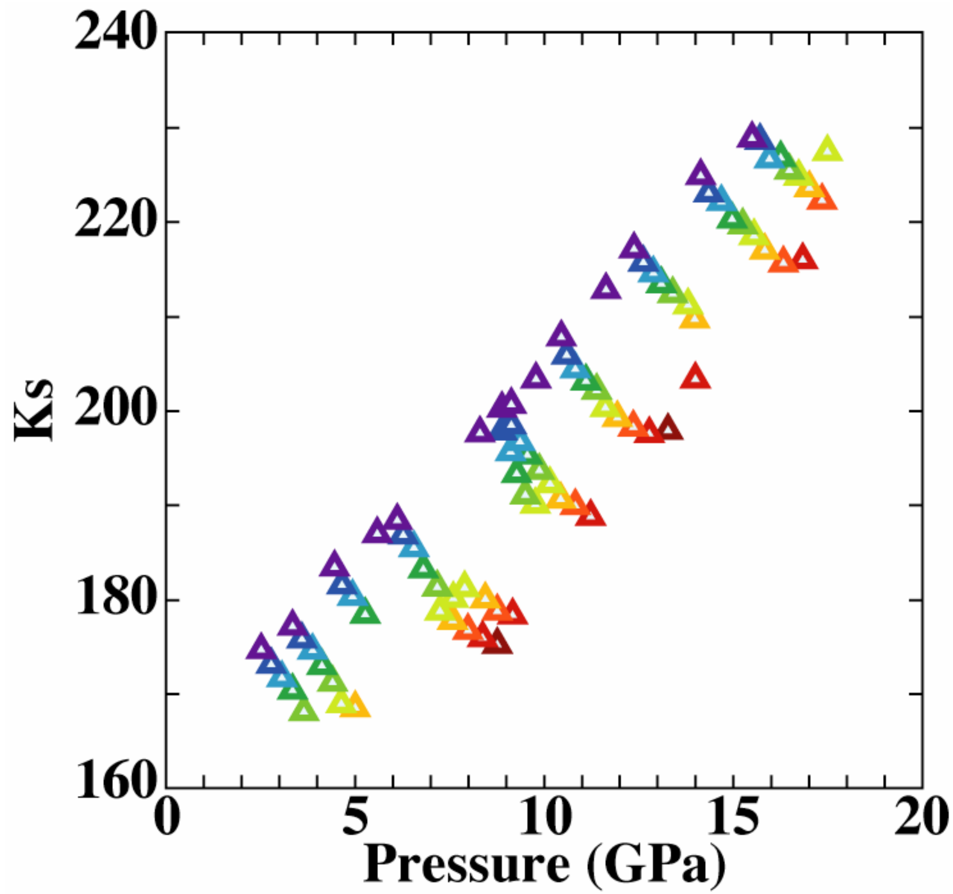
-olivine-wadsleyite transition corresponds to 410 km discontinuity
if we take account of the effect of iron of Mg#=~90-93.

However,
-**ringwoodite-perovskite transition locates at ~620 km depth and is difficult to cause 660 km discontinuity**.

Determination of isothermal bulk modulus without pressure

Determination of isothermal bulk modulus without pressure

Ks



Determination of isothermal bulk modulus without pressure

$$K_T = K_S/(1+\alpha\gamma T)$$

$$K_T = K_{T0}(1+2\varepsilon)^{5/2}(1+(3K'_T-5)\varepsilon) \qquad \varepsilon = \{(V_0/V)^{2/3}-1\}/2$$

$$K_S/(1+\alpha\gamma T) = 3K_{T(0,T)}(1+2\varepsilon)^{5/2}\varepsilon(1+3(K'_{T(T)}-4)\varepsilon/2)$$

$$\alpha = \alpha_0 + \partial\alpha/\partial P \times P \qquad K_{T(0,T)} = K_{T0} + \partial K_T/\partial T \times T$$

$$\partial\alpha/\partial P = (\partial K_{T(P)}/\partial T)/K_T^{\ 2} \qquad K'_{T(T)} = K'_{T0} + \partial^2 K_T/\partial PT \times T$$

$$\gamma = \gamma_0 \times \exp\{q_0/q_1[(V/V_0)^{q_1}-1]\} \qquad \partial K_{T(P)}/\partial T = \partial K_T/\partial T + \partial^2 K_T/\partial PT \times P$$

Fixed parameters

$$\alpha_0 = 2.6025\times10^{-5} + 1.3535\times10^{-8}\times T + 6.5687\times10^{-3}\times T^{-2} - 1.8281\times T^{-3}$$

Dubrovinsky and Saxena (1997)

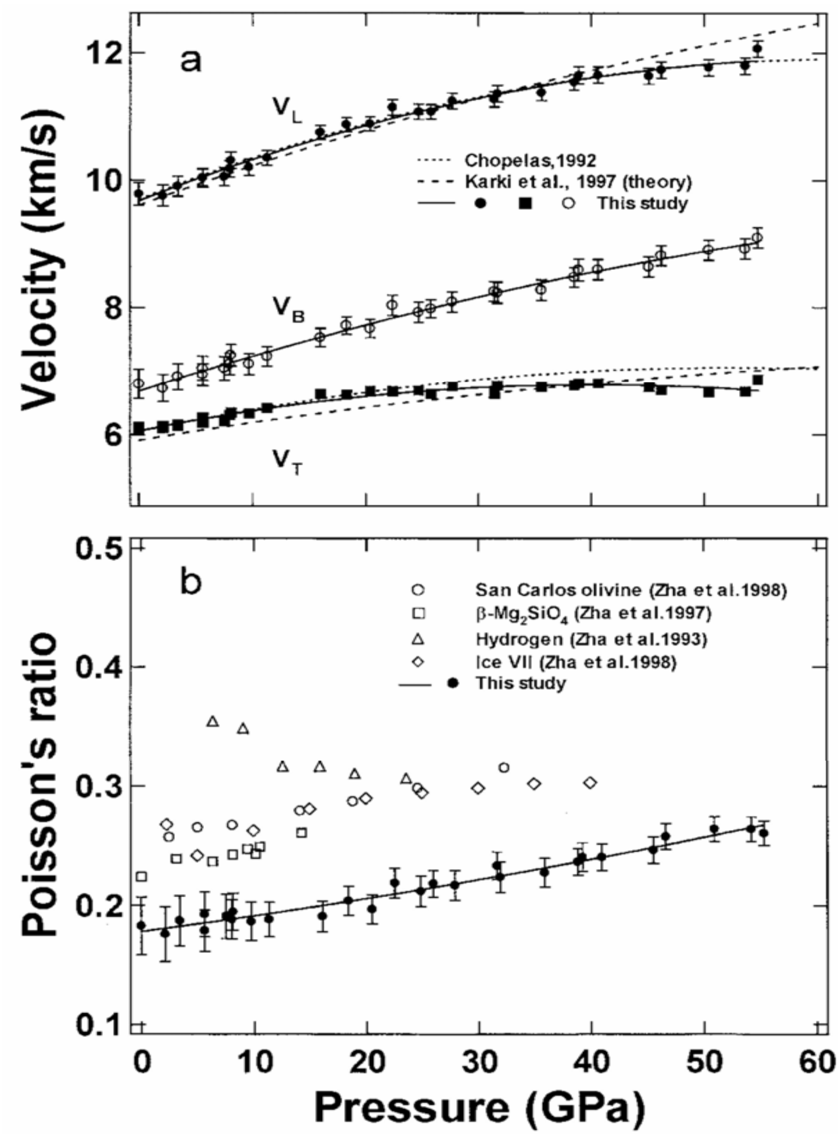
$$\gamma_0 = 1.524, q_0 = 1.65, q_1 = 11.8$$

Speziale et al. (2001)

Determined parameters

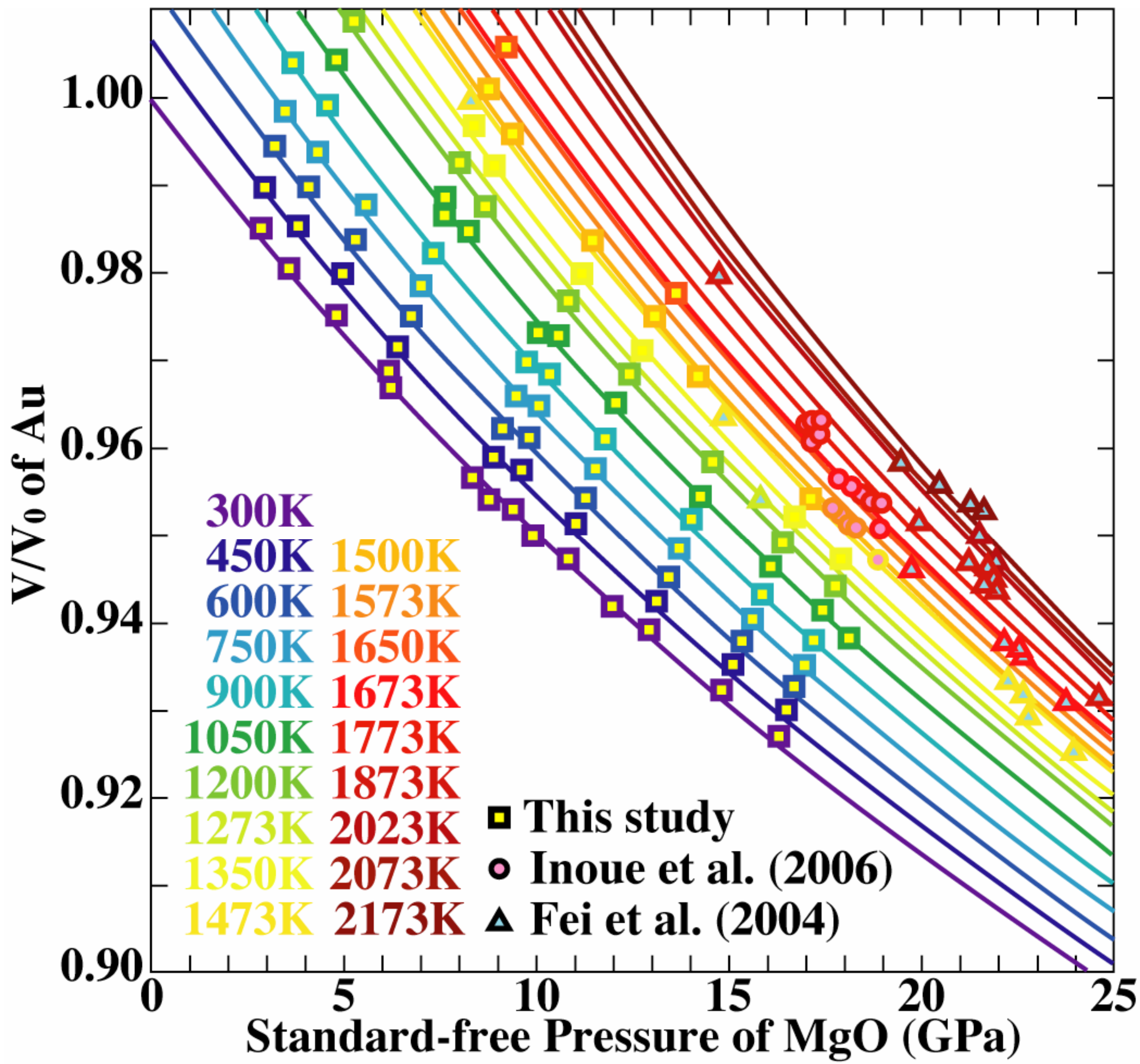
$$K_{T0},\ K'_{T0},\ \partial K_T/\partial T,\ \partial^2 K_T/\partial PT$$

Zha et al. (2000)



Zha et al. (2000)

P-V-T equation of state of Au (high-temperature third-order Birch-Murnaghan EoS)



$\alpha_0 = a + bT$

$a = 4.18(8)\times10^{-5}$

$b = 1.8(3)\times10^{-8}$

$K_{T0} = 166.44(fix)$

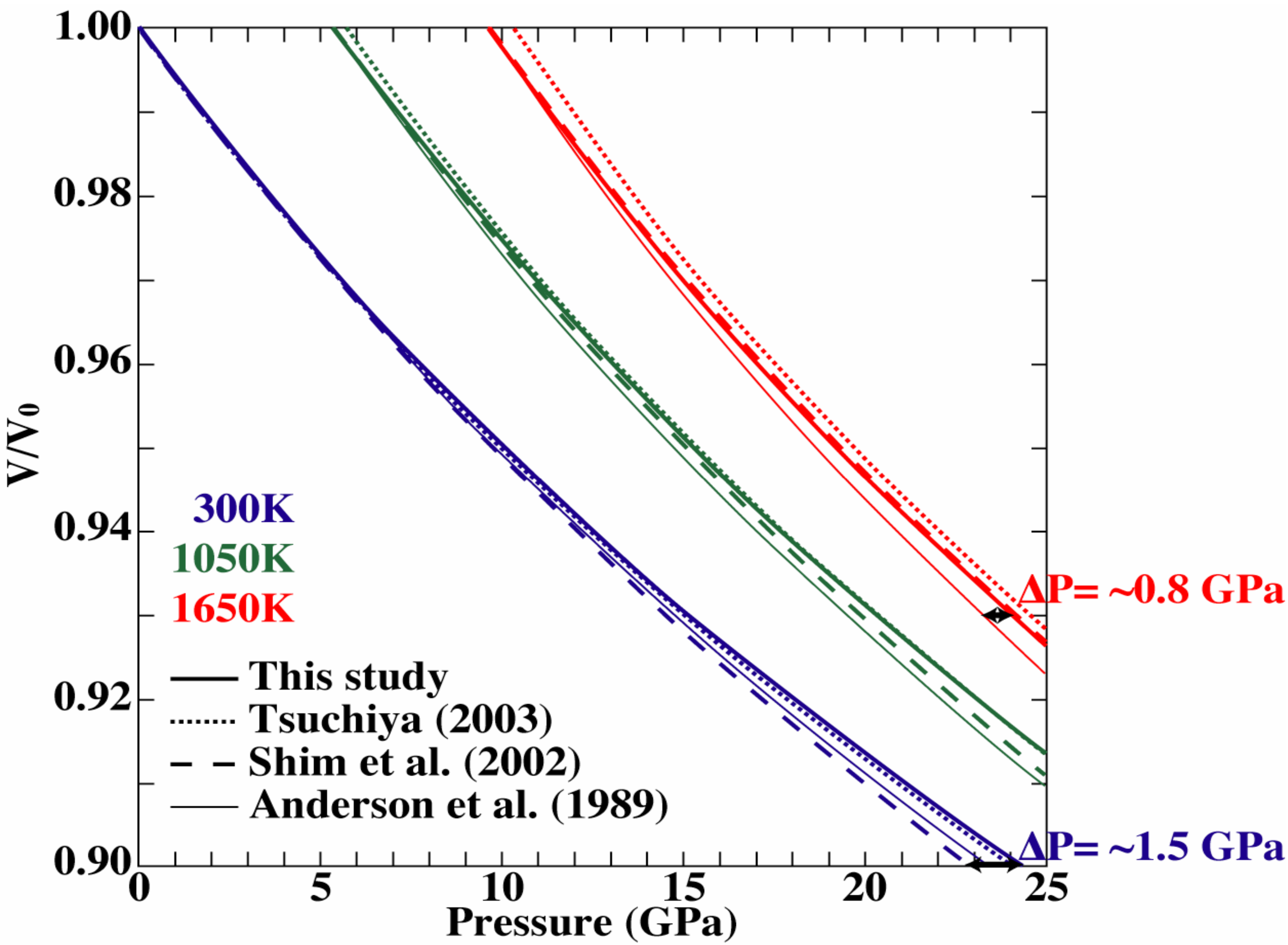
$K'_T = 6.3(2)$

$\partial K_T/\partial T = -0.045(2)$

K_{T0} and K'_{T0} of Au

	K_{T0}	K'_T
Ultrasonic		
Song et al. (2007)	166.44	6.56
P-V(-T) relation		
This study	**166.44 (fix)**	**6.3 (2)**
Shim et al. (2002)	167 (fix)	5.0 (2)
Heinz & Jeanloz (1984)	167 (11)	5.5 (8)
First-principle calculation		
Tsuchiya (2003)	166.7	6.12

P-V-T relations of Au (This study vs Previous studies)



Phase transition of Mg_2SiO_4 at the mantle transition zone