Accurate calculations of the high-pressure elastic constants based on the first-principles*

Wang Chen-Ju(王臣菊)[a], Gu Jian-Bing(顾建兵)[b], Kuang Xiao-Yu(邝小渝)[a)c)†], and Yang Xiang-Dong(杨向东)[a]

[a] Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China
[b] College of Physical Science and Technology, Sichuan University, Chengdu 610064, China
[c] International Centre for Materials Physics, Chinese Academy of Sciences, Shenyang 110016, China

(Received 14 December 2014; revised manuscript received 26 February 2015; published online 20 June 2015)

The energy term corresponding to the first order of the strain in Taylor series expansion of the energy with respect to strain is always ignored when high-pressure elastic constants are calculated. Whether the modus operandi would affect the results of the high-pressure elastic constants is still unsolved. To clarify this query, we calculate the high-pressure elastic constants of tantalum and rhenium when the energy term mentioned above is considered and neglected, respectively. Results show that the neglect of the energy term corresponding to the first order of the strain indeed would influence the veracity of the high-pressure elastic constants, and this influence becomes larger with pressure increasing. Therefore, the energy term corresponding to the first-order of the strain should be considered when the high-pressure elastic constants are calculated.

Keywords: accurate calculation, elastic constants, high-pressure, first-principles

PACS: 62.20.D–, 71.15.Mb, 71.15.Nc **DOI:** 10.1088/1674-1056/24/8/086201

1. Introduction

Accurate calculations of the high-pressure elastic constants based on the first-principles are crucial to predicting the high-pressure behaviors of the elastic properties and providing fundamental understanding of the properties of interatomic forces, mechanical stabilities,[1] and phase transition mechanisms of materials under high pressures.[2,3]

Among the existing first-principle approaches[4–35] to calculating the high-pressure elastic constants, total energy approach[4–12,18–22] is the most frequently used method. The kernel of this method is to expand the energy of the deformed system into Taylor series with respect to the strain[36] as shown below

$$U(X,\eta_{ij},S) = U(X,0,S)+V(X)\sum_{ij}T_{ij}(X)\eta_{ij} + \frac{1}{2}V(X)\sum_{ijkl}C^{S}_{ijkl}(X)\eta_{ij}\eta_{kl}+\cdots, \quad (1a)$$

$$F(X,\eta_{ij},T) = F(X,0,T)+V(X)\sum_{ij}T_{ij}(X)\eta_{ij} + \frac{1}{2}V(X)\sum_{ijkl}C^{T}_{ijkl}(X)\eta_{ij}\eta_{kl}+\cdots, \quad (1b)$$

where X is the reference state corresponding to the equilibrium state at a certain pressure, V denotes the volume of the system in X state, U and F are the internal energy and Helmholtz free energy respectively, S and T refer to the adiabatic and isothermal processes respectively. Subscript η_{ij} represents the element of the strain tensor, $T_{ij}(X)$ is the component of the stress tensor exerted on X state,

$$C^{T}_{ijkl}(X) = \frac{1}{V(X)}\frac{\partial^2 F}{\partial\eta_{ij}\partial\eta_{kl}}\bigg|_X$$

and

$$C^{S}_{ijkl}(X) = \frac{1}{V(X)}\frac{\partial^2 U}{\partial\eta_{ij}\partial\eta_{kl}}\bigg|_X$$

are the second-order elastic constants. Since the stress acting on the reference state X is nonzero, the energy term $V(X)\sum_{ij}T_{ij}(X)\eta_{ij}$ corresponding to the first order of the strain is also nonzero. As a consequence, $V(X)\sum_{ij}T_{ij}(X)\eta_{ij}$ should be taken into account when the elastic constants of state X are calculated. However, this term was not considered in most calculations[8,19,22,37] of the high-pressure elastic constants. Whether such a modus operandi would influence the results of the high-pressure elastic constants has remained unresolved so far.

To clarify this puzzling issue, we take the cubic tantalum (Ta) and hexagonal rhenium (Re), for example, and calculate their high-pressure elastic constants when the term of $V(X)\sum_{ij}T_{ij}(X)\eta_{ij}$ is considered and neglected respectively. The reasons for choosing the body-centered-cubic (bcc) Ta and hexagonal-close-packed (hcp) Re are as follows. One is that the two materials belong to different crystal systems, which could make the investigation in this paper have more stringency. And the other is that many previous studies[38–49] have shown that Ta and Re have relatively high stability at

*Project supported by the National Natural Science Foundation of China (Grant No. 11274235), the Young Scientist Fund of the National Natural Science Foundation of China (Grant No. 11104190), and the Doctoral Education Fund of Education Ministry of China (Grant Nos. 20100181110086 and 20110181120112).

†Corresponding author. E-mail: scu_kxy@163.com

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0 K, and can maintain their stable phases (bcc for Ta and hcp for Re) when the pressure increases to 500 GPa, which is conducive to calculating the high-pressure elastic constants and illuminating the confusing issue mentioned above. The rest of this paper is organized as follows. In Section 2, we present the computational method of the high-pressure elastic constants in detail. Results and discussion are given in Section 3. And the conclusions of the present study are drawn in Section 4.

2. Computational details

2.1. Density functional theory calculations

Structural optimizations and total energy calculations at 0 K are performed by using the Vienna *ab initio* simulation package (VASP).[50,51] The Perdew–Burke–Ernzerhof (PBE) version[52] of the general gradient approximation (GGA) is used for the electron exchange–correlation functional. Electrons of $5p^6 6s^2 5d^3$ for Ta and $5p^6 6s^2 5d^5$ for Re are treated as valence configurations. The interaction between the valence electrons and the remaining core electrons is described by the frozen core projector-augmented wave (PAW) method.[53] Energy convergence (1 mRy per atom) tests are performed to determine the cutoff energy and the number of k-points in whole pressure range for both metals, and the reasonable cutoff energy (400 eV for Ta and 450 eV for Re) and rational k-points ($18\times18\times18$ for Ta and $14\times14\times10$ for Re) are ascertained. Afterwards, the total energy of undeformed unit cell is calculated in a volume range of 0.45 $V_{0\text{expt}}$–1.1 $V_{0\text{expt}}$, where $V_{0\text{expt}}$ is the experimental equilibrium volume at zero pressure. Then the equation of states at 0 K for both metals are determined according to the fourth-order Brich–Murnaghan equation $E(V)=\sum_{n=1}^{4} a_n V^{-2n/3}$.[54] From the relation of $P=-(\partial E/\partial V)_{T=0}$, the P–V data are obtained directly, which is the basis of the elastic constants calculations at different pressures.

2.2. Elastic constants calculations

2.2.1. Cubic Ta

To determine the three elastic constants of cubic Ta, the following formula is first used:

$$B_{\mathrm{T}}=\frac{C_{11}+2C_{12}+P}{3}, \tag{2}$$

and its detailed derivations are given in Appendix A.

For calculating C_{11} and C_{12}, we adopt the volume conserving deformation gradient matrix, i.e.,

$$\alpha_{ij}=\begin{pmatrix} 1+\delta & 0 & 0 \\ 0 & 1-\delta & 0 \\ 0 & 0 & 1/(1-\delta^2) \end{pmatrix}, \tag{3}$$

which is obtained from the shear deformation of the (110) plane in the $[1\bar{1}0]$ direction. In Eq. (3), δ is the strain magnitude. In practice, it is set from -0.006 to 0.006 in steps of 0.001. Then the corresponding energy forms can be expressed as

$$E(\delta) = E(0)+(C_{11}-C_{12}-2P)V\delta^2+O(\delta^3) \text{ with } V(X)\sum_{ij}T_{ij}(X)\eta_{ij}, \tag{4a}$$

and

$$E(\delta) = E(0)+(\bar{C}_{11}-\bar{C}_{12})V\delta^2+O(\delta^3) \text{ without } V(X)\sum_{ij}T_{ij}(X)\eta_{ij}, \tag{4b}$$

where $E(0)$ represents the energy of the undeformed unit cell, V denotes the corresponding volume, C_{ij} and $\bar{C}_{ij}$ represents the elastic constants obtained respectively when the $V(X)\sum_{ij}T_{ij}(X)\eta_{ij}$ term is considered and ignored, P refers to the pressure exerted on the reference state, which comes from the $V(X)\sum_{ij}T_{ij}(X)\eta_{ij}$ term. Then C_{11} and C_{12} can be calculated with the help of formula (2) and the coefficient of the quadratic term obtained by the polynomial fitting of formula (4a). Similarly, $\bar{C}_{11}$ and $\bar{C}_{12}$ can be obtained with the aid of the formulas (2) and (4b).

In addition, the volume conserving deformation gradient matrix (5), which represents the deformation of the (100) plane shear in the [010] direction, is used to calculate the C_{44} ($\bar{C}_{44}$).

$$\alpha_{ij}=\begin{pmatrix} 1 & 0 & \delta \\ 0 & 1/(1-\delta^2) & 0 \\ \delta & 0 & 1 \end{pmatrix}. \tag{5}$$

The corresponding energy expressions are

$$E(\delta) = E(0)+(2C_{44}-2P)V\delta^2+0(\delta^4) \text{ with } V(X)\sum_{ij}T_{ij}(X)\eta_{ij}, \tag{6a}$$

and

$$E(\delta) = E(0)+(2\bar{C}_{44})V\delta^2+0(\delta^4) \text{ without } V(X)\sum_{ij}T_{ij}(X)\eta_{ij}. \tag{6b}$$

2.2.2. Hexagonal Re

With the aid of formulas (4) and (6), we can obtain $C_{11}-C_{12}$ ($\bar{C}_{11}-\bar{C}_{12}$) and C_{44} ($\bar{C}_{44}$) of Re in the same way as that in the case of Ta. To calculate C_{11} ($\bar{C}_{11}$), C_{12} ($\bar{C}_{12}$), C_{13} ($\bar{C}_{13}$), and C_{33} ($\bar{C}_{33}$) respectively, we first employ the following expression:

$$B_{\mathrm{T}}=\frac{C^2}{C_S}, \tag{7}$$

where

$$C^2=(C_{11}+C_{12})(C_{33}-P)-2(C_{13}+P)^2, \tag{8}$$

$$C_S = C_{11} + C_{12} + 2C_{33} - 4C_{13} - 6P. \quad (9)$$

Detailed derivations of the formula (7) are presented in Appendix A. In addition, the volume dependence of the equilibrium c/a rate is related to the difference in linear compressibility between along the a and along the c axes, which is described by the dimensionless quantity R

$$R = -\frac{\mathrm{d}\ln(c/a)}{\mathrm{d}\ln V} = \frac{M}{C_S}, \quad (10)$$

where

$$M = C_{33} - C_{11} - C_{12} + C_{13}. \quad (11)$$

The detailed deductions of Eq. (10) are shown in Appendix B. It should be pointed out that formulas (8), (9), and (11) can also be expressed by $\bar{C}_{ij}$ in the same way.

To calculate the C_S appearing in formulas (7) and (10), the volume-conserving deformation matrix (12) is used, i.e.,

$$\alpha_{ij} = \begin{pmatrix} 1+\delta & 0 & 0 \\ 0 & 1+\delta & 0 \\ 0 & 0 & 1/(1+\delta)^2 \end{pmatrix}. \quad (12)$$

The corresponding expressions of the energy are

$$F(\delta) = F(0) + (C_{11} + C_{12} + 2C_{33} - 4C_{13} - 6P)V\delta^2 + 0(\delta^3) \quad \text{with } V(X)\sum_{ij} T_{ij}(X)\eta_{ij}, \quad (13a)$$

and

$$F(\delta) = F(0) + (\bar{C}_{11} + \bar{C}_{12} + 2\bar{C}_{33} - 4\bar{C}_{13})V\delta^2 + 0(\delta^3) \quad \text{without } V(X)\sum_{ij} T_{ij}(X)\eta_{ij}. \quad (13b)$$

Then we can respectively obtain the C_{11} ($\bar{C}_{11}$), C_{12} ($\bar{C}_{12}$), C_{13} ($\bar{C}_{13}$), and C_{33} ($\bar{C}_{33}$) by solving Eqs. (4), (7), (10), and (13).

3. Results and discussion

3.1. Equilibrium structure

To verify the accuracy of the present calculations, we list the calculated lattice parameters, the values of equilibrium volume V_0, bulk modulus B_0, and their pressure derivative B_0' in Table 1, and compare them with the available experimental results.[55–60]

Table 1. Calculated values of equilibrium lattice parameter (in unit Å), atomic volume V_0 (in unit Å^3), bulk modulus B_0 (in unit GPa), and their pressure derivative B_0', together with the experimental results.[55–60] GGA–PBE denotes the generalized gradient approximation-Perdew Burke Ernzerhof, XRD the x-ray diffraction, DAC the diamond anvil cell.

	Method	a/Å	c/Å	c/a	V_0/Å^3	B_0/GPa	B_0'
Ta	Present work (GGA–PBE)	3.322	–	–	18.33	195	3.47
	Expt[55] (XRD in DAC)	3.304	–	–	18.04	194	3.52
	Expt[56] (XRD in DAC)	3.304	–	–	18.04	194	3.55
	Expt[57] (XRD in DAC)	3.304	–	–	18.03	195	3.40
Re	Present work (GGA–PBE)	2.762	4.457	1.614	14.72	361	4.11
	Expt[58] (XRD in DAC)	2.762	4.459	1.614	14.73	353	4.56
	Expt[59] (XRD in DAC)	2.762	4.455	1.613	14.72	372	4.05
	Expt[60] (XRD in DAC)	2.761	4.456	1.614	14.72	350	4.00

From Table 1, we can clearly see that the calculated lattice parameters of Ta and Re are in fair agreement (within 0.5%) with the experimental data.[45–50] And the equilibrium volumes, bulk modulus B_0 and their pressure derivatives B_0' for both Ta and Re are also shown to be in excellent agreement with the existing experimental results.[55–60] The good agreement indicates that the choices of PAW pseudopotential and GGA–PBE approximation are reasonable for the current study and the calculations are reliable.

3.2. Elastic constants

Having seen that the calculations of the present work are reliable, we now turn to the results of the high-pressure elastic constants.

The relationships between the pressure and elastic constants, obtained respectively when the energy term $V(X)\sum_{ij} T_{ij}(X)\eta_{ij}$ is considered and ignored, are displayed in Fig. 1. From the comparison shown in Fig. 1, we can clearly see that though C_{ij} and $\bar{C}_{ij}$ have the same upward tendency with pressure increasing, the values of elastic constant C_{ij} are not equal to the values of $\bar{C}_{ij}$ at nonzero pressures and the difference between them grows larger with the increase of pressure. In what follows, we take the calculated results of Ta for example. As the pressure increases, the values of $\bar{C}_{11}$ and $\bar{C}_{12}$ without the correction of the $V(X)\sum_{ij} T_{ij}(X)\eta_{ij}$ term respectively have errors about 12% ∼16% and 26% ∼ 43% in comparison with the corresponding true data C_{11} and C_{12}. Moreover, the deviation of $\bar{C}_{44}$ is high up to 53%∼71% with pressure increasing. This indicates that the energy term $V(X)\sum_{ij} T_{ij}(X)\eta_{ij}$ indeed will affect the accuracy of the high-pressure elastic constant. Furthermore, this influence will be-

come larger as pressure increases, especially when the value of the pressure is comparable to that of the elastic constant. Therefore, the energy term $V(X)\sum_{ij} T_{ij}(X)\eta_{ij}$ should be included in expression (1) when the high-pressure elastic constant is calculated. Otherwise, the calculated results can neither explain the corresponding experimental phenomenon exactly, nor predict the high-pressure elastic property behavior accurately.

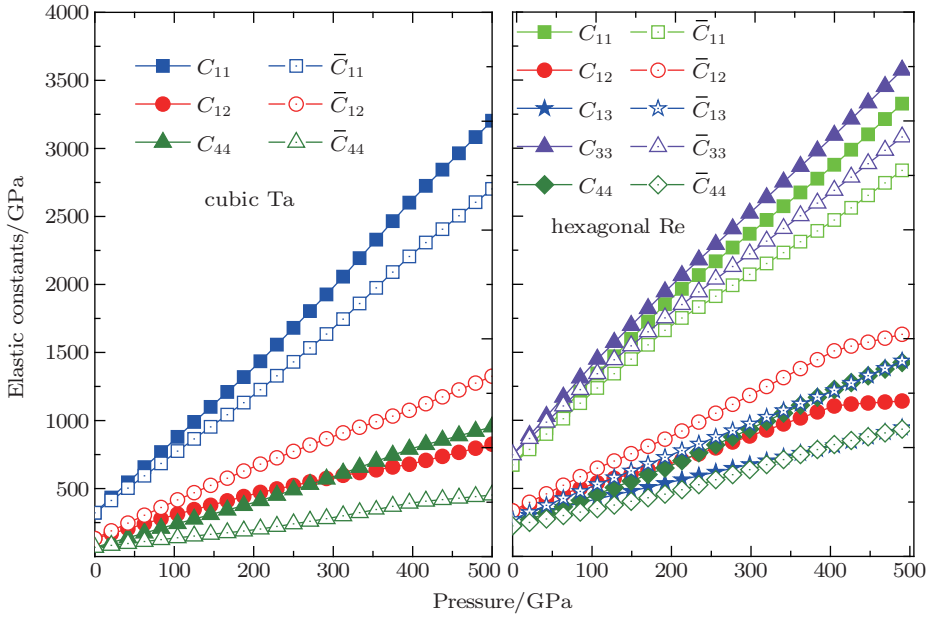


Fig. 1. (color online) Pressure dependences of the elastic constants of Ta and Re. Solid symbols represent the elastic constants of C_{ij} obtained when the energy term $V(X)\sum_{ij} T_{ij}(X)\eta_{ij}$ is considered, and the empty symbols denote the elastic constants of $\bar{C}_{ij}$ obtained when the energy term $V(X)\sum_{ij} T_{ij}(X)\eta_{ij}$ is ignored.

4. Conclusion

Through the calculations of the high-pressure elastic constants of the cubic Ta and hexagonal Re when the energy term corresponding to the first-order of the strain is considered and ignored respectively, we find the energy term corresponding to the first-order of the strain indeed will affect the calculated results of the high-pressure elastic constants and such an influence grows larger with pressure increasing. Therefore, the energy term corresponding to the first-order of the strain in the Taylor series expansion of the total energy with respect to the strain should not be ignored when the high-pressure elastic constants are calculated.

Appendix A: Derivation of the bulk modulus B_{T}

Since the bulk modulus B_{T} of cubic crystal can be obtained from that of the hexagonal crystal when $B_{11} = B_{33}$ and $B_{13} = B_{12}$, the bulk modulus of the hexagonal crystal is first derived.

To obtain the bulk modulus B_{T}, we assume that the volume V_1, corresponding to a certain hydrostatic pressure P, becomes V_2 under a small uniform and isotropic (hydrostatic) compression. Accordingly, the strain tensor can be expressed as

$$\begin{pmatrix} e_{11} & 0 & 0 \\ 0 & e_{22} & 0 \\ 0 & 0 & e_{33} \end{pmatrix} = \begin{pmatrix} \mathrm{d}a/a & 0 & 0 \\ 0 & \mathrm{d}a/a & 0 \\ 0 & 0 & \mathrm{d}c/c \end{pmatrix}. \quad \text{(A1)}$$

And the change of the volume can be written as

$$\begin{aligned} \mathrm{d}V = V_2 - V_1 &= V_1\left[(1+\mathrm{d}a/a)^2(1+\mathrm{d}c/c) - 1\right] \\ &\approx V_1(2\mathrm{d}a/a + \mathrm{d}c/c). \end{aligned} \quad \text{(A2)}$$

According to the definition of the stress–strain coefficient, we can obtain

$$\Delta T_{ij} = \sum_{kl} B_{ijkl} e_{kl}, \quad \text{(A3)}$$

where B_{ijkl} is the stress–strain coefficient, e_{kl} is the element of the strain tensor (A1), and the subscripts i, j, k, and l vary from 1 to 3 respectively. Since ΔT_{ij} is the change of the stress, induced by the small hydrostatic compression, it can be written as

$$\Delta T_{ij} = -\Delta P \delta_{ij}, \quad \text{(A4)}$$

where the symbol δ_{ij} is the Kronecker delta (unity when $i = j$, zero otherwise).

Therefore, equation (A3) becomes

$$\sum_{k} B_{ijkk} e_{kk} = -\Delta P \delta_{ij}. \quad \text{(A5)}$$

For the hexagonal crystal, the matrix of the stress–strain coefficients (in Voigt notation) is

$$B_{ij} = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{12} & B_{11} & B_{13} \\ B_{13} & B_{13} & B_{33} \end{pmatrix}. \tag{A6}$$

So equation (A3) can be written as

$$\begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{12} & B_{11} & B_{13} \\ B_{13} & B_{13} & B_{33} \end{pmatrix} \begin{pmatrix} \mathrm{d}a/a \\ \mathrm{d}a/a \\ \mathrm{d}c/c \end{pmatrix} = -\mathrm{d}P \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \tag{A7}$$

Subsequently, we can obtain

$$2\,\mathrm{d}a/a + \mathrm{d}c/c = -\mathrm{d}P \frac{B_{11}+B_{12}+2B_{33}-4B_{13}}{B_{33}(B_{11}+B_{12})-2B_{13}^2}. \tag{A8}$$

With the help of Eqs. (A2) and (A8), the bulk modulus $B_{\mathrm{T}} = -V_1\,\mathrm{d}P/\mathrm{d}V$ of the hexagonal crystal can be expressed as

$$B_{\mathrm{T}} = \frac{B_{33}(B_{11}+B_{12})-2B_{13}^2}{B_{11}+B_{12}+2B_{33}-4B_{13}}. \tag{A9}$$

Using the transformation relationship

$$B_{ijkl} = \frac{1}{2}(T_{il}\delta_{jk} + T_{jl}\delta_{ik} + T_{ik}\delta_{jl} + T_{jk}\delta_{il} - 2T_{ij}\delta_{kl}) + C_{ijkl}, \tag{A10}$$

provided by Wallace,[36] we obtain the bulk modulus expressed in terms of the elastic constant

$$B_{\mathrm{T}} = \frac{(C_{11}+C_{12})(C_{33}-P)-2(C_{13}+P)^2}{C_{11}+C_{12}+2C_{33}-4C_{13}-6P}. \tag{A11}$$

This is Eq. (7) appeared in Section 2 of the present paper.

For cubic crystal, we have

$$B_{11} = B_{33} \quad \text{and} \quad B_{13} = B_{12}. \tag{A12}$$

Substituting Eq. (A12) into Eq. (A9), the bulk modulus of cubic crystal can be obtained as

$$B_{\mathrm{T}} = \frac{B_{11}+2B_{12}}{3}. \tag{A13}$$

Then equation (2) can be obtained by combining the expressions of Eqs. (A10) and (A13).

Appendix B: Derivation of the dimensionless quantity *R*

According to the definition of the linear compressibility,[61] we express the linear compressibilities along the a and c axes respectively as

$$\beta_a = -\frac{1}{a}\frac{\mathrm{d}a}{\mathrm{d}P} \tag{B1}$$

and

$$\beta_c = -\frac{1}{c}\frac{\mathrm{d}c}{\mathrm{d}P}. \tag{B2}$$

With the aid of Eq. (A7), we can obtain

$$\mathrm{d}a/a = -\mathrm{d}P \frac{B_{33}-B_{13}}{B_{33}(B_{11}+B_{12})-2B_{13}^2} \tag{B3}$$

and

$$\mathrm{d}c/c = -\mathrm{d}P \frac{B_{11}+B_{12}-2B_{13}}{B_{33}(B_{11}+B_{12})-2B_{13}^2}. \tag{B4}$$

Then expressions (B1) and (B2) become

$$\beta_a = \frac{B_{33}-B_{13}}{B_{33}(B_{11}+B_{12})-2B_{13}^2} \tag{B5}$$

and

$$\beta_c = \frac{B_{11}+B_{12}-2B_{13}}{B_{33}(B_{11}+B_{12})-2B_{13}^2}. \tag{B6}$$

Accordingly, the coefficient $\beta_{c/a}$ can be expressed as

$$\beta_{c/a} = \beta_a - \beta_c = \frac{B_{33}-B_{11}-B_{12}+B_{13}}{B_{33}(B_{11}+B_{12})-2B_{13}^2}. \tag{B7}$$

Finally, we obtain the dimensionless quantity R as

$$R = B_{\mathrm{T}}\beta_{c/a} = -\frac{\mathrm{d}\ln(c/a)}{\mathrm{d}\ln V} = \frac{(B_{33}-B_{11}-B_{12}+B_{13})}{B_{11}+B_{12}+2B_{33}-4B_{13}}. \tag{B8}$$

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