Strain- and stress-induced changes on second-order elastic coefficient and its relationship with third-order elastic coefficient

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Abstract

To describe elastic wave propagation in a medium under stress or strain, the second-order elastic constants (SOEC) need to be modified. Early studies have shown this can be accomplished by introducing additional third-order elastic constants (TOEC) [1]. In this study, we reevaluate these accommodations theoretically and provide *ab initio* verifications. We first examine the effect of hydrostatic stress, i.e., we describe the pressure derivative of SOEC; then, as a more general case, we investigate the modifications needed for the SOEC under hydrostatic and deviatoric stress. We show that in both cases the modifications of the SOEC are linear combinations of SOEC and TOEC. The relationships are tested on NaCl and MgO with *ab initio* calculated SOEC and TOEC vs. pressure. The methods to compute finite-pressure TOEC are also self-consistently tested.

[1] R. N. Thurston, K. Brugger, *Phys. Rev.* **133**, A1604–A1610 (1964).

Introduction

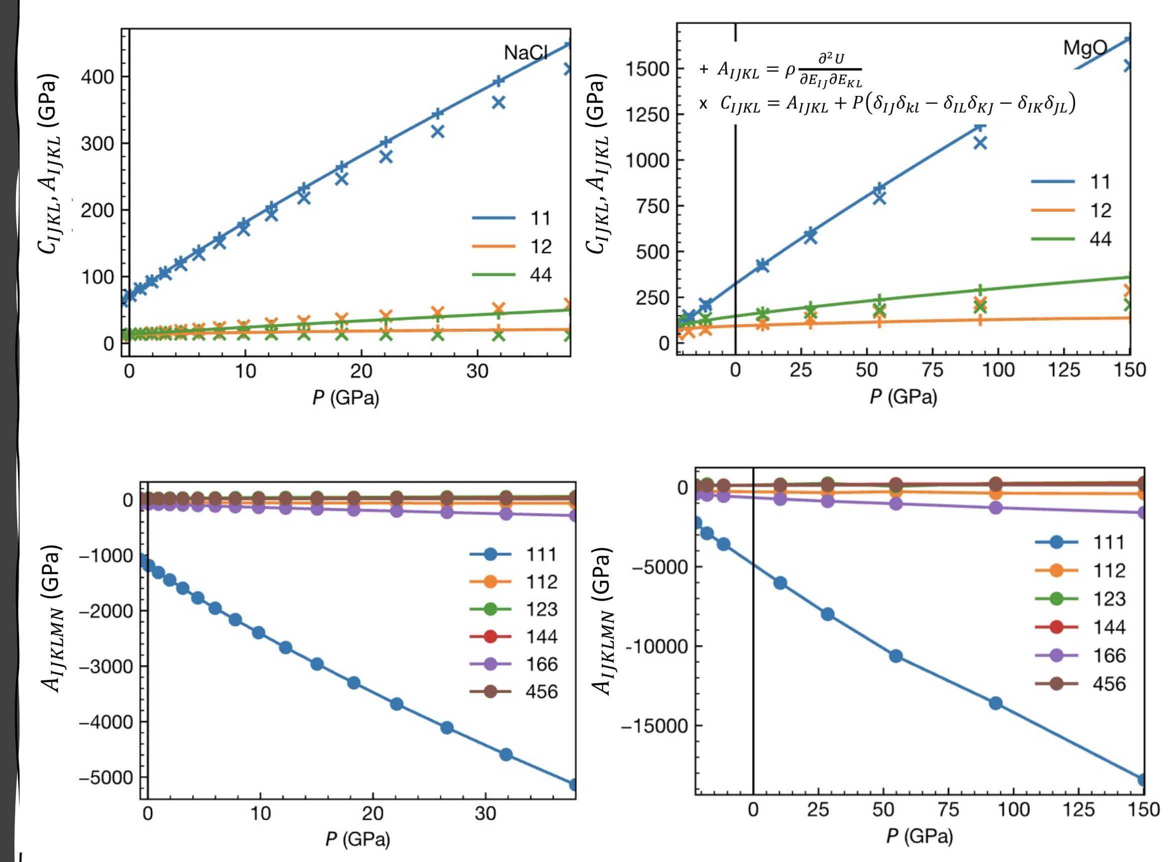
A heterogeneous distribution of stress and strain is common in many geophysical fields of study. For example, anisotropy in the lower mantle, which affects seismic wave propagation, is anticipated to be controlled by strain and texture (Couper et al., 2020). Practical applications, such as hydrocarbon reservoir characterization and volcano monitoring, would benefit from knowledge of the effects of strain and stress on elastic moduli and the propagation of mechanical waves (Sripanich et al., 2021). A recent review by Sripanich et al. (2021) has examined three viable approaches to address the effects of stress changes on wave propagation. This includes an approach based on adiabatic pressure derivatives, third-order elasticity (TOE), and micro-mechanical structures. Following this review, our study focuses on strain and stress effects related on elastic moduli. We review and clarify the theoretical foundation of TOE to address these strain/stress effects and more deeply explore the connection between TOEC and pressure derivatives of SOEC with validations based on *ab initio* results.

Method

- **DFT software**: Quantum ESPRESSO
- **Exchange-correlation functional**: LDA
- **Pseudopotential type**: Ultrasoft
- ***k*-point sampling**: 8 x 8 x 8 for NaCl, 12 x 12 x 12 for MgO

SOEC, TOEC vs. pressure

To calculate SOEC and TOEC simultaneously, we followed Zhao et al.'s (2007) recipe, where elastic constants are obtained as linear combinations of expansion coefficients and strain energy is expanded to the fourth order. However, the effective elastic constants C_{IJKL} (Thurston 1965) need to be distinguished from the second derivatives of the internal energy A_{IJKL} for finite pressure. The following figures show our results for SOEC and TOEC:

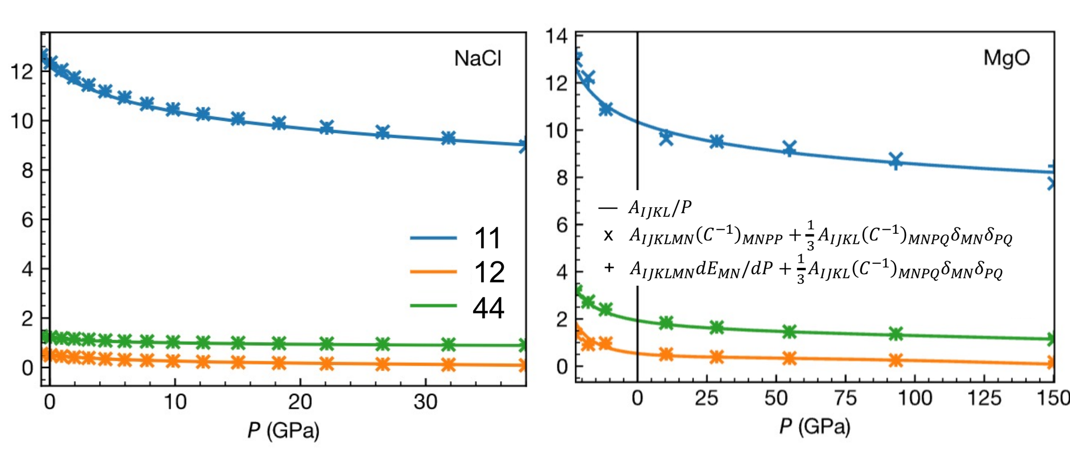


Pressure derivatives of SOEC

Pressure derivatives of SOEC were calculated in two ways. A numerical derivative of SOEC vs. P was compared to TOEC predictions. The formula for predicting the P derivative with TOEC is similar to previously reported ones (Barsch, 1967):

$$\frac{\partial C_{IJKL}}{\partial P} = A_{IJKLMN}(C^{-1})_{MNPQ}\delta_{PQ} + \frac{1}{3}A_{IJKL}(C^{-1})_{MNPQ}\delta_{MN}\delta_{PQ}$$

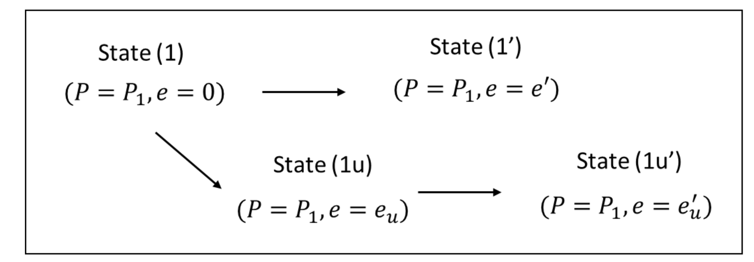
The following figure shows numerical derivatives of SOEC compared to TOEC predictions:



Effects of stress/strain on elastic constants

For validation, we determined the change in elastic constants under induced strain/stress. We calculated the change in elastic constants before and after the strain/stress are applied. Then we compare our theoretical predictions based on TOE theory to *ab initio* calculations. Two cases are tested, one under hydrostatic conditions and one under uniaxial stress/strain.

To determine changes in elastic constants, we calculate A_{IJKL} for an initial hydrostatic state (1) and a uniaxial state (1u). Supplementary states (1') and (1u') are also introduced as "initial" and "final" states for strain-stress calculation the tensor terms. The following figure summarizes the states discussed above.



The change in SOEC could be measured under a uniform reference frame (all under state (1)) or in their own frames as a direct difference.

Uniform reference frame

To address the change in different reference frames, the following equation is tested:

$$\Delta A = JF^{-1}_{II'}F^{-1}_{JJ'}F^{-1}_{KK'}F^{-1}_{LL'}A_{I'J'K'L'}(V, e_{MN}) - A_{IJKL}(V, 0) \quad (1)$$

$$= A_{IJKLMN}e_{MN} \quad (2)$$

Direct difference

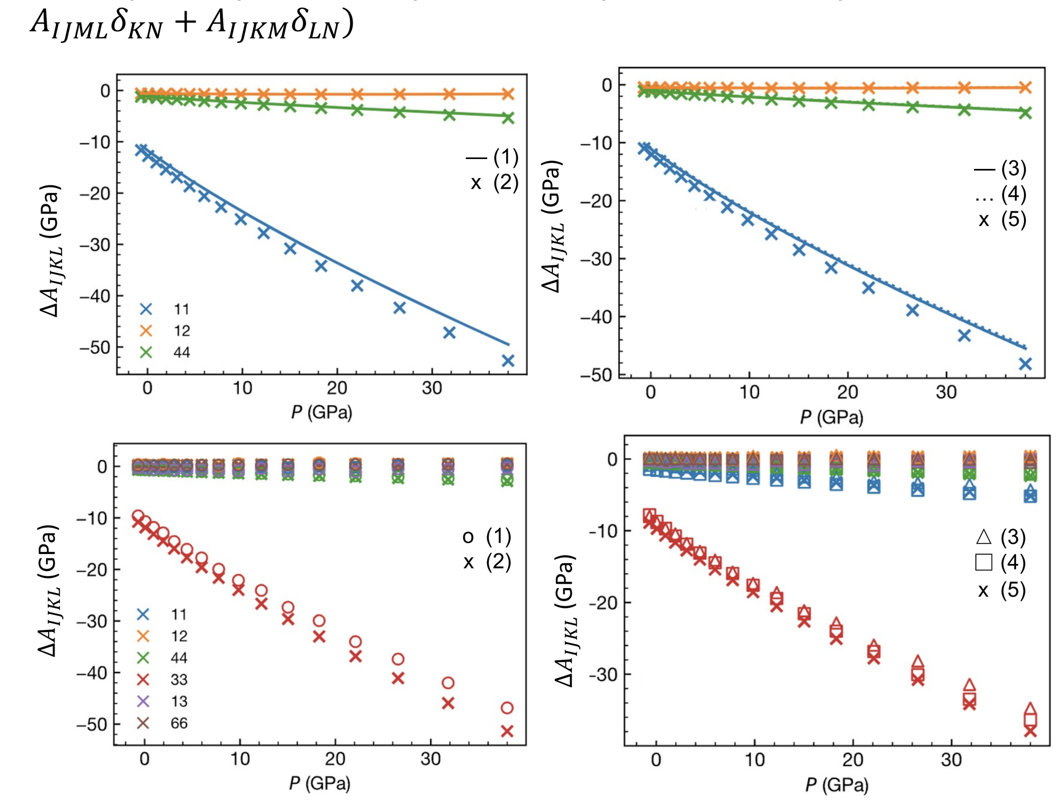
To address the change in different reference frames, the following equation is tested (Eq. 4 from Tromp et al., 2019; Tromp & Trampert, 2018):

$$\Delta A = A_{IJKL}(V, e) - A_{IJKL}(V, 0) \quad (3)$$

$$= A'_{IJKL}\Delta P - \frac{1}{4}\left(A'_{MJKL}\tau^I_M + A'_{IMKL}\tau^J_M + A'_{IJML}\tau^K_M + A'_{IJKM}\tau^L_M\right) \quad (4)$$

$$= C_{IJKLMN}e_{MN} \quad (5)$$

where $C_{IJKLMN} = \frac{\partial \Xi^{IJKL}}{\partial E_{MN}} = A_{IJKLMN} - A_{IJKLMN}\delta_{MN} + \frac{1}{2}(A_{NJKL}\delta_{IM} + A_{INKL}\delta_{JM} + A_{IJNL}\delta_{KM} + A_{IJKN}\delta_{LM} + A_{MJKL}\delta_{IN} + A_{IMKL}\delta_{JN} + A_{IJML}\delta_{KN} + A_{IJKM}\delta_{LN})$

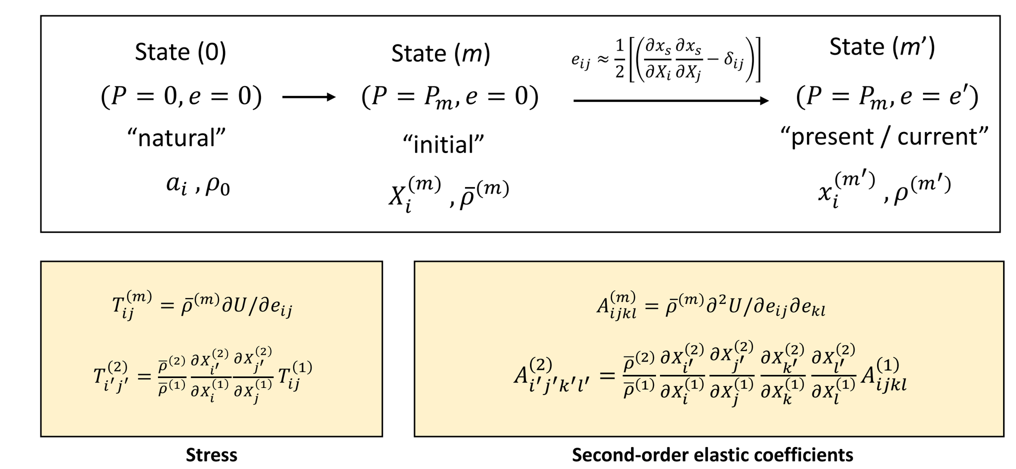


Frame of reference

On an additional note, since each strain, stress, SOEC, and TOEC is defined as a difference or a derivative, they are associated with at least two states. Therefore, we need to clarify which state each of these tensors is referring to. Below we summarize three states.

- **Natural frame**: this is the unstressed state, the external stress is 0 GPa.
- **Initial (reference) state / intermediate frame**: this is usually a hydrostatically pre-stressed state, the tensor is said to be measured or calculated for this state.
- **Final (current) state**: this occurs when additional strain or stress is applied to the reference state.

The definition of stress and SOEC under these states, and equation for how to change the reference state is shown in the figure below (Thurston, 1965)



Conclusions

In this study, we reevaluate the the effects of stress/strain on SOEC and TOEC theoretically and provide *ab initio* verifications. We first examine the effect of hydrostatic stress, i.e., we describe the pressure derivatives of SOEC; then, as a more general case, we investigate modification of the SOEC under hydrostatic and deviatoric stresses. We show in that both cases the required modification of the SOEC is a linear combination of SOEC and TOEC. The relationships are tested on NaCl and MgO with *ab initio* calculated SOEC and TOEC vs. pressure. The method to compute finite-pressure TOEC is also self-consistently tested.

Acknowledgments

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