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ABSTRACT
Non-hydrostatic stresses have a unique influence on materials. To understand the effect of non-hydrostatic stress on NaCl, one of the most widely used pressure calibrant in high-pressure experiments, the lattice constants, density, elastic modulus, Young’s modulus, and phase transitions of the B1 and B2 phases of NaCl were calculated under hydrostatic and non-hydrostatic stresses. The effects of non-hydrostatic stresses on the lattice constants and Young’s modulus show the Poisson effect. The effect of non-hydrostatic stresses on lattice constants increases linearly with increasing differential stress, however, these effects decrease with increasing pressure. Therefore, non-hydrostatic stresses do not affect the NaCl acting as a pressure scale to indicate pressure values in high-pressure experiments, but it may not accurately reflect the state of stress. The state of non-hydrostatic stress is complex in high-pressure experiments, but we only considered one non-hydrostatic state in this study; thus, more work is needed to clarify the effect of non-hydrostatic stress.

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I. INTRODUCTION
Diamond anvil cells (DACs) have long been extensively used to generate high pressure on materials for research purposes. However, maintaining hydrostatic conditions under extremely high pressures has long been a great challenge, and the effects of non-hydrostatic stress caused by pressure-transmitting media (PTM) solidification will become more and more ineligible with increasing pressure. Non-hydrostatic stress has been reported to have a unique influence on materials. Powder diffraction lines tend to broaden significantly under non-hydrostatic stresses. A number of compounds show strong dependence of phase-transition pressure and sequence on non-hydrostatic stress. Studies of the state of non-hydrostatic stress in high-pressure experiments have thus received considerable attention. Two distinct theories have been proposed, namely anisotropic elasticity theory (AET) and isotropic elasticity theory (IET). These theories have been used to analyze the state of non-hydrostatic stress in high-pressure experiments by deriving the relationship between lattice strain, d-spacing, and diffraction data. Estimation of non-hydrostatic stress using IET and AET requires the knowledge of the crystal-structure parameters and elastic moduli of the material under hydrostatic stress. Owing to the difference in the lattice strain and elastic constant of materials under non-hydrostatic and hydrostatic stress, quantitative studies of lattice parameters under non-hydrostatic stress are essential to understanding the state of non-hydrostatic stress under high pressure.

Pressure has been measured in high-pressure experiments on the basis of the relationship between the pressure and volume of pressure-scale materials. Sodium chloride (NaCl) is one of the most widely used pressure calibrants in high-pressure experiments due to its high compressibility and simple crystal structure. At ambient temperature, NaCl transforms from the B1 phase (NaCl-type structure, Fm3-m) to the B2 phase (CsCl-type structure, Pm3-m) at approximately 30 GPa. Accurate information on this phase boundary is useful for X-ray-diffraction experiments at high pressure.
pressure and temperature.\cite{36} A large pressure gradient was observed in \( \text{NaCl} \) in DAC high-pressure experiments, in which the pressure varied from 0 to 12 GPa.\cite{37} Thus, clearly understanding the effects of non-hydrostatic stress on \( \text{NaCl} \) is important to determining the pressure in, and to the analysis of experimental results of, high-pressure experiments. Furthermore, accurate determination of pressure is also important to understanding the composition and temperature of the Earth’s core and fundamental high-pressure phenomena through comparison of theoretical and experimental results.\cite{38} First-principles simulations are reliable for calculating the properties of materials,\cite{39–42} including the state of non-hydrostatic (differential) stress and its effects on materials at atomic scale.\cite{43–46} Therefore, the structure and elasticity of the B1- and B2-phases of \( \text{NaCl} \) under non-hydrostatic and hydrostatic stresses were calculated by the first-principles method in this study.

II. SIMULATIONS DETAILS

First-principles calculations were performed using density-functional-theory (DFT)\cite{47,48} and the plane-wave pseudopotential technique, as implemented in CASTEP codes.\cite{49} The generalized gradient approximation (GGA) with PBE parameterization \cite{50} was used to describe exchange-correlation interactions, an ultrasoft pseudopotential was employed to model electron-ion interactions, and a \( 5 \times 5 \times 5 \) Monkhorst pack grid of \( k \) points was adopted for sampling the Brillouin zone. A convergence criterion of \( 5 \times 10^{-7} \) a.u. on the total energy was used in the self-consistent field (SCF) calculations. The energy cutoff for the plane-wave basis was chosen as 800 eV. The total energy was used in the self-consistent field (SCF) calculations. The lattice constants under non-hydrostatic stresses were found to deviate from those under hydrostatic stress. The calculated lattice constants \( a \) and \( b \) (\( a = b \)) under non-hydrostatic stresses are larger than their equivalent hydrostatic values, while the \( c \) values are smaller; that is, the effect of non-hydrostatic stresses on the lattice constants shows the Poisson effect, consistent with previous results.\cite{51,52} The lattice constants of B1- and B2-phase \( \text{NaCl} \) decrease non-linearly with increasing pressure, consistent with previous results.

The previous results indicate as follow: Decker\cite{53}; Feldman et al.;\cite{54} Liu and Bassett;\cite{55} Ono et al.;\cite{56} Sata et al.;\cite{57} Bukowsk and Aidum;\cite{58} Fei et al.\cite{59}

III. RESULTS AND DISCUSSION

A. Lattice parameter

Figure 2 shows the lattice constants of \( \text{NaCl} \) as a function of pressure and differential stress. Furthermore, partial enlargement is used to present the details in the figure 2. Non-hydrostatic stresses were generated by applying additional pressures in the \( z \) direction (\( c \) axis) during the pressuring in this work. The B1- and B2-phase \( \text{NaCl} \) will not exhibit cubic symmetry under non-hydrostatic stress. The lattice constants under non-hydrostatic stresses were found to deviate from those under hydrostatic stress. The calculated lattice constants \( a \) and \( b \) (\( a = b \)) under non-hydrostatic stresses are larger than their equivalent hydrostatic values, while the \( c \) values are smaller; that is, the effect of non-hydrostatic stresses on the lattice constants shows the Poisson effect, consistent with previous results.\cite{51,52} The lattice constants of B1- and B2-phase \( \text{NaCl} \) decrease non-linearly with increasing pressure, consistent with previous results.

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TABLE I. Zero-pressure lattice constants and bulk modulus of NaCl.

|           | B1 phase (Pm3-m) | B2 phase (Pm3-m) |
|-----------|------------------|------------------|
|           | $a$              | K                | $a$              | K                | Ref.          |
| Theory    |                  |                  |                  |                  |              |
|           | 5.695            | 23.3             | 3.506            | 24.7             | This study    |
|           | 5.646            | 21.44            | 3.483            | 29.12            | Cowley, et al.|
|           | 5.64             | 28.5             | 3.41–3.57        | 24.4–35.6        | Cohen and Gorden |
|           | 5.67             | 24.2             | 3.458            | 28.11            | Ono, et al.   |
|           | 5.51–5.80        | 22.8–32.5        | 3.458            | 28.45            | Cohen and Gorden |
|           | 5.636            | 24.94            | 3.458            | 26.65            | Ueda, et al.  |
|           |                  |                  | 3.435            | 25.6             | Apra, et al.  |
| Experiment|                  |                  |                  |                  |              |
|           | 5.634            | 25.87            | 3.469            | 36.2             | Brown         |
|           | 5.64             | 23.8             | 3.458            | 30.69            | Hofmeister    |
|           | 5.618            | 27.05            | 3.442            | 35.4             | Decker        |
|           | 5.64             | 24.2             | 3.444            | 30.62            | Birch         |
|           |                  | 23.88            |                  |                  | Heinz and Jeanloz |
|           |                  |                  | 3.469            | 30.69            | Fei, et al.  |
|           |                  |                  | 3.442            | 35.4             | Ono, et al.   |
|           |                  |                  | 3.444            | 30.62            | Sims, et al.  |

FIG. 2. Lattice constants of B1- and B2-phase NaCl under different stresses; Partial enlargements of figures appear as insets.
Changes of lattice constants, $a$, of B1- and B2-phase NaCl under pressure received considerable attention from different researchers; $^{31,38,59,63–66}$ however, these research results are not exactly accordant (Figure 2). Our calculated $a$ are bigger than all previous results under hydrostatic stress. However, the $a$ of B1- and B2-phase NaCl of the previous researches are the same as partly calculated results of non-hydrostatic stresses. Therefore, we might boldly imagine one of the possible reasons for the difference between the simulation and the experimental results is that perfect hydrostatic stress cannot be maintained during the high pressure experiment.

The differences in lattice constants of B1- and B2-phase NaCl between non-hydrostatic and hydrostatic stress are presented in Figure 3. The effect of non-hydrostatic stress on lattice constants increases linearly with increasing differential stress. However, such effects decrease with increasing pressure. The differences in the lattice constants ($a$, $b$, and $c$) under hydrostatic stress compared to non-hydrostatic stresses with differential stress were fitted by a linear equation; the fitted coefficients are listed in Table II. The effect of non-hydrostatic stress on the $c$ axis are larger than that on the $a$ and $b$ axes because of the simultaneous increase in the $a$ and $b$ axes, while only the $c$ axis decreases under non-hydrostatic stresses. The excellent linear relationship of the effect of non-hydrostatic stresses on the lattice constants of NaCl can be used to deduce the differential stresses in high-pressure experiments.

B. Density

Changes in NaCl density (cell volume) with pressure are commonly used to indicate pressure in high-pressure experiments.
TABLE II. Linear fitted coefficient of difference of lattice constants under hydrostatic stress from non-hydrostatic stresses with differential stress. The linear equation is described as $D = D_0 + S_{D0} \times S_D$, where $D$ (in Å) indicates the differences in lattice constants under hydrostatic and non-hydrostatic stresses; $S_D$ (in GPa) indicates the differential stress.

| Lattice constant | $P$ (GPa) | $D_0$ | $S_{D0}$ | $D_0$ | $S_{D0}$ |
|------------------|-----------|-------|----------|-------|----------|
| $a/b$            | 1         | $-8.22E-04$ | 0.04387 | $-4.83E-04$ | 0.01347 |
| $c$              |           | $-0.01075$  | $-0.06976$ | $-0.0011$  | $-0.02859$ |
| $a/b$            | 10        | $-4.43E-04$ | 0.01492  | $-3.79E-04$ | 0.00957  |
| $c$              |           | $0.00199$   | $0.02694$ | $-0.0600$  | $-0.0175$ |
| $a/b$            | 20        | $3.97E-04$  | $0.00909$ | $5.53E-04$ | 0.00673  |
| $c$              |           | $-0.00131$  | $-0.01728$ | $1.38E-04$ | $-0.0138$ |
| $a/b$            | 30        | $1.52E-04$  | $0.00605$ | $9.39E-05$ | 0.00577  |
| $c$              |           | $-3.42E-04$ | $-0.01157$ | $-3.29E-04$ | $-0.0110$ |
| $a/b$            | 40        | $-4.48E-04$ | $0.0059$  | $3.36E-04$ | 0.00488  |
| $c$              |           | $8.46E-05$  | $-0.00939$ | $-6.66E-04$ | $-0.00941$ |
| $a/b$            | 50        | $-6.56E-04$ | $0.00465$ | $-8.67E-05$ | $-0.00804$ |

The densities of B1- and B2-phase NaCl under hydrostatic and non-hydrostatic stresses are shown in figure 4. There is no difference among the calculated densities, even from the partial enlarged figure, under hydrostatic and non-hydrostatic pressure from the figure 4. The result indicates that non-hydrostatic stresses have a limited effect on the density of B1- and B2-phase NaCl at high pressure; that is, the equations of state (EOS) of B1- and B2-phase NaCl under hydrostatic stress are same as those under non-hydrostatic pressure. Therefore, non-hydrostatic stresses explored in this work do not affect NaCl acting as a pressure scale to indicate pressure.

![FIG. 4. Density of B1- to B2-phase with different stress conditions. Partial enlargement of the figure appears as an inset.](image-url)
values in high-pressure experiments, but also may not accurately reflect the state of stress. These results are consistent with experimental results on ruby in which ruby was used as a pressure scale to at least 52.5 GPa in high-pressure experiments under non-hydrostatic stresses.

The previous results indicate as follow: Decker;31 Feldman et al.;63 Liu and Bassett;64 Ono et al.;65 Sata et al.; Bukowinska and Aidum;59 Fei et al.38

The experimental results show no obvious non-hydrostatic effect on cell volume of B2 phase NaCl, consistent with our calculated results. However, our results are different from previous results on the effects of non-hydrostatic stress on the densities of forsterite12 and calcite. The densities of calcite and forsterite increase or decrease under different differential stresses, relative to their equivalent values under hydrostatic pressure, which depends on the state of differential stress. The reasons may be differences in crystal symmetry of NaCl compared with forsterite and calcite. NaCl belongs to a cubic system and forsterite and calcite belong to an orthorhombic system.

Previous results31,38,59,63–66 of density of B1- and B2-phase NaCl at high pressure also listed in the figure 4. Our calculated densities are smaller than all previous results, but the calculated change trends in lattice constants with pressure are consistent with the previous results. These differences may be attributed to under-binding resulting from the use of the GGA. And our calculations are carried out at 0 GPa, so zero-point corrections to the elastic constants will very likely improve the agreement between the calculated and reported results. The K and G values of NaCl under non-hydrostatic stress are the same as those under hydrostatic stress. The K value of B2 phase NaCl is larger than that of B1-phase NaCl throughout the pressure range explored in this work. However, the G value of B2-phase NaCl is smaller than that of B1-phase NaCl at low pressure (<13.5 GPa) and increases when the pressure is higher than 13.5 GPa. Changes of K caused by the B1- to B2-phase phase transition are not consistent among different researchers. Hofmeister35 and Heinz and Jeanloz61 suggest decreases in K value, but a small increase is indicated in other works.37,59,60,65–67 The results of our calculation are consistent with those indicating an increase of K value.

D. Young’s modulus

The Young’s modulus describes the characteristics of how a material responds to linear stress. Therefore, we calculated the Young’s modulus (Y) of the a and c axes to understand the differences between elastic properties in different directions under non-hydrostatic stress (Figure 6). The values of Ya (=Yb) and Yc, which represent the Young’s modulus in a-, b-, and c-axis directions, under non-hydrostatic stress are different than those under...
hydrostatic stress. Like the effect of non-hydrostatic stress on lattice constant, the values of $Y_a (=Y_b)$ under non-hydrostatic stresses are larger than their equivalent hydrostatic values, while the values of $Y_c$ are smaller. Effects of non-hydrostatic stress on the Young’s modulus increase with increasing differential stress. That effect of non-hydrostatic stress on $Y_c$ is larger than that on the $Y_a$ and $Y_b$ axes shows the different effect of non-hydrostatic stress on the Young’s modulus in different directions.

### E. The B1-B2 phase transition

The B1-B2 phase transition of NaCl is of considerable interest as a model for other structural phase transformations, including those of geophysical importance, as it is one of the simplest first-order nondisplacive transitions. The energy-volume relationships of B1- and B2-phase of NaCl under hydrostatic and non-hydrostatic stresses are shown in figure 7. We calculated the properties of NaCl.
at 0 K, so the total energies of B1- and B2-phase NaCl are equal to their enthalpy. Therefore, the intersection points of the energy-volume curves of B1- and B2-phase NaCl are equivalent to the phase-transition points, and, thus, the corresponding pressures are the phase equilibrium pressures. Li and Jeanloz \cite{Li2011a} extrapolated their experimental result for the NaCl B1- to B2-phase phase transition to 0 K and found good agreement with the results derived from first-principles simulations. In addition, the previous works proved that properties of alkali halides, including NaCl, can be computed accurately using the first-principles method. \cite{Li2011b, Li2011c} NaCl transforms from B1 to B2 phase at approximately 29.5 GPa from the calculated energy-volume results, which is consistent with previous results. \cite{Johansen1984, Johansen1985, Johansen1986, Johansen1987}

To achieve clear understanding, the energy-volume result under hydrostatic stress is also individually plotted in figure 6. The phase equilibrium pressure of the B1- to B2-phase phase transition under hydrostatic stress is the same as that under non-hydrostatic stresses. As with the density and elastic modulus, non-hydrostatic stress did not change the transition pressure in the B1- to B2-phase phase transition in this study. This result, however, is different than the effect of non-hydrostatic stress on the B1- to B2-phase phase-transition pressure of KCl. The non-hydrostatic stress reduced the B1- to B2-phase phase-transition pressure of KCl. \cite{Caspersen2004}

IV. CONCLUSION

The lattice constants, density, elastic modulus, Young’s modulus, and energy-cell volume relationship of B1- and B2-phase NaCl were calculated under hydrostatic and non-hydrostatic stresses. Results show that the values of the lattice constants and Young’s modulus of B1- and B2-phase NaCl under non-hydrostatic stresses deviate from those under hydrostatic stress. The effect of non-hydrostatic stresses on the lattice constants shows the Poisson effect, consistent with previous results. The effects of non-hydrostatic stress on lattice constants increase linearly with increasing differential stress, and such effects decrease with increasing pressure. However, the non-hydrostatic stresses explored in this study have no effect on the density (i.e., the equation of state), elastic modulus, and phase-transition pressure of B1- and B2-phase NaCl. Therefore, non-hydrostatic stress does not affect NaCl acting as a pressure scale to indicate stress values in the high-pressure experiment; however it may not accurately reflect the state of stress. The state of non-hydrostatic stress is complex in high-pressure experiments. Since just one of the non-hydrostatic states was considered in this study, more work is needed to clarify the effect of non-hydrostatic stress and understand the high-pressure experimental results.

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