

## Equation of state of NaCl

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### Introduction

Sodium chloride (NaCl) is a most important alkali halide that is used as a pressure calibrant in laboratory measurements of compression data. NaCl has a stable B1-type structure up to a pressure of ~30 GPa, and its phase transition into a B2-type structure has been confirmed. Numerous attempts to investigate the EOS and thermoelastic properties have been carried out on B1-type NaCl. However, reliable data for the high-pressure B2-type NaCl phase are not available. The bulk modulus of B2-type NaCl at room temperature has been repeatedly measured experimentally in previous studies. In contrast, previous theoretical studies using first-principles calculations have investigated the physical properties of NaCl, including its bulk modulus at 0 K. However, the uncertainty in first-principles calculations is non-negligible, because the discrepancy in the values of the bulk modulus and the zero-pressure volume from previous calculations is ~50 % and ~10 %, respectively. We noticed that the scatter of the experimental bulk modulus values was much smaller than that obtained from calculations. This indicates that experiments are more accurate than first-principles calculations for determining the bulk modulus at room temperature. In contrast, high temperature data performed by the diamond anvil cell experiments have a significant uncertainty, because the heating condition is unstable. Recently, the first-principle molecular dynamics method has been used to calculate the thermoelastic properties of materials under extreme high-pressure and high-temperature conditions [1]. In this study, we used density functional theory to investigate the thermal pressure of B2-type NaCl. We also used the experimental data to determine the room temperature EOS of B2-type NaCl. The combination of the first-principles calculations and the high-pressure experiments led us to determine a reliable EOS for B2-type NaCl over a wide range of pressures and temperatures.

### Experimental

High-pressure X-ray diffraction experiments were performed using a laser-heated diamond anvil cell high-pressure apparatus. The starting materials of pure NaCl have a B1-type structure. High-pressure X-ray diffraction experiments were carried out in a motor-driven diamond anvil cell [2]. A small sample of polycrystalline NaCl was sandwiched between pellets of MgO powder, and this was loaded into a hole in a rhenium gasket. A few grains of

powdered ruby were also loaded into the sample chamber to carry out a preliminary pressure calibration. Gold powder mixed with NaCl sample was used as the primary pressure calibrant. The sample was heated after compression or decompression using an infrared laser to minimize any pressure inhomogeneity in the sample. The sample was probed using angle-dispersive X-ray diffraction, employing the 13A or NE1A synchrotron beam line at KEK. The angle-dispersive X-ray diffraction patterns were obtained on an image plate system.

### Results and Discussion

After the pressure was increased directly at room temperature, an X-ray diffraction pattern of the sample was recorded. The acquired diffraction data showed a strain-broadening of the diffraction peaks, resulting from the large differential stress that was induced in the diamond anvil cell as the pressure was increased. As the differential stress causes a significant systematic bias for the relationship between pressure and structural properties, diffraction patterns including the strain-broadening are not suitable for this work. Therefore, the sample was heated after each change in pressure to relax the differential stress. After heating, the strain-broadening of each peak in the diffraction pattern disappeared. This implies that the differential stress in the sample decreased after heating. Only diffraction data after heating were used in this study. The high-pressure phase of sodium chloride remained the B2-type structure in the space group Pm3-m to the highest pressure attained. A fit of the volume-pressure data using the Vinet EOS. The results of the fit of our  $P$ - $V$ - $T$  data including the high-pressure experiments and the first-principles molecular dynamics calculations were summarized in our publication [3]. In conclusion our method combined between experiments and calculations predicts accurate equations of state for the ionic crystals. Thus, this method may prove useful to geophysical and astrophysical issues to investigate physical properties of crystals under extreme high pressure and temperature.

### References

- [1] Ono et al., J. Appl. Phys., 103, 023510 (2008).
- [2] Ono et al., J. Phys. Condens. Matter, 19, 036205 (2007).
- [3] Ono, J. Phys. Conf. Ser., 215, 012196 (2010).

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