Equation of state and thermodynamic Grüneisen parameter of monoclinic 1,1-diamino-2,2-dinitroethylene

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Abstract

In situ synchrotron x-ray diffraction experiments were conducted on 1,1-diamino-2,2-dinitroethylene (FOX-7) at pressures up to 6.8 GPa and temperatures up to 485 K. Within the resolution of the present diffraction data, our results do not reveal evidence for a pressureinduced structural phase transition near 2 GPa, previously observed in several vibrational spectroscopy experiments. Based on unit-cell volume measurements, the least-squares fit using the third-order Birch–Murnaghan equation of state (EOS) yields $K_0 = 12.6 \pm 1.4$ GPa and $K_0\_ = 11.3 \pm 2.1$ for the α-phase of FOX-7, which are in good agreement with recently reported values for the deuterated sample, indicating that the effect of hydrogen–deuterium substitution on the compressibility of FOX-7 is negligibly small. A thermal EOS is also obtained for the α-phase of FOX-7, including pressure dependence of thermal expansivity, $(\partial\alpha/\partial P)_T = -7.0 \pm 2.0 \times 10^{-5}\,K^{-1}\,GPa^{-1}$, and temperature derivative of the bulk modulus, $(\partial K_T/\partial T)_P = -1.1 \times 10^{-2}\,GPa\,K^{-1}$. From these EOS parameters, we calculate heat capacity at constant volume (C_V) and thermodynamic Gruneisen parameter (γ_{TH}) as a function of temperature. At ambient conditions, the calculated γ_{TH} is 1.055, which is in good agreement with the value (1.09) previously obtained from density functional theory (DFT). The obtained C_V, however, is 13% larger than that calculated from the first-principles calculations, indicating that the dispersion correction in the DFT calculations may need to be further improved for describing intermolecular interactions of molecular crystals.

Keywords: equation of state, phase transformation, FOX-7, high explosive, pressure
(Some figures may appear in colour only in the online journal)
near 389 K [3–5], $\beta \rightarrow \gamma$ transition at ~446 K [6, 7], and $\gamma \rightarrow \delta$ transition at ~483 K [7, 8]. Upon further heating the decomposition occurs at temperatures above 523 K [7, 9]. The α phase crystallizes in a monoclinic $P2_1/n$ structure and is most stable under ambient pressure and temperature conditions. Based on single-crystal x-ray diffraction, the β phase is determined to be orthorhombic with space group $P2_12_12_1$ [4], whereas the γ-phase can be indexed by space group $P2_1/n$ [6]. At temperatures above 483 K, both differential scanning calorimetry measurement and infrared spectroscopy experiments indicate the presence of the δ-phase [7–9] although its crystal structure is currently still not known. Under static compression, several spectroscopy studies reported the existence of highpressure polymorphs of phase-I and phase-II at both ambient [10–13] and elevated temperatures [7, 9], with the $\alpha \rightarrow$ I transition occuring around 2 GPa and I → II transition above
5 GPa. The phase transitions are manifested by the appearance of new vibrational modes or discontinuous frequency shifts above the transition pressures. Although there exists some evidence from x-ray [14, 15] and neutron [16, 17] diffraction showing phase changes in the 4.0–4.5 GPa range under roomtemperature compression, there is some discrepancy between the results of vibrational spectroscopy and diffraction experiments for the phase transition near 2 GPa, which has not been observed in any diffraction studies.

In this work, we conducted *in situ* synchrotron x-ray diffraction experiments on FOX-7 in order to further examine structural phase stability under high pressure (P) and temperature (T). From unit-cell volume measurements under high P–T conditions, we derived a thermal EOS for the monoclinic α-phase, including pressure dependence of volumetric thermal expansivity and temperature derivative of the bulk modulus. Based on these EOS parameters, we also calculated the heat capacity at constant volume and thermodynamic Gruneisen parameters as a function of temperature.

Experimental methods

The polycrystalline FOX-7 sample was obtained through a cooperative agreement with the Totalförsvarets forskningsinstitut (FOI, Swedish Defense Research Agency). Synchrotron x-ray diffraction experiments were conducted in a cubic anvil apparatus [18] using energy-dispersive technique at beamline X17B2 of the National Synchrotron Light Source, Brookhaven National Laboratory. The detail of cell assembly used in the experiments has been described in [18]. Briefly, we used a mixture of amorphous boron and epoxy resin as pressure transmitting medium and amorphous carbon as heating element. The starting FOX-7 sample was loaded into a boron nitride (BN) container, 1.0 mm inner diameter and 2.0 mm length, and was sandwiched between two layers of NaCl powders. The temperatures were measured by a W/Re25%-W/Re3% thermocouple and pressures were determined from the Decker's EOS for NaCl [19]. During the course of experiments,

diffraction patterns were collected for both sample and NaCl in the close vicinity of the thermocouple junction. Over the *P*–*T* range of this study the estimated errors in temperature measurements are less than 10 K and are less than 0.2 GPa in the pressure measurements.

Two experiments were conducted in this work, an isothermal compression experiment at room temperature up to 6.76 GPa and an 'isobaric' heating experiment from 300 K to 485 K at a constant load of 10 tons (corresponding to 0.74 to 1.31 GPa due to the combined effects of thermal pressure and stress relaxation). In each experiment, diffraction data were collected for both FOX-7 and NaCl under selected *P*–*T* conditions. The unit-cell parameters for the monoclinic α phase were obtained from the Le Bail fit of the observed patterns using the GSAS software [20].

Results and discussion

Shown in figure 1(a) are diffraction patterns collected at selected pressures during room-temperature compression. As pressure is increased, diffraction peaks began to broaden and gradually lose their intensities due to the combined effects of crystallographic texture and non-hydrostatic sample environment. In the pressure range of 0–4.88 GPa, all diffraction patterns could be refined with the monoclinic $P2_1/n$ structure for the α-phase of FOX-7, as exemplified in figure 1(b). Our observations hence do not reveal any evidence for a structural phase transition around 2 GPa, which has been identified in several high-pressure spectroscopy experiments [7, 9–13]. However, due to the limited number of diffraction peaks observed in our experiment for a monoclinic structure, the present data do not have sufficient resolution to detect small changes in molecular geometry and associated structural parameters. To further look into a possible phase transition, we plot in figure 1(c) the d-spacing values as a function of pressure for the two most intense peaks of the α-phase, 0 2 1 and 0 2 2. Apparently, there is no visible discontinuity in the trend of variations and hence no evidence of a phase transition near 2 GPa. Based on recent simulations using density functional theory (DFT) reported in [16], the observed changes in the experimental vibrational frequencies can be attributed to a subtle second-order phase transition at 1.89 GPa, which involves small conformational changes in the internal geometries of molecules. However, it would be difficult to detect such changes in high-pressure diffraction experiments.

At a higher pressure of 5.69 GPa, two new diffraction peaks, as indicated by two red arrows in figure 1(a), start to appear with an intense peak at the d-spacing of 2.69 A, suggesting the presence of a new phase. Upon further increase in pressure, the new phase continues to grow but it still coexists with the α-phase of FOX-7 at 6.76 GPa, the highest pressure of this experiment. This pressure-induced phase transition is hence kinetically sluggish, at least at room temperature. As can be seen in figure 1(c), the d-spacing values determined in this work for the new phase line up nicely with the value of 2.73 A at 4.24 GPa reported in [16] for the ε-phase of FOX-7. However, there are some notable differences between this

study and [16] for the α–ε transition in both the observed onset pressures (5.69 GPa versus 3.63 GPa) and hysteresis regions for the metastable α phase (ΔP = 5.69–>6.76 GPa versus ΔP = 3.63–4.14 GPa). While we do not have definite explanations for the discrepancy, the underlying cause is likely associated with one or a combination of the following differences between the two studies: internal pressure standard (NaCl versus Pb), pressure medium (solid NaCl + BN versus methanol/ethanol liquid), and isotope composition in the starting samples (proton H versus deuteron D). Most recently, a synchrotron single-crystal x-ray diffraction experiment reports a transition pressure of 4.5 GPa for the α–ε phase transition [17]. The high-pressure ε phase possesses a triclinic structure with P1 space group and is made of planar molecular layers as compared to zig-zagging layers in the low-pressure monoclinic phase [16, 17]. With regard to isotope differences, it is well knwon that the hydrogen–deuterium (H–D) substitution in hydrogen bonded systems can affect the A—X…B bond in the crystal structure (where A is a donor, X is H or D, and B is an acceptor), which would lead to modifications of the bond geometry (e.g. [21, 22]) and in turn affect the structural stability of molecules. Such structural effect, the so-called geometric isotope effect, is commonly linked with changes in bond vibrations. Most recently, Tao *et al* investigated the effect of H–D substitution on the high-pressure stability of FOX-7 using Raman spectroscopy [23]. The authors, however, concluded that the H–D substitution does not affect the onset pressure for the phase transition near 4.5 GPa.

Figure 2(a) shows diffraction patterns collected during heating under a constant load force. No apparent changes were observed as temperature increases from 300 K to 485 K, and all patterns in this temperature range could be refined with the monoclinic α-phase of FOX-7, as exemplified in figure 2(b). The commonly reported $\alpha \rightarrow \beta$ and $\beta \rightarrow \gamma$ transitions at ambient pressure are thus not observed even under moderate pressures of ~1.2 GPa. The α and β phases of FOX-7, however, are very similar in the internal structure, and the subtle difference in the molecular geometries cannot be resolved with our energy-dispersive data. To gain further insight into possible phase transitions, the d-spacing values for the 0 2 1 and 0 2 2 peaks of α-phase are plotted in figure 2(c), which show smooth and monotonic increase with temperature up to 485 K and no sign of phase transitions given the fact that the $\alpha \rightarrow \beta$ transition at ambient pressure is accompanied by a 2% increase in the unit-cell volume [4]. On the other hand, the present observations are consistent with recent results of high P–T spectroscopy experiments, which showed steep dT/dP slopes for the phase transitions between high-temperature polymorphs of FOX-7 [9]. As a result, both the α–β and β–γ phase boundaries are terminated at the γ–δ boundary at pressures below 1.2 GPa. The β and γ polymorphs of FOX-7 are thus energetically unfavorable under high pressure and have very limited stability fields in the P–T space.

Figure 1. (a) Selected diffraction patterns of FOX-7 collected during room-temperature compression. Diffraction data were collected at the

fixed Bragg angle of 6.458 88°. The red arrows indicate the two new diffraction peaks for the high-pressure phase of FOX-7, referred to as
ε-phase in [16, 17]. In both figures 1(a) and 2(a), 0 2 1 and 0 2 2 are the two strongest peaks for the α-phase, and asterisks denote the peak
positions of hexagonal boron nitride (*h*-BN); (b), an example of the Le Bail fit at 4.88 GPa and 300 K. In both figures 1(b) and 2(b), data are
shown as plus signs, and the solid red curve is the best fit to the data. Tick marks below the pattern show the positions of allowed reflections
for P21/*n* FOX-7 (black color) and *h*-BN (red color). The lower curve in pink represents the difference between the observed and calculated
profiles; (c), d-spacing values as a function of pressure for the 0 2 1 and 0 2 2 diffraction lines of the α-phase and the strongest diffraction
line of the ε-phase.

Figure 3 shows the lattice parameters obtained from the Le Bail fits for the α-phase of FOX-7 during room-temperature compression. Although there are some scatters due to limited number of diffraction lines for the monoclinic structure, our data clearly show that the crystallographic *b*-axis, which lies in the direction perpendicular to the wave-shaped layers of molecules in the crystal structure [17], is substantially more compressible than the *a*- and *c*-axes. Over the 0–4.88 GPa pressure range where the α-phase is structurally stable, the normalized lattice parameters are approximately 0.98, 0.90 and 0.96, respectively, for $a/a0$, $b/b0$ and $c/c0$, which are in reasonably good agreement with those reported in [16].

The refined unit-cell volumes from the room-temperature compression experiment are plotted as a function of pressure in figure 4(a). The volume–pressure data were analyzed using an Eulerian finite-strain EOS [24], commonly known as the Birch–Murnaghan EOS. In this EOS, the pressure is expressed to third order in strain *f* by:

$$P = (3f + 1)^{5/2} f K_0 \left[1 + \xi f + \ldots\right] \quad (1)$$

with $\xi = 3/4(4 - K_0')$ and $f = 1/2[(V/V_0)^{-2/3} - 1]$, where K_0 and K_0' are, respectively, isothermal bulk modulus and its pressure derivative at 300 K. The least-squares fit using the thirdorder EOS yields $K_0 = 12.6 \pm 1.4$ GPa and $K_0' = 11.3 \pm 2.1$ for the α-phase of FOX-7, which are in good agreement with recently reported values for the deuterated sample [16], $K_0 = 11.8 \pm 0.5$ GPa and $K_0' = 11.4 \pm 1.0$. Based on this comparison, the effect of H–D substitution on the compressibility of FOX-7 is negligibly small, within the mutual experimental errors. Note that the errors reported here for EOS parameters are those of the least-squares fitting; uncertainties in the measurements of pressure and unit-cell volume are not included for error estimation.

Figure 2. (a) Selected diffraction patterns of FOX-7 collected during heating at a constant load of 10 tons. Diffraction data were collected
at the fixed Bragg angle of 6.460 94°. The calculated pressures increase with increasing temperature due to the effect of thermal pressure;
(b), an example of the Le Bail fit at 1.28 GPa and 485 K; (c), d-spacing values as a function of temperature for the 0 2 1 and 0 2 2 diffraction
lines of the α-phase.

Figure 3. Variation of lattice parameters as a function of pressure
for the α-phase FOX-7 at room temperature. The observations

reveal that the crystallographic *b*-axis is substantially more compressible than the *a*- and *c*-axes. The errors in the refined lattice parameters are smaller than the size of the symbols (see, for example, figures 1(b) and 2(b)).

To study thermal expansion of the α-phase under high pressure, we measured the unit-cell volumes in the temperature range of 300–485 K under a constant load of 10 tons. The measured pressures increase from 0.74 to 1.31 GPa due to the combined effects of stress relaxation and thermal pressure (figure 2(a)). Based on the EOS data shown in figure 4(a), we corrected the unit-cell volumes corresponding to a constant pressure of 1.0 GPa, and the corrected isobaric data are shown in figure 4(b). Note that this correction scheme assumes that the compressibility at elevated temperatures up to 485 K is the same as at ambient temperature, which would introduce errors if α-phase of FOX-7 has relatively large temperature derivative of the bulk modulus. The volumetric thermal expansivity at 1.0 GPa is derived from the equation

$$V_{T,P} = V_{0,P} \exp \int_T \alpha_T dT \quad (2)$$

where $V_{0,P}$ and $V_{T,P}$ are unit-cell volumes at 300 K and a given higher temperature, respectively, and α_T is given in the form of $\alpha_T = \alpha_0 + \alpha_1 T$. From the volume data of figure 4(b), we obtain $\alpha_0 = 1.2(2) \times 10^{-5}$ K^{-1} and $\alpha_1 = 3.9(6) \times 10^{-7}$ K^{-2}. Also plotted in figure 4(b) are the volume–temperature data previously determined at ambient pressure for the α-phase of FOX-7 [4]. Over the 300–373 K range, the calculated average thermal expansion coefficients are 2.1×10^{-4} K^{-1} at ambient pressure and $1.4 \pm 0.2 \times 10^{-4}$ K^{-1} at 1.0 GPa. The thus-determined pressure derivative of thermal expansion, $(\partial\alpha/\partial P)_T$, is $-7.0 \pm 2.0 \times 10^{-5}$ K^{-1} GPa^{-1}. From the thermodynamic identity:

$$\left(\frac{\partial K_T}{\partial T}\right)_P = -\left(\frac{\partial^2 P}{\partial T^2}\right)_V \left(\frac{\partial V}{\partial P}\right)_T \quad (3)$$

the temperature derivative of the bulk modulus, $(\partial K_T/\partial T)_P$, is found to be -1.1×10^{-2} GPa K^{-1}.

The Gruneisen parameter is an important physical quantity for describing thermoelastic behavior of materials under high pressure and temperature. It is dimensionless and often denoted by γ. Because of the equivalency between many thermodynamic properties and their derivatives, there are several formulations of the Gruneisen parameter that are physically valid but yet have different interpretation of its meaning. The macroscopic or thermodynamic definition, γ_{TH}, is given by

$$\gamma_{TH} = \alpha_T K_T V / C_V \quad (4)$$

where the parameters on the right hand side of equation are familiar thermodynamic properties of bulk modulus (K_T as in equation (1)), thermal expansion (α_T as in equation (2)), and heat capacity. Of these properties the measurement of heat capacity at constant volume (C_V) is especially challenging. However, it is experimentally much more convenient to measure heat capacity at constant pressure (C_P) than at constant volume. Thermodynamically, C_V can be converted from C_P and other thermodynamic parameters using the following equation

$C_V = C_P - \__T K V T.$
^{2}
$_T$ (5)

For the α-phase of FOX-7, recently reported C_P data [25, 26] are shown as a function of temperature in the upper panel of figure 5. Also plotted in figure 5 is C_V obtained from equation (5) and thermoelastic parameters discussed earlier. For the α-phase of FOX-7, the thermodynamic Gruneisen parameters calculated from equation (4) are shown as a function of temperature in the lower panel of figure 5. However, there have been

Figure 4. (a) Pressure–volume data measured at room temperature for the α-phase of FOX-7. Errors in the volume measurements are smaller than the size of plotted symbols. The curve represents the results of least-squares fit using equation (1); (b) volume–temperature data at atmospheric pressure (solid circles) and 1.0 GPa (solid squares) for the α-phase of FOX-7. The 1-bar data were taken from [4] based on single-crystal x-ray diffraction. The 1.0 GPa data were corrected based on high-temperature data measured at pressures of 0.74–1.31 GPa and EOS data shown in figure 4(a). The curves represent the results of least-squares fit using equation (2). Thermal expansion coefficients represent the average values over the temperature range of 300–373 K. The errors in the unit-cell volume measurements are smaller than the size of the symbols (see, for example, figures 1(b) and 2(b)).

so far no experimental data of γ_{TH} or C_V published for any polymorphs of FOX-7. At ambient conditions, our calculated γ_{TH} is 1.055, which argrees well with the value (1.09) previously obtained from *ab initio* calculations within the local-density and quasiharmonic approximations [31]. The heat capacity at constant volume has also been reported as a function of pressure based on the vibrational frequencies calculated from the dispersion-corrected DFT simulations [16]. At ambient conditions, the calculated C_V is 147.5 J mol^{-1} K^{-1}, which is more than 13% smaller than the value (167.1 J mol^{-1} K^{-1}) we obtained from equation (5). Although there have been several simulations using DFT on crystalline FOX-7 [27, 28], it is known that an accurate description of the intermolecular interactions in molecular crystals using conventional DFT methods requires implementation of appropriate dispersion corrections, the socalled DFT-D method [29, 30]. In this regard, the dispersion correction in the DFT calculations need to be further improved for FOX-7 to accurately describe intermolecular interactions, especially the phonon or vibrational properties.

Summary

We conducted *in situ* synchrotron x-ray diffraction experiments on FOX-7 at pressures up to 6.8 GPa and temperatures up to 485 K. We show that upon heating at 1.0–1.3 GPa the α phase of FOX-7 remains stable in the temperature range of the experiment. Consistent with previous high-pressure infrared spectroscopy and neutron diffraction experiments, a structural phase transformation from α-phase to ε-phase is observed between 4.88 and 5.69 GPa during room-temperature compression. From the *P–V–T* measurements, thermoelastic parameters including pressure dependence of thermal expansivity and temperature derivative of the bulk modulus were derived for the first time for the α-phase of FOX-7. Based on the EOS thus determined, we calculate heat capacity at constant volume and thermodynamic Gruneisen

parameter as a function of temperature. At ambient conditions, the calculated γ_{TH} is in good agreement with the value previously obtained from DFT calculations. The C_V obtained in this work is more than 13% larger than the value obtained from DFT calculations, indicating that the dispersion correction in the DFT calculations need to be further improved for the α-phase FOX-7 to accurately describe intermolecular interactions.

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Figure 5. Heat capacity (upper panel) and thermodynamic Gruneisen parameter (lower panel) plotted as a function of temperature for the α-phase of FOX-7 at ambient pressure. The experimental C_P is from [25]. C_V and γ_{TH} are calculated from equations (5) and (4), respectively.

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