I. INTRODUCTION

The discovery of the superconductivity with a critical transition temperature ($T_c$) of 26 K in LaFeAsO$_{1-x}$F$_x$ has opened research activity in a family of superconductors. Since then, four types of superconductors, ReFeAsOF (Re = Ce, Pr, Nd, Sm, etc.), AFe$_2$As$_2$ (A = Ba, Sr, Ca), A'FeAs (A' = Li, Na), and FeSe(FeTe), have been found. The $T_c$ is enhanced up to 55 K either by chemical substitution Re for La or by introducing oxygen vacancies. This type of superconductors, with such high $T_c$’s but without the copper oxide plane, is likely to have a different mechanism from cuprates. It is believed that the superconductivity in ReFeAsOF and AFe$_2$As$_2$ is related to the spin-density-wave (SDW) anomaly in the Fe-As layer. Application of high pressure or chemical doping suppresses the SDW order and drives the superconducting transition. Among those superconductors, the binary compound of $\alpha$-FeSe is a safe system due to the absence of the toxic arsenic. At ambient pressure, FeSe which has a $T_c$ of 8 K has an PbO-type tetragonal structure, with FeSe layers stacked along the $c$ axis. Partial substitution of Te for Se enhances the $T_c$ to 10 K. The $T_c$ is further increased by application of pressure reaching 27 K at 1.48 GPa (Ref. 9) and 37 K at 7–8 GPa.10,11

The compound $\alpha$-FeTe has structure similar to tetragonal $\alpha$-FeSe at ambient pressure. Neutron-scattering experiments revealed that an antiferromagnetic (AF) transition and structural transition in $\alpha$-FeTe take place at the same temperature (~65 K). At ambient pressure, $\alpha$-FeTe has a tetragonal phase at room temperature. This phase transforms to an orthorhombic structure at temperature below 65 K, different from $\alpha$-FeSe in which the structure transforms from a tetragonal phase to a triclinic phase at temperature below 105 K. Theoretical calculations for the FeTe and FeSe compounds indicated that $\alpha$-FeTe adopts multiple Fermi surface similar to ReFeAsO$_{1-x}$F$_x$, with hole and electron pockets at the zone center and corners, respectively. An AF instability was found in these two compounds at ground state. However, the strength of instability in $\alpha$-FeTe is stronger than that in $\alpha$-FeSe. This implies that $\alpha$-FeTe should have a higher $T_c$ than $\alpha$-FeSe after the suppression of the AF transition. Experimental studies showed that the AF transition is tightly correlated with structural properties. The pressure-induced lattice collapse was discovered in tetragonal (T) phase of single crystal Fe$_{1.05}$Te at room temperature through x-ray and neutron-diffraction measurements. A remarkable compression along the $c$ axis (~5%) was observed upon increasing pressure from the ambient condition to 4 GPa. Indexed results demonstrate that the crystallographic structure remains unchanged after the collapse, revealing that the collapse does not break symmetry of crystal structure. The Fe-spin state change was proposed to account for the lattice collapse. The equations of state for the T phase and pressure-induced collapsed T phase were determined from the diffraction measurements.

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II. EXPERIMENTAL DETAILS

The sample was synthesized by solid state reaction at ambient pressure, as described previously. Phase purity was assessed with powder x-ray diffraction to be a single phase with tetragonal symmetry, as shown in Fig. 1. Temperature dependence of resistance (R) and magnetization (M) obtained at ambient pressure exhibited that R-T and M-T curves of the sample have anomalies at the same temperature near 65 K, as shown in Figs. 2(a) and 2(b). The abrupt de-
crease in resistance and magnetization below 65 K is related to the first-ordered tetragonal-monoclinic phase transition, consistent with our previous experimental results.18

Angle-dispersive x-ray diffraction (XRD) measurements were carried out at the Beijing Synchrotron Radiation Facility (BSRF). A monochromatic x-ray beam with a wavelength of 0.6199 Å was used. The XRD images were collected using a charge-coupled device (CCD) detector, and the XRD geometry was calibrated with CeO2. High pressure was created by using a pair of diamond anvils with low birefringence. Diamond anvils used were cut with a 300 μm culet. A spring steel gasket with a 100 μm hole in diameter and 50 μm thickness was adopted. The single crystal sample was loaded into the gasket hole with silicon oil to maintain the sample in a hydrostatic pressure environment. Pressure was determined by ruby fluorescence at room temperature.19

Time-of-flight neutron-diffraction experiments were performed at the SNAP (spallation neutron source and pressure) beamline of the spallation neutron source at Oak Ridge National Laboratory. The powder sample used in the neutron diffraction experiment was ground from the same single-crystalline sample that was used for the other experiments. Pressure was generated by boron nitride (BN) toroidal anvils in a Paris-Edinburgh high-pressure cell. The wide opening of this kind of cell allows the angular coverage of 38–142° horizontal and ±34° vertical in the configuration with the distance from sample to detector of 50 cm. The neutron-diffraction data were time focused from three detector modules spanning 45°, with its central module at 90° from the incident beam. A collimation with a 2 mm hole in diameter was used to narrow the beam to the sample size and effectively reduce the background. The wavelength range of the neutrons was in the range from 0.5 Å to 3.7 Å. The sample was contained in a chamber of approximately 5 mm in diameter bored in a TiZr gasket filled with a 4:1 mixture of deuterated methanol and ethanol. The methanol and ethanol mixture can remain fluid up to 10 GPa at room temperature, thus offering quasihydrostatic pressure conditions.

![X-ray diffraction pattern of a single crystal Fe1.05Te obtained at ambient pressure and room temperature](image)

FIG. 1. (Color online) X-ray diffraction pattern of a single crystal Fe1.05Te obtained at ambient pressure and room temperature with Cu Kα radiation.

### III. RESULTS AND DISCUSSIONS

Figure 3(a) shows the x-ray diffraction patterns of Fe1.05Te at ambient and high pressures at room temperature. It is seen that only the (003) reflection of the single-crystalline sample can be detected over the angular range available. No peaks were found in the diffraction measurements with increasing pressure up to 11.5 GPa. This indicates that no phase transition occurs over the pressure range studied. However, distinct shift of peak (003) was observed upon increasing pressure to 4 GPa at which the lattice parameter c decreases about 0.3 Å, signaling pressure-induced lattice distortion in this material.

High-pressure neutron diffraction (ND) was measured on polycrystalline Fe1.05Te sample in order to examine the observed lattice distortion. Figure 3(b) shows the ND patterns obtained at various pressures. All peaks collected at 0.7 GPa can be indexed well as a tetragonal structure. No peak was found under pressure up to 7 GPa, entirely consistent with the high-pressure XRD results. The computed lattice parameters c and a are compared at different pressures, as shown in Fig. 4. The two sets of the c values derived from ND and XRD measurements are in good agreement. A remarkable reduction in c axis was observed under applied pressure, as seen in Fig. 4(a). The c value is reduced about 5% at ~4 GPa. With further increasing pressure, the c value slowly decreases. The striking reduction in c is interpreted as a lattice collapse in the T phase of Fe1.05Te. To distinguish pressure-induced collapsed T phase from the “normal” T phase, we call the high-pressure form as cT. Figure 4(b) shows the pressure dependence of the lattice parameter a. Unlike the c axis, the a value exhibits a monotonic decrease with increasing pressure. The different behaviors along the a and c axis indicate that the pressure-induced lattice collapse only occurs along the c direction.

Figure 5 shows the unit cell volumes (V) as a function of pressure (P) in the T and cT phase of Fe1.05Te. No visible discontinuity was found in the P-V curve, further supporting

![Resistance and magnetization as a function of temperature of the sample at ambient pressure, showing tetragonal-to-monoclinic phase transition at the same temperature near 65 K.](image)

FIG. 2. (a) Resistance and (b) magnetization as a function of temperature of the sample at ambient pressure, showing tetragonal-to-monoclinic phase transition at the same temperature near 65 K.
that no phase transition takes place when the lattice collapses. The data were fitted by the third-order Birch-Murnaghan equation of state:

\[
P = \frac{3}{2}B_0\left\{\left(\frac{V}{V_0}\right)^{-7/3} - \left(\frac{V}{V_0}\right)^{-5/3}\right\} + \frac{3}{4}(B'_0 - 4)\left(\frac{V}{V_0}\right)^{-2/3} - 1\right\}
\]

where \(B_0\) is the isothermal bulk modulus at zero pressure, \(B'_0\) is the pressure derivative of \(B_0\) evaluated at zero pressure, and \(V/V_0\) is the ratio of high-pressure volume and zero-pressure volume of the sample. The resulting parameters are listed in Table I. We obtained \(B_0 = 31.3 \pm 1.45\) GPa and \(B'_0 = 6.6 \pm 1.2\) for the T phase, and \(B_0 = 86.7 \pm 6.6\) GPa and \(V_0 = 88.7 \pm 0.4\) (Å)³ for the cT phase when \(B'_0\) was fixed at 4. These results provide crucial information for further theoretical and experimental investigations of the high-pressure behavior of FeTe parent compound.

The lattice collapse in tetragonal phase was also found in CaFe₂As₂ compound at 2.5 GPa where the \(c\) parameter is reduced about \(\sim 1\) Å. First-principle study and high-pressure inelastic neutron-scattering results indicated that this strange behavior is caused by the strong suppression of Fe-spin state. As a result, the Fe-As bonding reduces and the corresponding As-As bonding enhances. These results indicated that the spin state of iron is a key factor that controls the lattice distortion in CaFe₂As₂ system. Pressure-induced lattice collapse in \(\alpha\)-FeTe should have the similar origin to
TABLE I. Bulk modulus $B_0$, volume at ambient pressure $V_0$ and pressure derivative $B'_0$ of tetragonal phase T and collapsed tetragonal phase cT in Fe$_{1+8}$Te compound.

<table>
<thead>
<tr>
<th>$P$ (GPa)</th>
<th>Phase</th>
<th>$V_0$ ($\text{Å}^3$)</th>
<th>$B'_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0–4</td>
<td>T</td>
<td>$31.3 \pm 1.45$</td>
<td>6.6 $\pm$ 1.2</td>
</tr>
<tr>
<td>4–7</td>
<td>cT</td>
<td>$86.7 \pm 6.6$</td>
<td>8.8 $\pm$ 0.4</td>
</tr>
</tbody>
</table>

CaFe$_2$As$_2$. Pressure may change Fe-spin state which leads to the reduction in the Fe-Te bonding. Compared to CaFe$_2$As$_2$, the contraction along the $c$ direction of FeTe compound should be small because the iron radii of Te is larger than that of As. If that would be the case, the lattice collapse in the FeTe compound should be slightly weaker than that in CaFe$_2$As$_2$. The Fe-spin state change must play an important role in the lattice collapse of the FeTe compound.

IV. CONCLUSION

We have investigated high-pressure behaviors of single crystal and polycrystalline Fe$_{1+8}$Te compound through the measurements of x-ray and neutron diffractions at 300 K. Pressure-induced lattice collapse was found around 4 GPa at which the T phase “transforms” to the cT phase. The equations of state for the T and cT phase were determined from x-ray and neutron-diffraction measurements. These results are expected to simulate further theoretical calculations on the electronic structure of this material at high pressure.

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