

## Supplementary Materials

for

### Unveiling the crystallization behavior of amorphous Te driven by pressure

Chong Qiao<sup>1</sup>, Chongze Wang<sup>2</sup>, Chengyan Liu<sup>3</sup>, Qundao Xu<sup>4</sup>, Shaojie Yuan<sup>4</sup>,  
Shengzhao Wang<sup>1</sup>, Songyou Wang<sup>5</sup>, Ming Xu<sup>4,\*</sup> and Xiangshui Miao<sup>4</sup>

<sup>1</sup>*School of Mathematics and Physics, Nanyang Institute of Technology, Nanyang 473004, China*

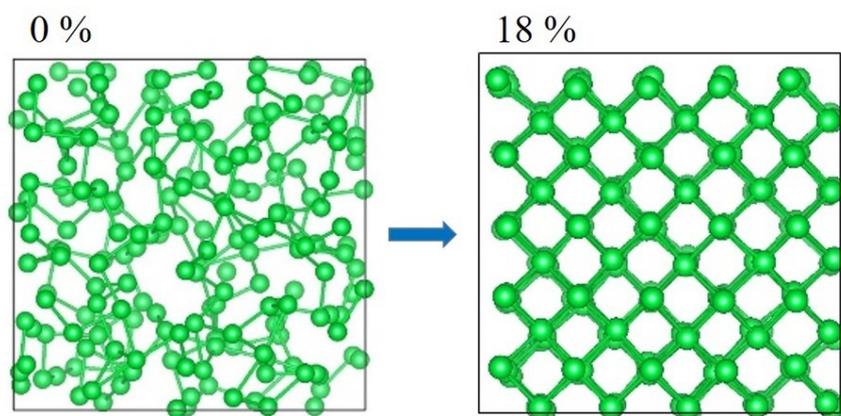
<sup>2</sup>*Institute of Quantum Materials and Physics, Henan Academy of Sciences, Zhengzhou 450046, China*

<sup>3</sup>*Henan Key Laboratory of Quantum Materials and Quantum Energy, School of Quantum Information Future Technology, Henan University, Kaifeng, Henan 475001, China*

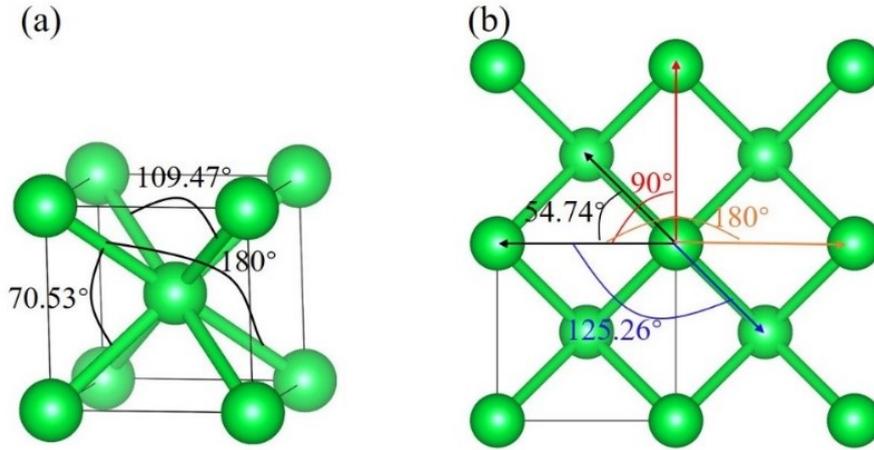
<sup>4</sup>*School of Integrated Circuits, Huazhong University of Science and Technology, Wuhan 430074, China*

<sup>5</sup>*Shanghai Ultra-Precision Optical Manufacturing Engineering Center and Department of Optical Science and Engineering, Fudan University, Shanghai 200433, China*

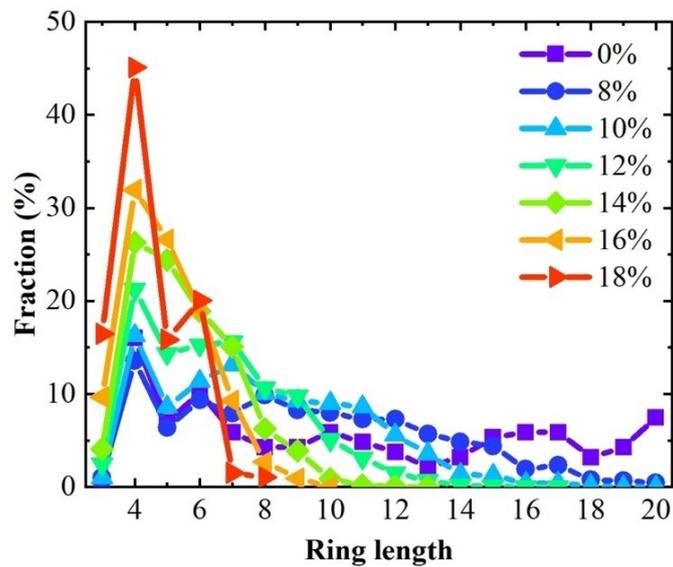
\*Corresponding author. E-mail address: mxu@hust.edu.cn



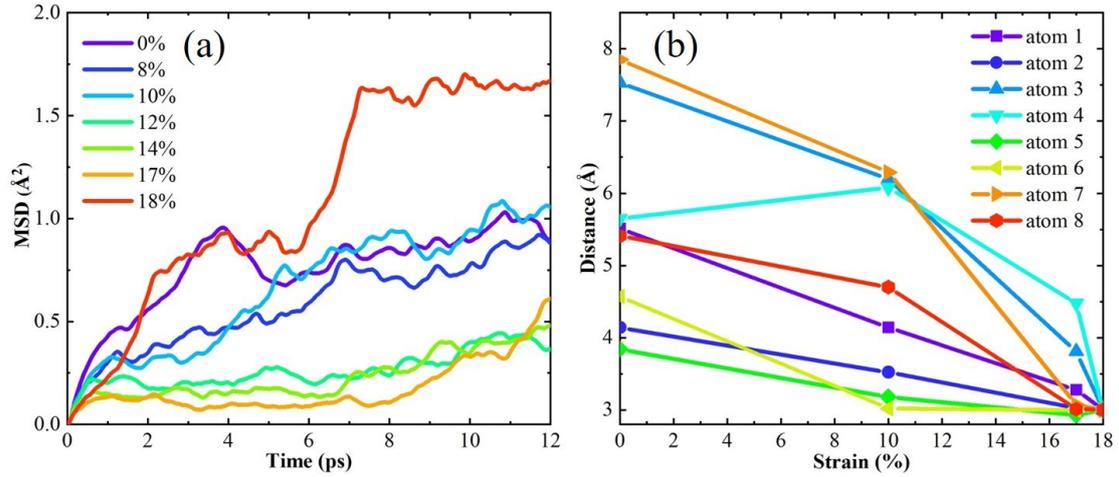
**Fig. S1.** In the initial configuration at strain of 0 %, the atoms are randomly distributed, while they are arranged in an orderly manner in the final state at strain of 18 %, demonstrating that amorphous Te undergoes a transition to the crystalline phase under compression.



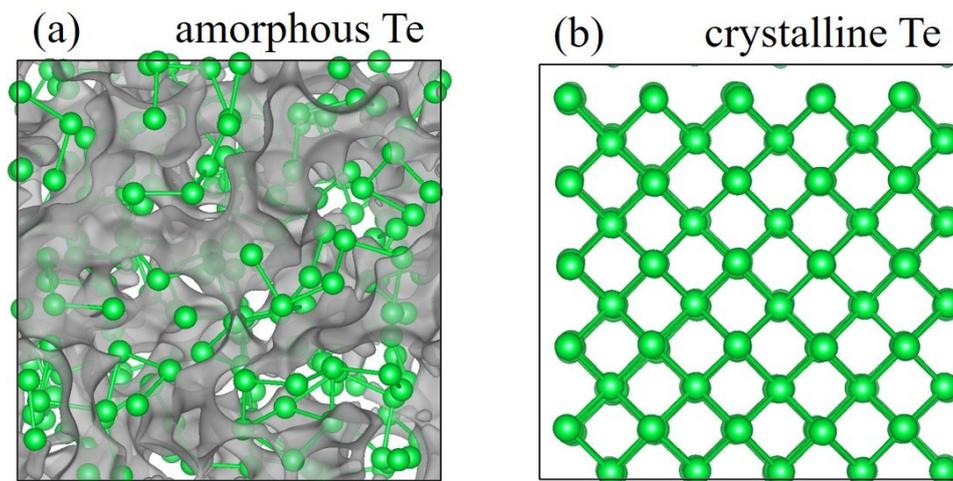
**Fig. S2.** The bond-angle relations of BCC Te in first (a) and second (b) atomic shells, respectively. Obviously, the bond-angle relations concentrate on 70.53° and 109.47° in the first atomic of BCC structure. For the second atomic shell, the bond-angle relation is mainly in the form of 90° and 180°. However, due to the atomic thermal fluctuation, the atoms in the first shell may move to the second shell, forming the bond-angle relations of 54.74° and 125.26°.



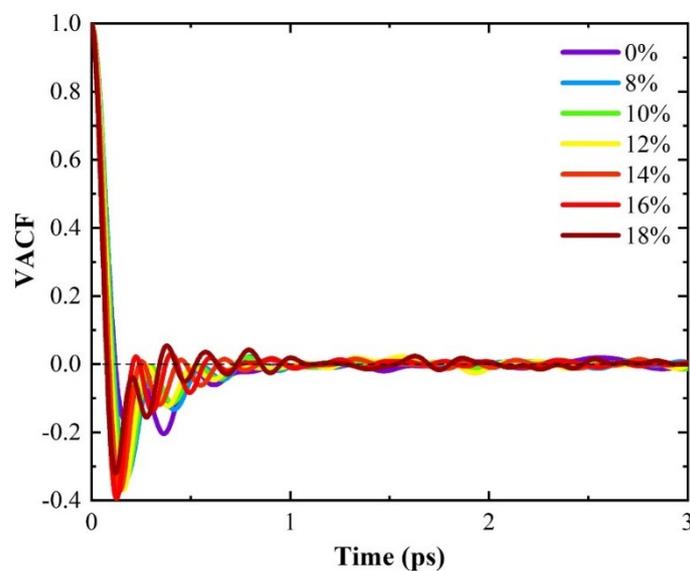
**Fig. S3.** The distributions of rings at different strains. The fraction of 4-fold ring increases with the strain, implying that the amorphous network becomes denser.



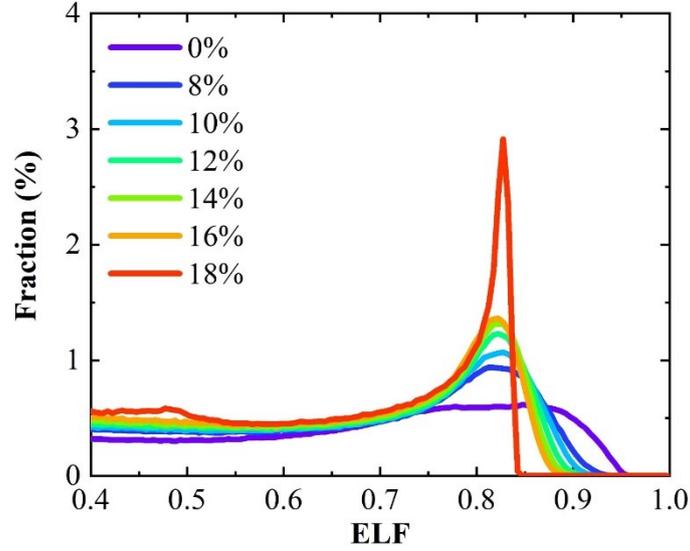
**Fig. S4.** The mean square displacement (MSD) (a) of amorphous Te in the compression process, and the distance variations (b) of the atoms bonded to the central atom of BCC phase. As the strain increases from 0 % to 10 %, the MSD increases to  $\sim 1.0 \text{ \AA}^2$  at 12 ps, indicating that atoms possess the stronger motion ability. This is because there is sufficient space in the amorphous Te to allow for atomic diffusion. As the strain increases from 12% to 17%, the MSD decreases to approximately  $0.5 \text{ \AA}^2$  at 12 ps, suggesting the movement ability of the atoms has been suppressed. This is because that the space for atomic diffusion is reduced. However, when the strain changes to 18 %, the MSD initially increases to  $\sim 1.6 \text{ \AA}^2$  within 7.3 ps, and then fluctuates only slightly over time. This indicates that the considerable atomic rearrangement is driven by the high stress before reaching the stable configuration. From Fig. S4(b), the atomic distances to the central atom decrease with the increasing strain. At the strain of 0 %, the distances of atoms 2, 5 and 6 to the central atom are relatively small, while the distances of atoms 1, 3, 4, 7 and 8 to the central atom are relatively large, indicating that some atoms are located around the central atom, while others are far away from the central atom in initial amorphous Te. At strain of 17 %, most of the atoms are squeezed close to the central atom. However, they finally bond to the central atom with the same distances at the strain of 18 %. It indicates that the formation of the BCC Te also depends on the long-range atomic diffusion, in addition to the local diffusion.



**Fig. S5.** The distributions of voids in amorphous (a) and crystalline (b) Te at the strains of 0 % and 18%, respectively. The voids are randomly distributed in the amorphous Te, whereas there is no void in crystalline Te.



**Fig. S6.** The velocity autocorrelation functions (VACF) of amorphous Te in the compression process. Usually, the VACF begins at 1.0, and gradually converges to zero with time. The VACF at the larger strain takes more time to converge, illustrating that the atomic motion is suppressed in the compression process.



**Fig. S7.** The electron localization functions (ELF) of amorphous Te at different strains.

Usually, the electron is completely localized for  $ELF=1.0$ , which is the characteristic of covalent bonds. While the electron is completely delocalized for  $ELF=0.5$ , which is a typical characteristic of metal bonds. The obvious peak is observed at 0.83 for crystalline Te at strain of 18 %, indicating that electrons have a distinct tendency to be localized in the regions between atoms. Therefore, the Te–Te bond in crystalline Te should be weak covalent bond.

**Table S1.** The atomic coordinates (CONTCAR) of final BCC structure of Te.

CONTCAR

1.0000000000000000

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0.0000000000000000 17.5427000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.5427000000000000

Te

250

Direct

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