

## Insight into the Role of Oxygen in Phase-Change Material GeTe

Linggong Zhu<sup>1,2</sup>, Zhen Li<sup>1</sup>, Jian Zhou<sup>1</sup>, Naihua Miao<sup>1,2</sup> and Zhimei Sun<sup>1,2,\*</sup>

<sup>1</sup>School of Materials Science and Engineering, Beihang University, Beijing 100191, China

<sup>2</sup>Center for Integrated Computational Materials Engineering, International Research Institute for Multidisciplinary Science, Beihang University, Beijing 100191, China

\*Corresponding Author. Email: [zmsun@buaa.edu.cn](mailto:zmsun@buaa.edu.cn)

### Content

1. Movie1: Crystallization of GeTe-O system in the first 180 ps
2. Movie2: annealing of crystalline GeTe-O at 1100 K over 9 ps.
3. FigureS1: Radial distribution functional  $g(r)$  for the snapshots in the crystallization simulations. The  $g(r)$  at 180 ps presents the more ordered structure in the case of GeTe than GeTe-O, indicating the higher crystallization speed for GeTe.

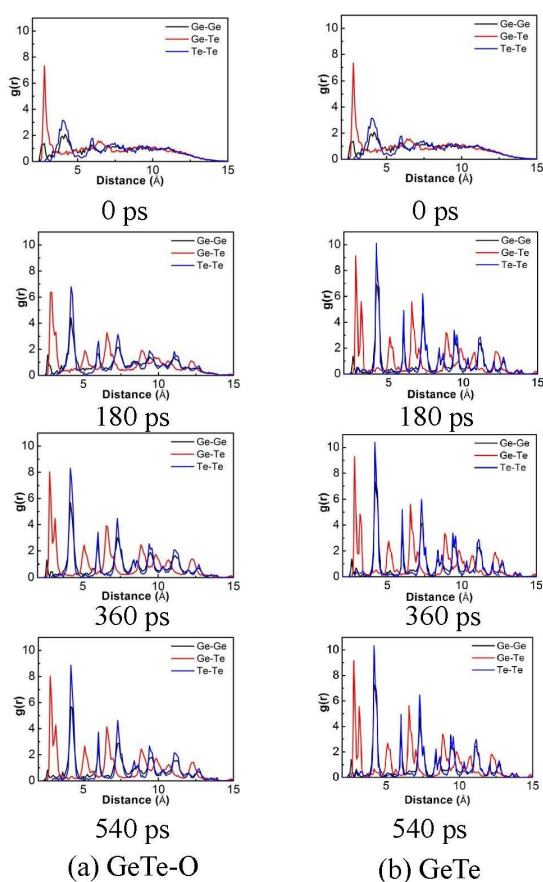


Figure S1: Radial distribution functional ( $g(r)$ ) for the snapshots in the

crystallization simulations of (a) GeTe-O and (b) Ge-Te systems, the corresponding atomic structures of these snapshots can be found in Fig. 7. Since the doping concentration of oxygen is rather low in GeTe-O system, the coordination environments of O is omitted in (a), for clearer comparison.