

Machine-Learning molecular dynamics simulations of Shock Response and Spallation Behavior in PPTA Crystals

Lei Liu¹, Jingfu Shi¹, Di Song², Changqing Miao^{1*}

1 National Key Laboratory of Science and Technology on Advanced Composites in Special Environment, Harbin

Institute of Technology, Harbin 150001, P. R. China.

2 School of Mechanical and Electrical Engineering, University of Electronic Science and Technology of China,

Chengdu, Sichuan 611731, PR China.

* Corresponding author Email: miaocq@hit.edu.cn

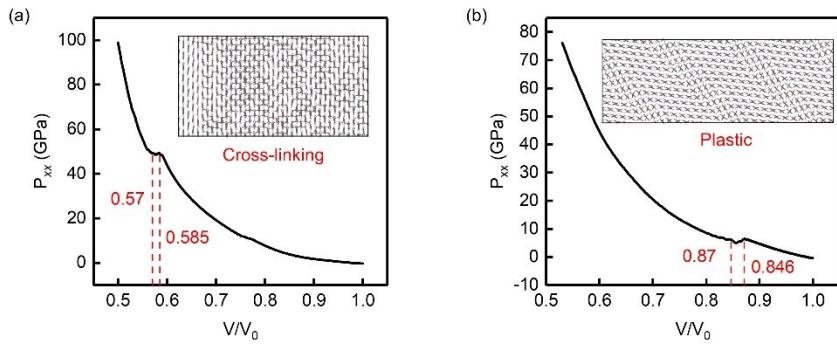


Fig. S1. The compressive stress (P_{xx}) as a function of relative volume (V/V_0) during dynamic compression along (a) the a-axis and (b) the b-axis of the PPTA crystal, respectively.

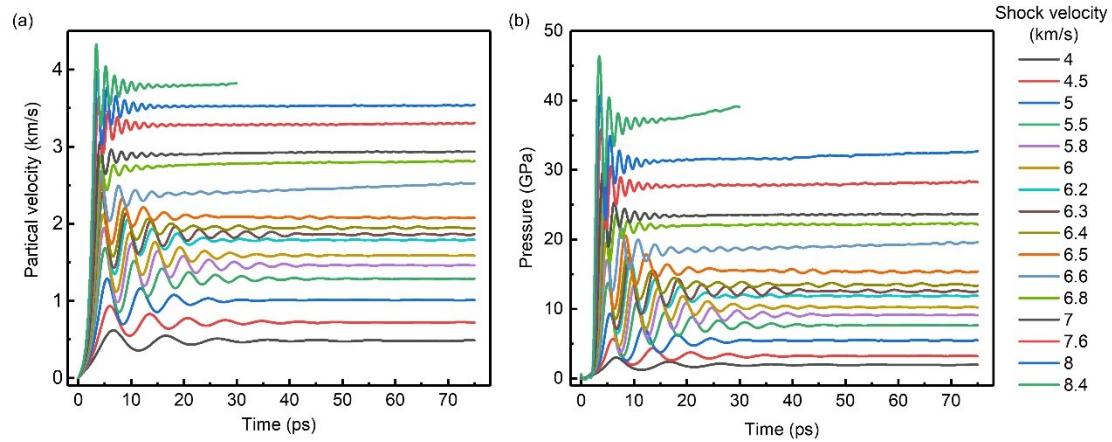


Fig. S2. Under shock compression along the a-axis of the PPTA crystal, the variations of (a) particle velocity and (b) system pressure with time at different shock velocities.

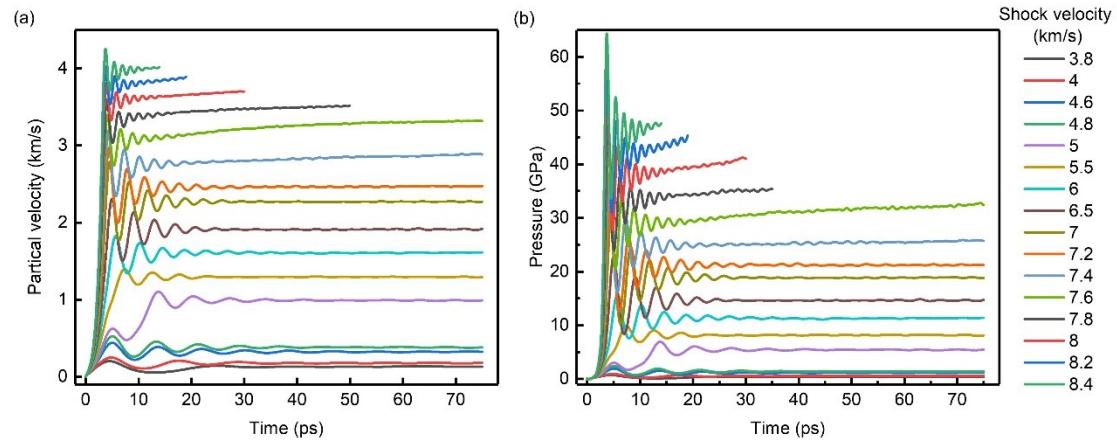


Fig. S3. Under shock compression along the b-axis of the PPTA crystal, the variations of (a) particle velocity and (b) system pressure with time at different shock velocities..

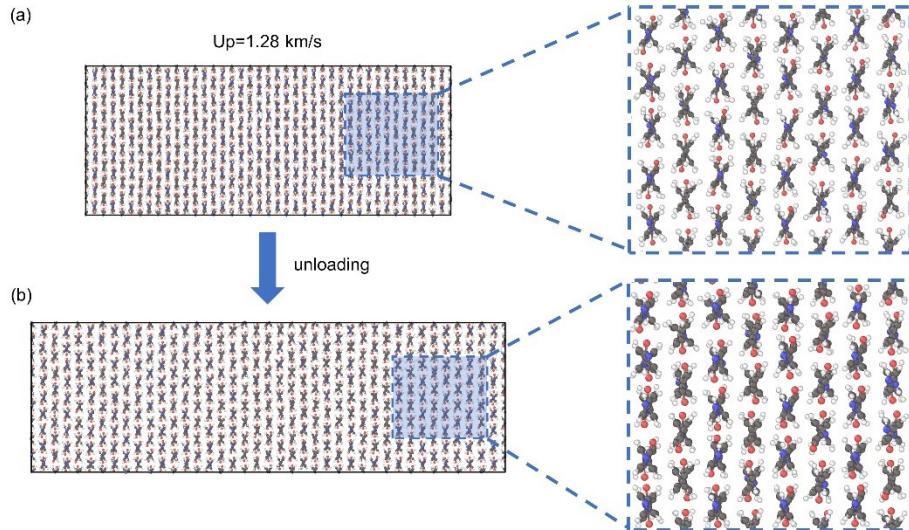


Fig. S4. Under shock compression along the a-axis of the PPTA crystal, (a) the atomic structure after shock compression and (b) the atomic structure after unloading and re-equilibration are shown for the elastic regime (using $U_p=1.28\text{km/s}$ as an example). The deformation in the elastic regime is almost entirely recoverable upon unloading.

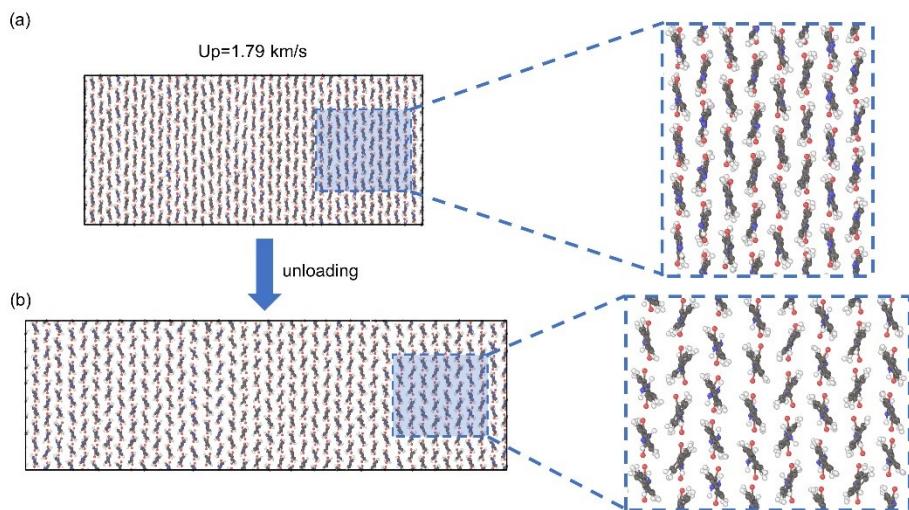


Fig. S5. Under shock compression along the a-axis of the PPTA crystal, (a) the atomic structure after shock compression and (b) the atomic structure after unloading and re-equilibration are shown for the plastic regime (using $U_p=1.79\text{km/s}$ as an example). The deformation in the plastic regime is not recoverable upon unloading.

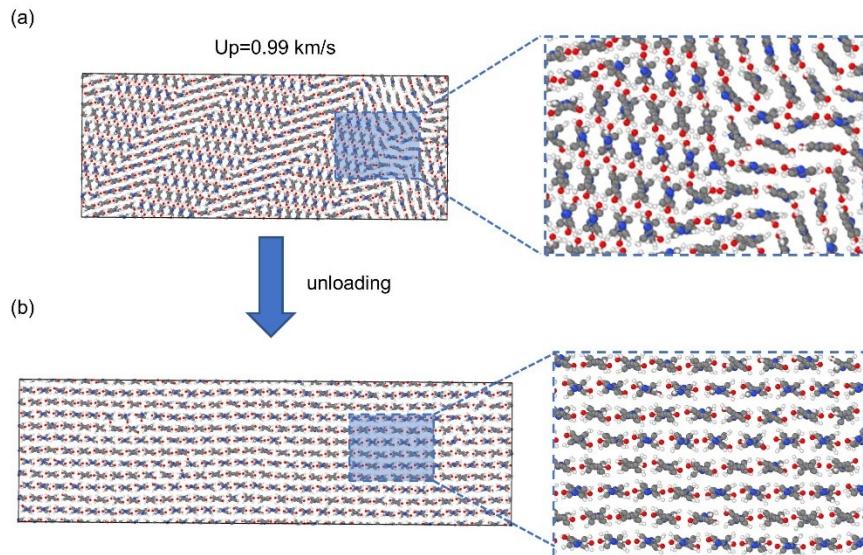


Fig. S6. Under shock compression along the b-axis of the PPTA crystal, (a) the atomic structure after shock compression and (b) the atomic structure after unloading and re-equilibration are shown for the plastic regime (using $U_p=0.99\text{km/s}$ as an example). The deformation in this regime is almost entirely recoverable upon unloading.