

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

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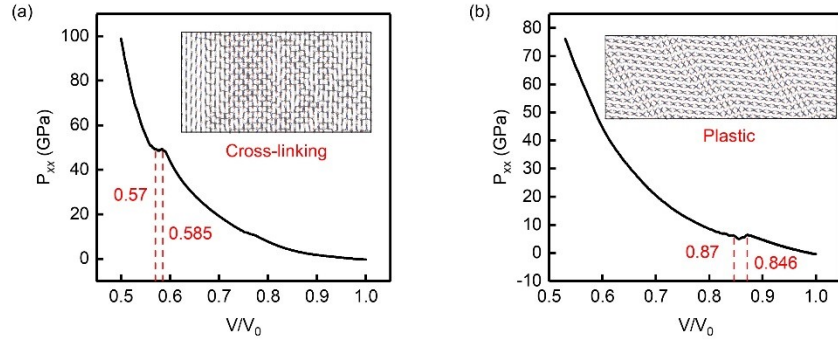


Fig. S1. The compressive stress (P_{xx}) as a function of relative volume (V/V_0) during dynamic compression along (a) the a-axis and (b) the b-axis of the PPTA crystal, respectively.

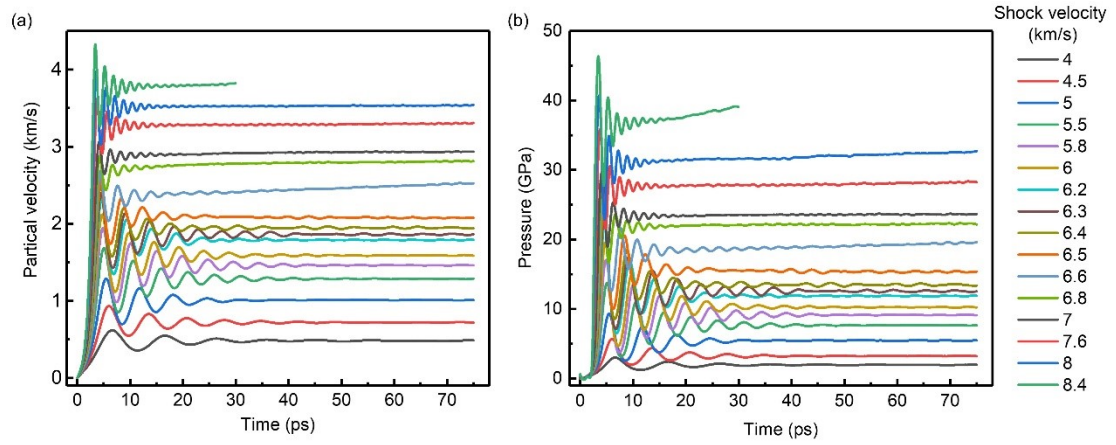


Fig. S2. Under shock compression along the a-axis of the PPTA crystal, the variations of (a) particle velocity and (b) system pressure with time at different shock velocities.

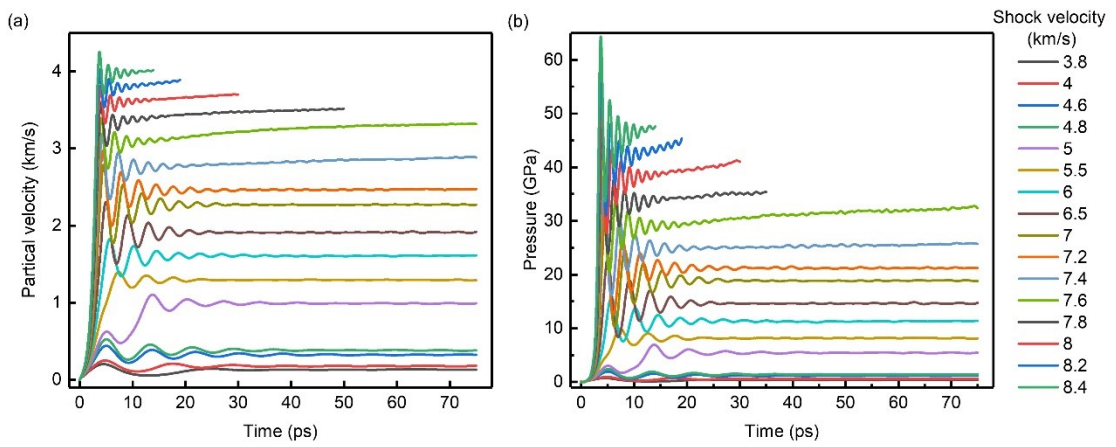


Fig. S3. Under shock compression along the b-axis of the PPTA crystal, the variations of (a) particle velocity and (b) system pressure with time at different shock velocities..

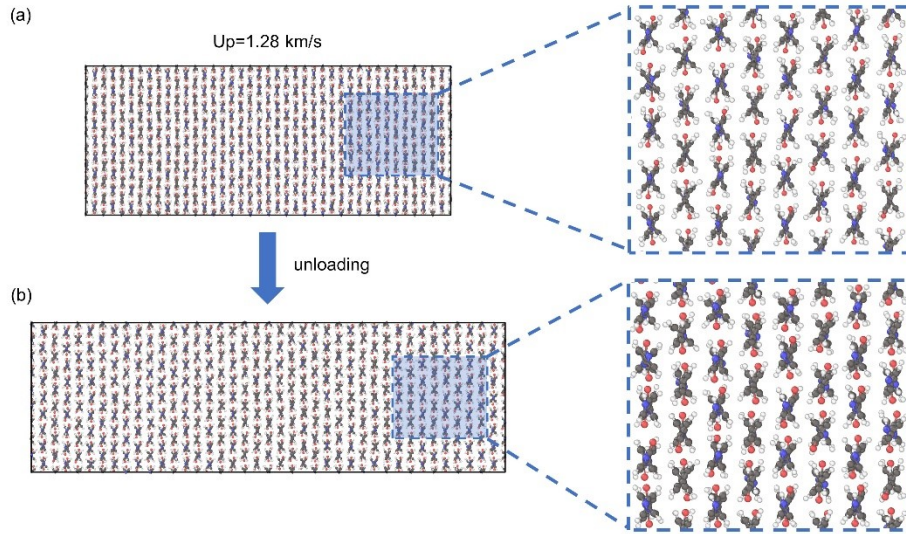


Fig. S4. Under shock compression along the a-axis of the PPTA crystal, (a) the atomic structure after shock compression and (b) the atomic structure after unloading and re-equilibration are shown for the elastic regime (using $U_p = 1.28 \text{ km/s}$ as an example). The deformation in the elastic regime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

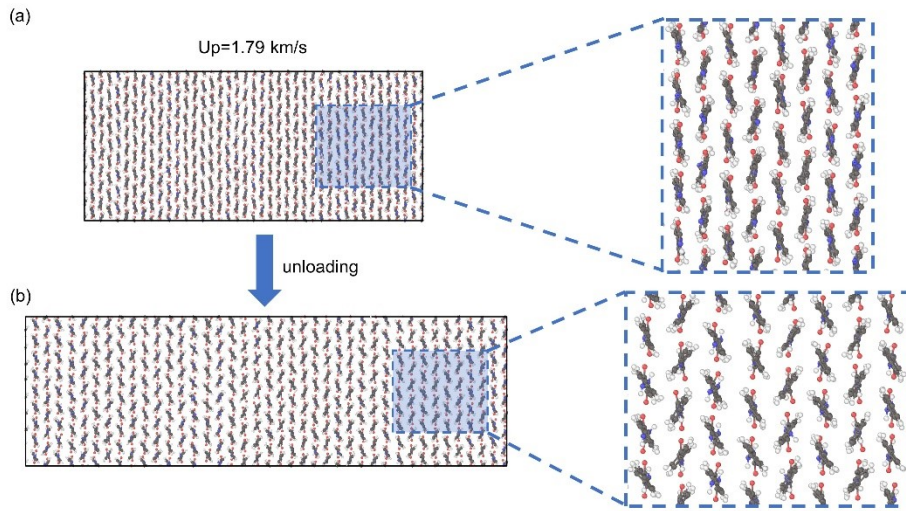


Fig. S5. Under shock compression along the a-axis of the PPTA crystal, (a) the atomic structure after shock compression and (b) the atomic structure after unloading and re-equilibration are shown for the plastic regime (using $U_p = 1.79 \text{ km/s}$ as an example). The deformation in the plastic regime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

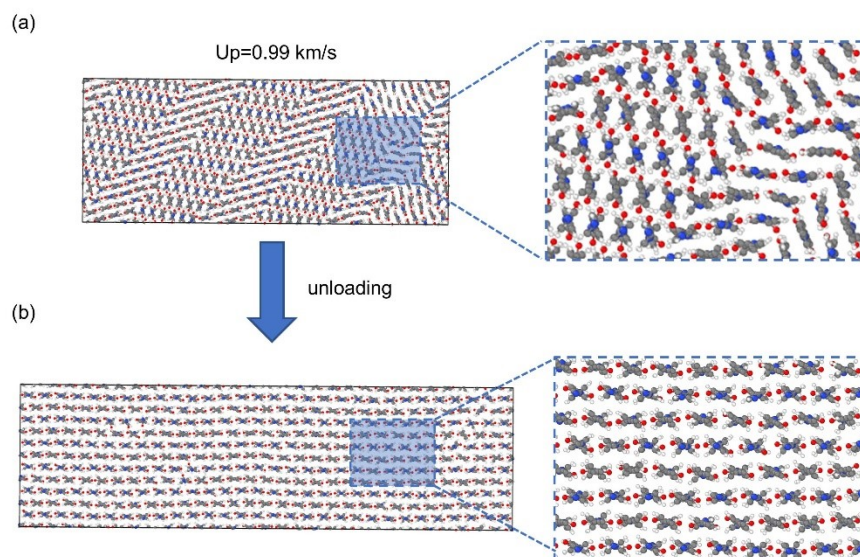


Fig. S6. Under shock compression along the b-axis of the PPTA crystal, (a) the atomic structure after shock compression and (b) the atomic structure after unloading and re-equilibration are shown for the plastic regime (using $U_p=0.99$ km/s as an example). The deformation in this regime is almost entirely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