Electronic Supplementary Information (ESI) Available

Hot Spot Formation and Chemical Reaction Initiation in Shocked HMX Crystal with a Nanovoid: A Large-Scale Reactive Molecular Dynamics Study

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Table S1. Bond order cutoff values for various atom pairs. The algorithm of molecule recognition in the fragment analysis uses these values.

	C	H	O	N
C	0.55	0.40	0.60	0.30
H		0.55	0.40	0.55
O			0.65	0.40
N				0.55

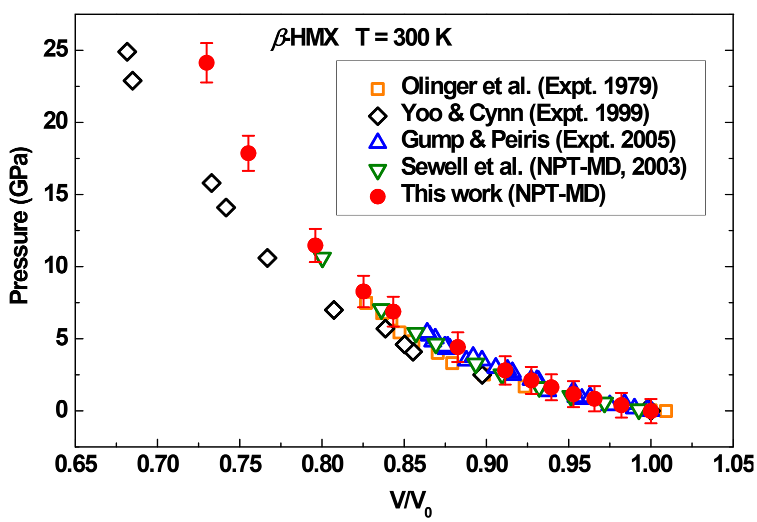


Figure S1. EOS for β-HMX under hydrostatic compression at T = 300 K. The red fitted circles are the results from this work; the orange open squares are the experimental results from Olinger et al.;[78] the black open diamonds are the experimental results from Yoo and Cynn;[79] the blue open up triangles are the experimental results from Gump and Peiris;[80] the green open down triangles are the theoretical results from Sewell et al.[81] The result from ReaxFF-lg is in excellent agreement with the experimental result from Gump and Peiris[80] and the theoretical result from Sewell et al.[81] Gump and Peiris[80] used a relatively pure batch of HMX thrice recrystallized in acetone, with the hope of obtaining the properties of pure materials, making it a good case with which to compare theoretical results for perfect crystal.

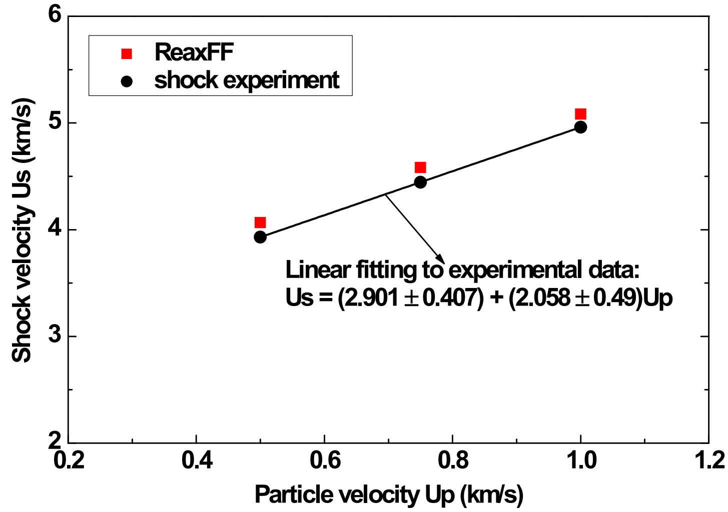


Figure S2. The relation between shock velocity (U_s) and particle velocity (U_p) for perfect single crystal HMX obtained from ReaxFF-MD simulations and shock experiments.[82] The line represents the linear fitting to the experimental data: $U_s = (2.901 \pm 0.407) + (2.058 \pm 0.49)U_p$ for $0.59 < U_p < 1.04$ km/s. The density of the HMX crystal is 1.89 g/cm^3 for both the MD simulation and the shock experiment. The U_s predicted by ReaxFF is a little higher than but is within the error range of experimental result, indicating good agreement.

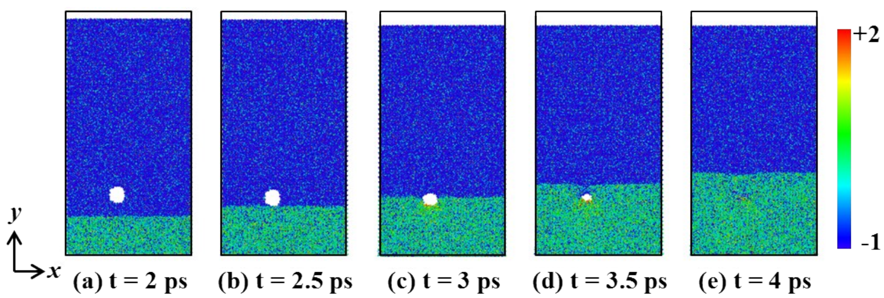


Figure S3. The illustrations of shock wave propagation and void collapse during 2 ~ 4 ps for the case of R = 2 nm and U_p = 1 km/s. Atoms are color coded by the magnitude of atom velocity along y direction: duck blue represents -1 km/s, cyan 0 km/s, kelly 1 km/s, and red +2 km/s. The maximal velocity for a few atoms reaches 1.20 km/s.

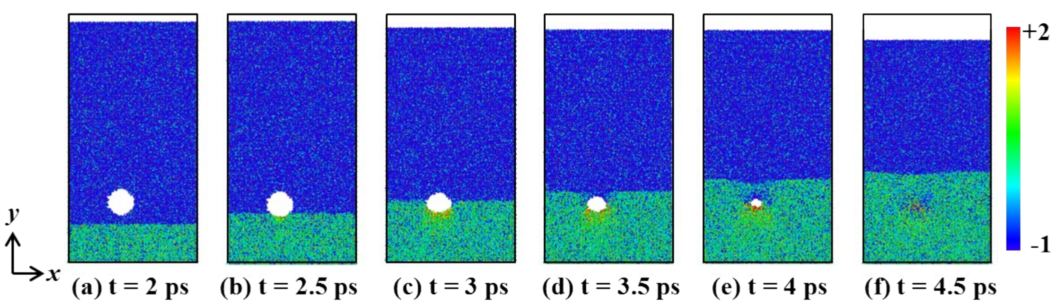


Figure S4. The illustrations of shock wave propagation and void collapse during 2 ~ 4.5 ps for the case of R = 3 nm and U_p = 1 km/s. Atoms are color coded by the magnitude of atom velocity along y direction: duck blue represents -1 km/s, cyan 0 km/s, kelly 1 km/s, and red +2 km/s. The maximal velocity for a few atoms reaches 1.79 km/s.

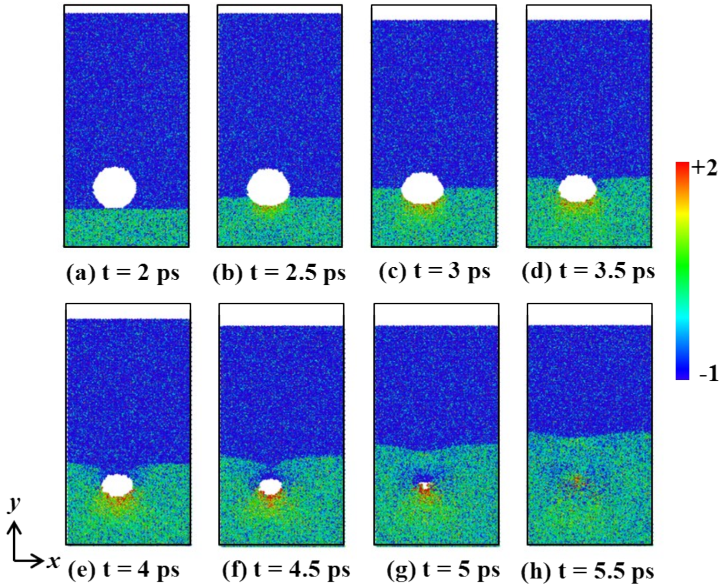


Figure S5. The illustrations of shock wave propagation and void collapse during 2 ~ 5.5 ps for the case of R = 5 nm and U_p = 1 km/s. Atoms are color coded by the magnitude of atom velocity along y direction: duck blue represents -1 km/s, cyan 0 km/s, kelly 1 km/s, and red +2 km/s. The maximal velocity for a few atoms reaches 2.92 km/s.

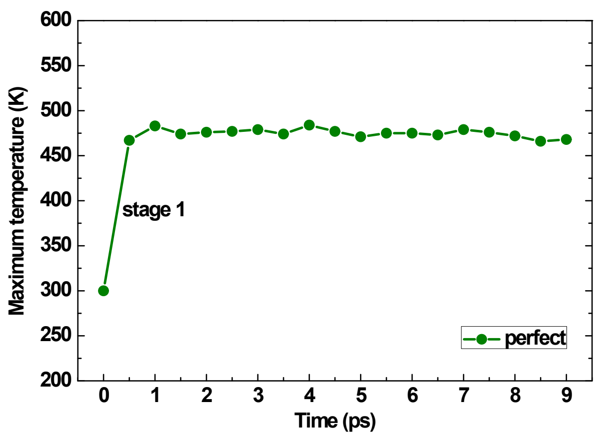


Figure S6. The time evolution of the maximum temperature for the perfect crystal under an impact velocity of 1 km/s

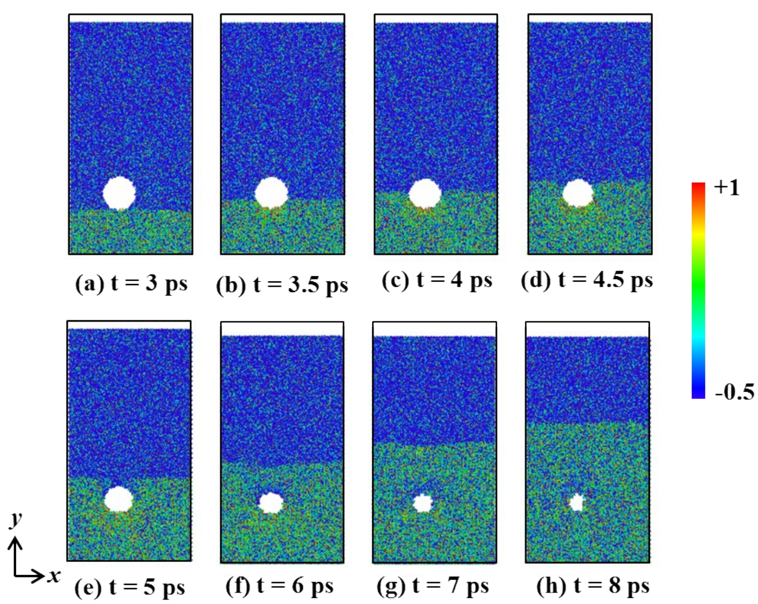


Figure S7. The illustrations of shock wave propagation and void collapse for the case of R = 4 nm and U_p = 0.5 km/s. Atoms are color coded by the magnitude of atom velocity along y direction: duck blue represents -0.5 km/s, cyan 0 km/s, kelly 0.5 km/s, and red +1 km/s. The maximal velocity for a few atoms reaches 0.58 km/s.

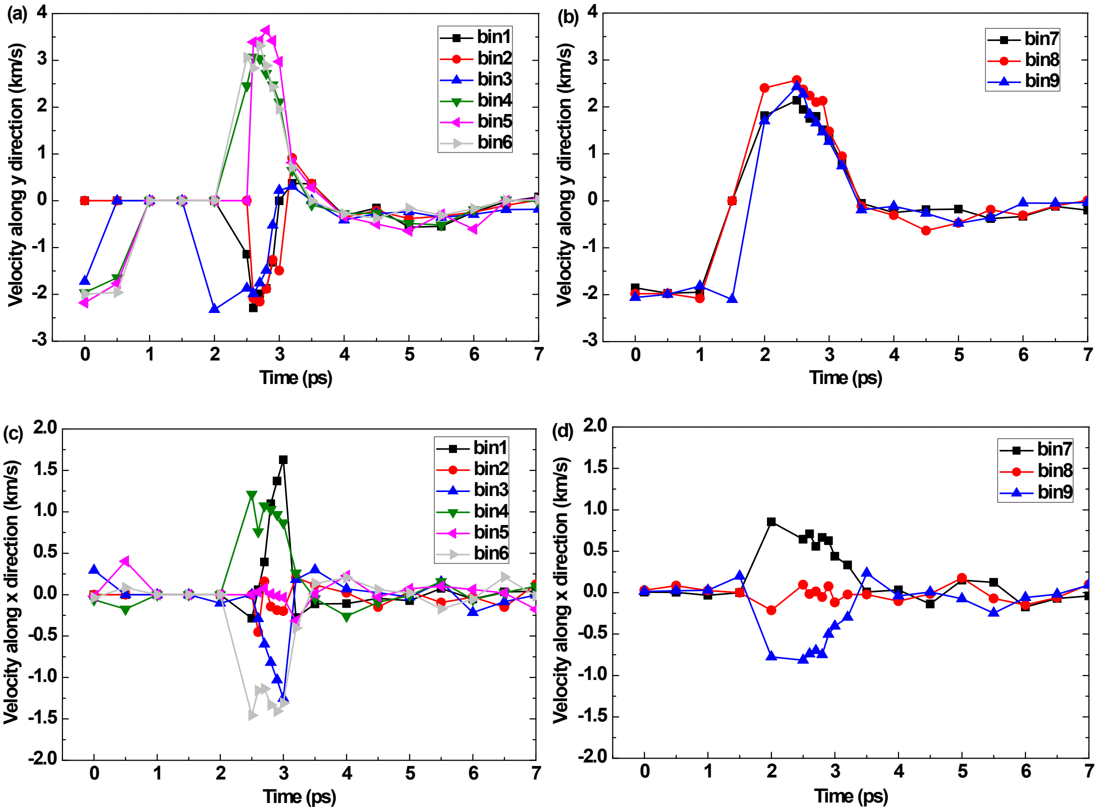
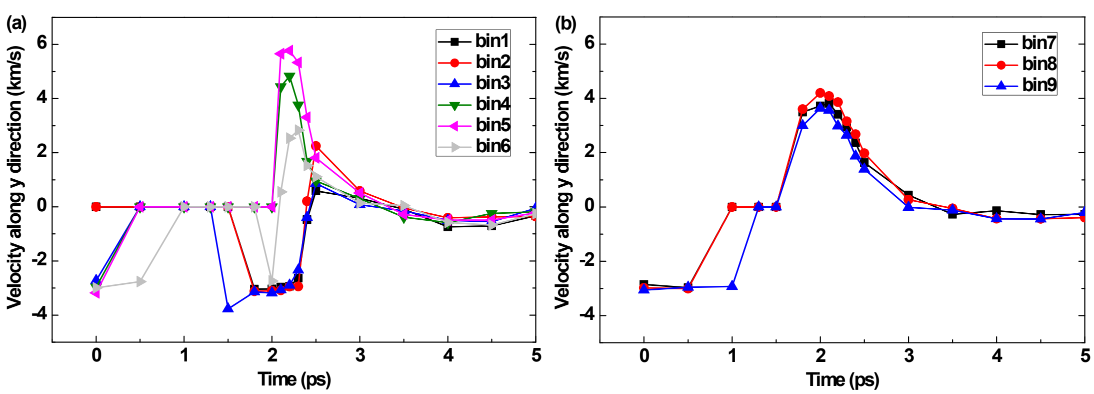


Figure S8. The averaged atom velocities as a function of time for the atoms in the bins as indicated in the parentheses of Table 1 for the crystal containing a 4 nm radius void under the impact velocity of 2 km/s. (a) and (b) represent the velocity along y direction; (c) and (d) represent the velocity along x direction.



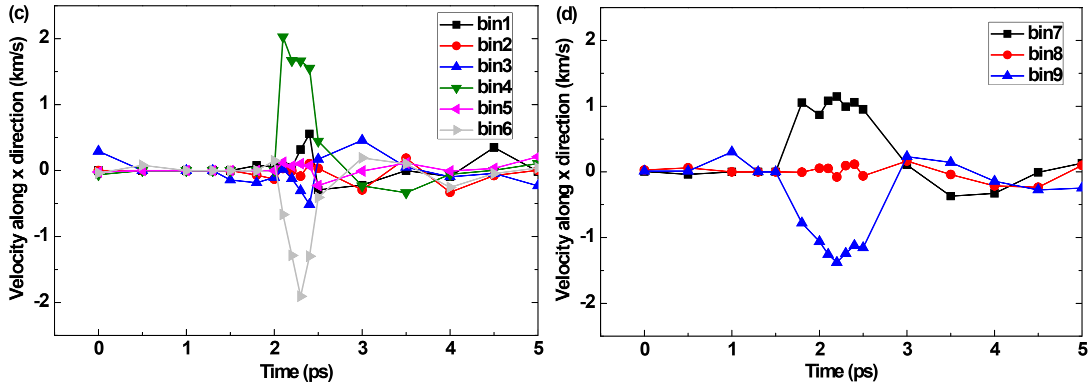


Figure S9. The averaged atom velocities as a function of time for the atoms in the bins as indicated in the parentheses of Table 1 for the crystal containing a 4 nm radius void under the impact velocity of 3 km/s. (a) and (b) represent the velocity along *y* direction; (c) and (d) represent the velocity along *x* direction.

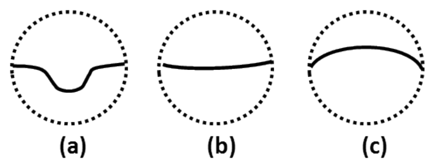


Figure S10. The simple illustrations of representative void shape during void collapse for the crystal containing a 4 nm radius void under the impact velocities of 1 (a), 2 (b), and 3 km/s (c). The difference in the dominant collapse mechanism leads to different void shapes during void collapse.

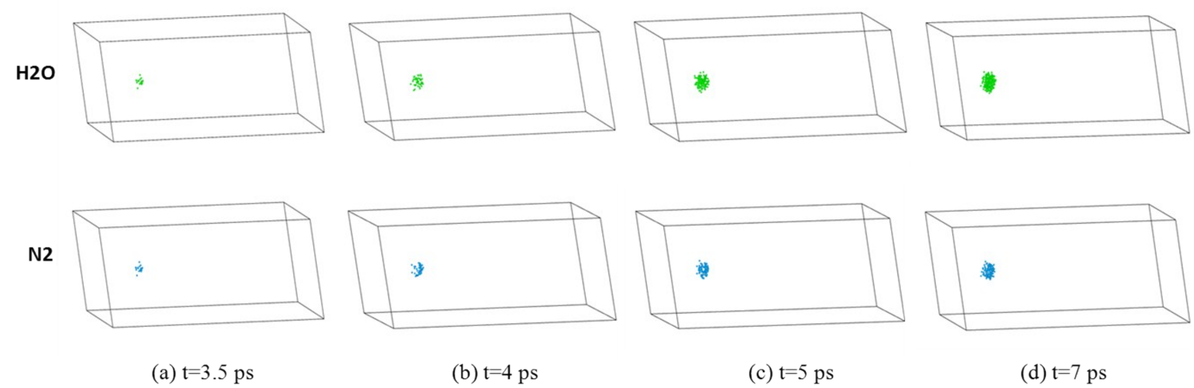


Figure S11. The spatial distributions of H_2O (top row) and N_2 (bottom row) at various times for the crystal containing a 4 nm radius void under the impact velocity of 2 km/s

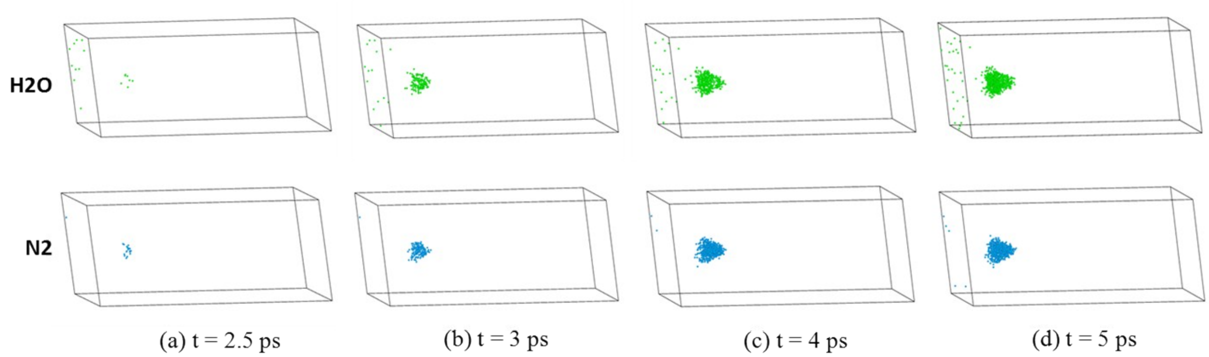


Figure S12. The spatial distributions of H_2O (top row) and N_2 (bottom row) at various times for the crystal containing a 4 nm radius void under the impact velocity of 3 km/s