Electronic Supplementary Information (ESI)

A Reactive Molecular Dynamics Study on the Anisotropic Sensitivity in Single Crystal

**α-Cyclotetramethylene Tetranitramine**

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Table S1 The averaged full stress tensors for the seven uniaxially compressed structures after NVT-MD relaxation (unit: GPa)

Shock plane	P	P_{xx}	P_{yy}	P_{zz}	P_{xy}	P_{xz}	P_{yz}
(010)	9.549	8.544	13.447	6.657	0.181	0.237	0.089
(001)	10.164	7.638	10.431	12.421	-0.124	-0.117	-0.212
(100)	10.305	11.994	9.304	9.616	-0.082	0.148	0.110
(110)	10.218	12.396	9.411	8.845	0.013	0.017	0.080
(011)	10.097	7.716	10.509	12.065	-0.033	0.035	0.127
(111)	10.099	8.935	9.163	12.200	0.007	0.779	0.122
(101)	10.484	9.397	10.068	11.985	-0.363	0.913	-0.082

Table S2. Bond order cutoff values for various atom pairs. The algorithm of molecule recognition in the fragment analysis uses these values.

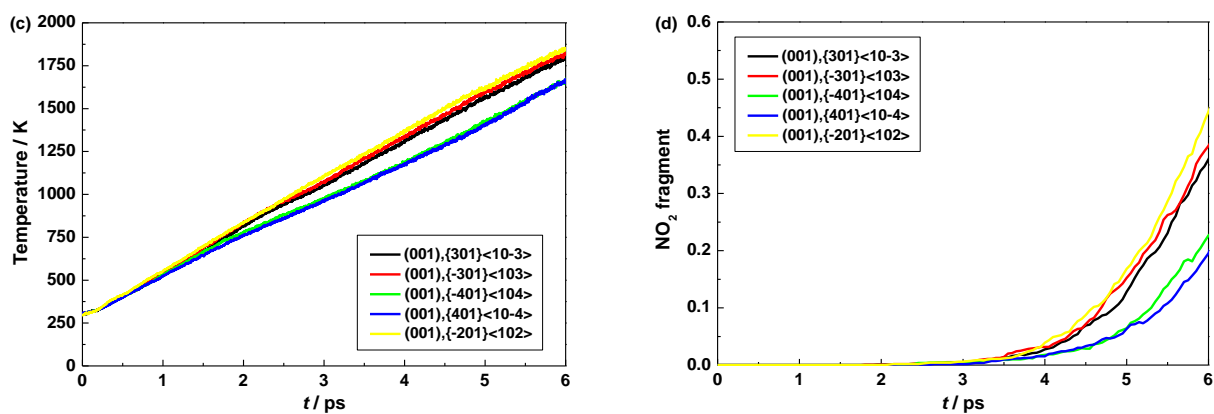|	C	H	O	N
C	0.55	0.40	0.60	0.30
H		0.55	0.40	0.55
O			0.65	0.40
N				0.55
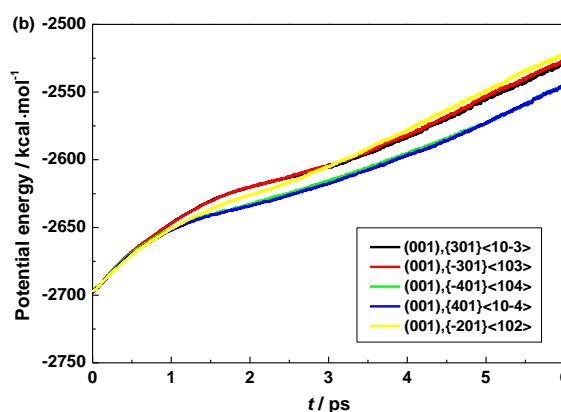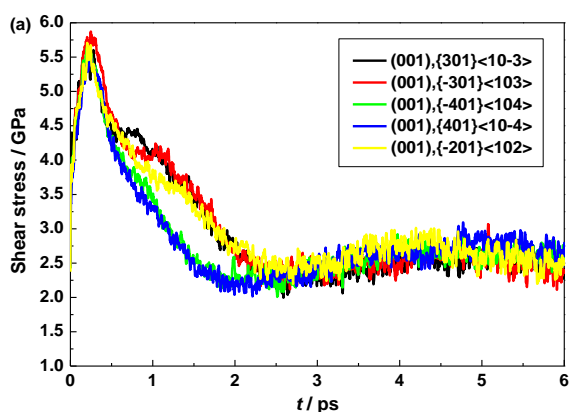
Fig. S1 Time evolutions of shear stress (a), potential energy per HMX molecule (b), temperature (c), and NO$_2$ fragment per HMX molecule (d) for the five possible slip systems along shock direction normal to the (001) plane during shear simulations.
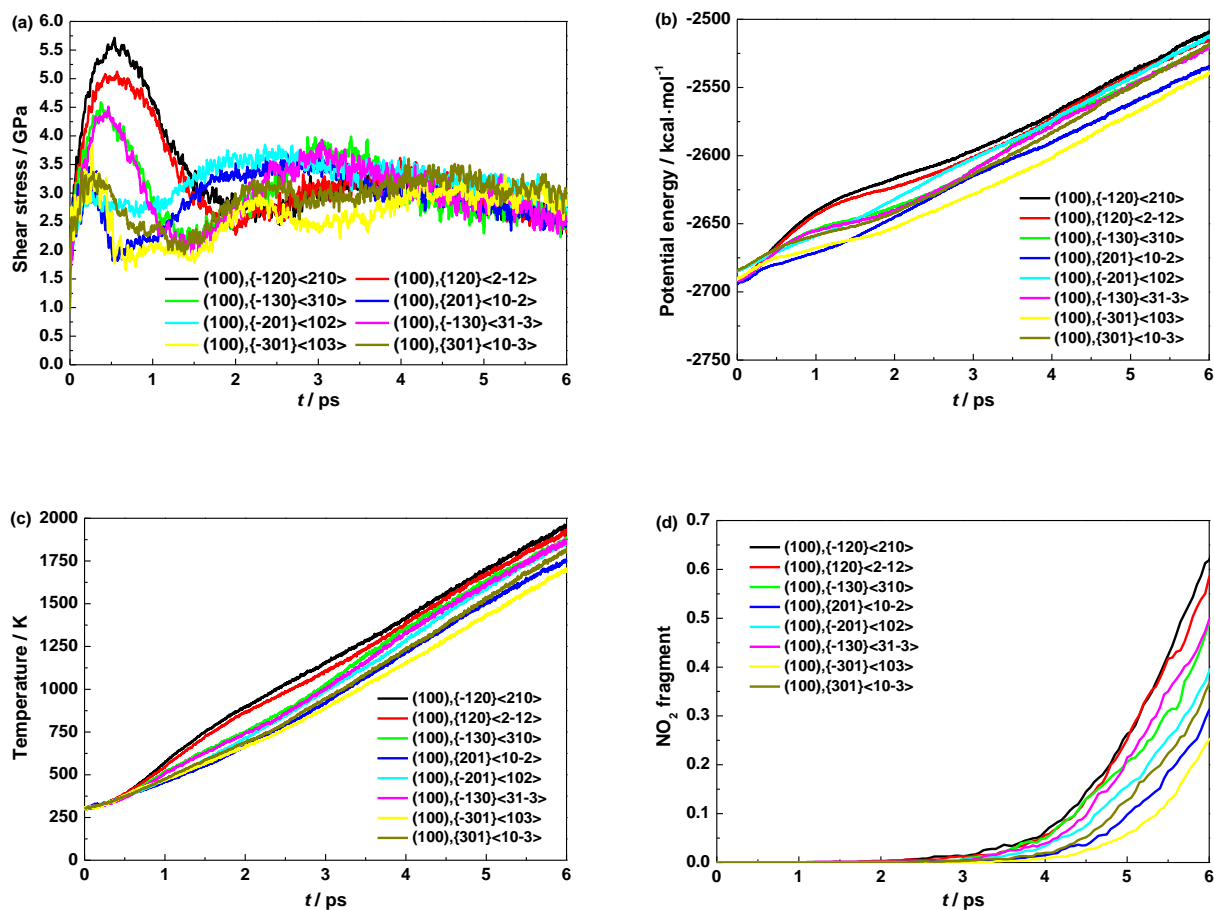

Fig. S2 Time evolutions of shear stress (a), potential energy per HMX molecule (b), temperature (c), and NO$_2$ fragment per HMX molecule (d) for the eight possible slip systems along shock direction normal to the (100) plane during shear simulations.
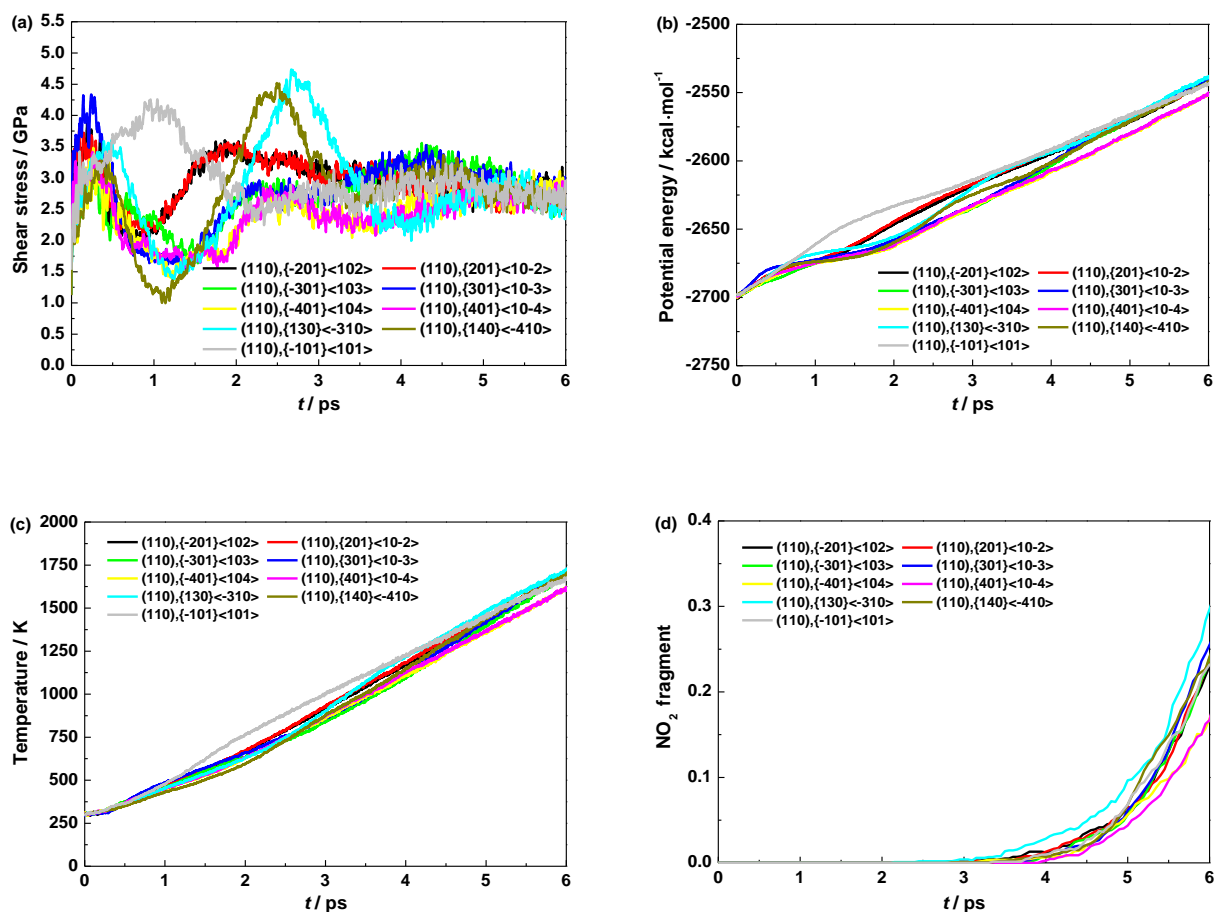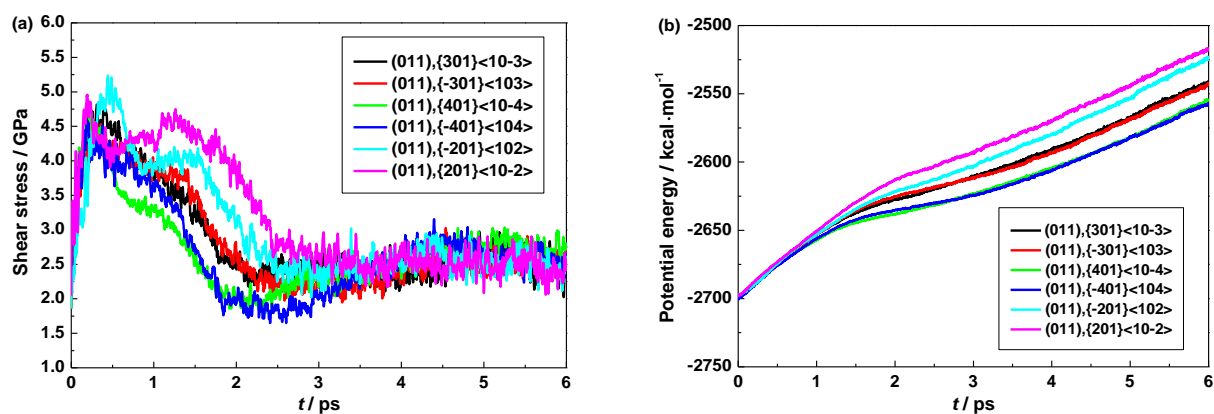
2

Fig. S3 Time evolutions of shear stress (a), potential energy per HMX molecule (b), temperature (c), and NO_2 fragment per HMX molecule (d) for the eight possible slip systems along shock direction normal to the (110) plane during shear simulations.
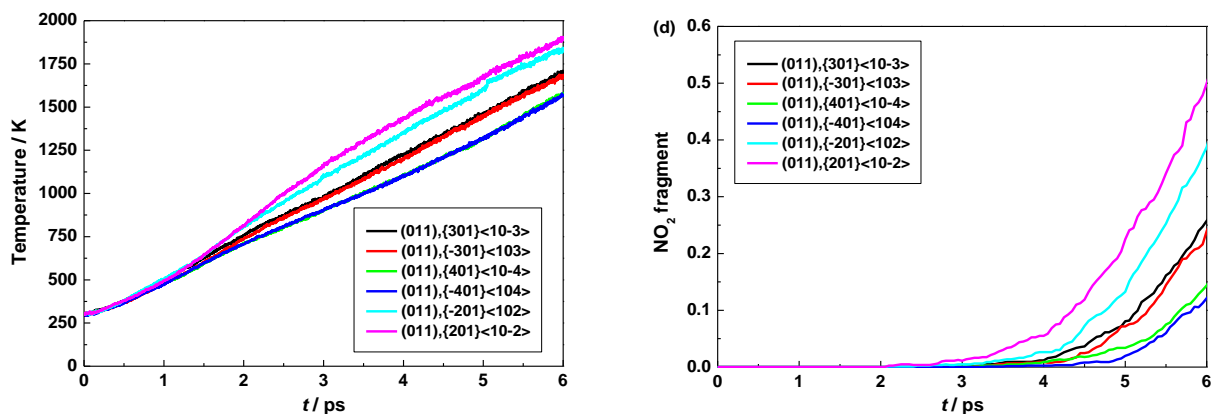
Fig. S4 Time evolutions of shear stress (a), potential energy per HMX molecule (b), temperature (c), and NO$_2$ fragment per HMX molecule (d) for the eight possible slip systems along shock direction normal to the (011) plane during shear simulations.
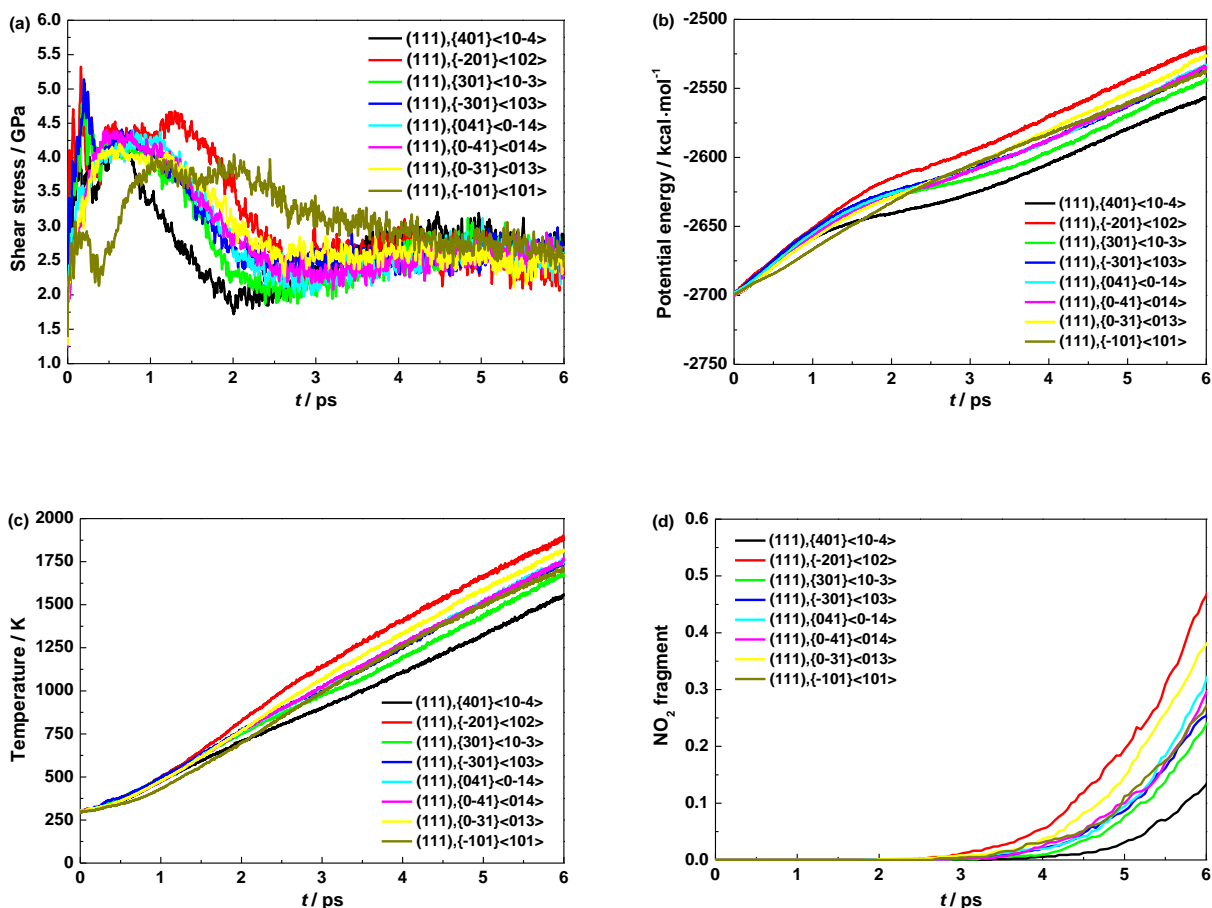

Fig. S5 Time evolutions of shear stress (a), potential energy per HMX molecule (b), temperature (c), and NO$_2$ fragment per HMX molecule (d) for the eight possible slip systems along shock direction normal to the (111) plane during shear simulations.
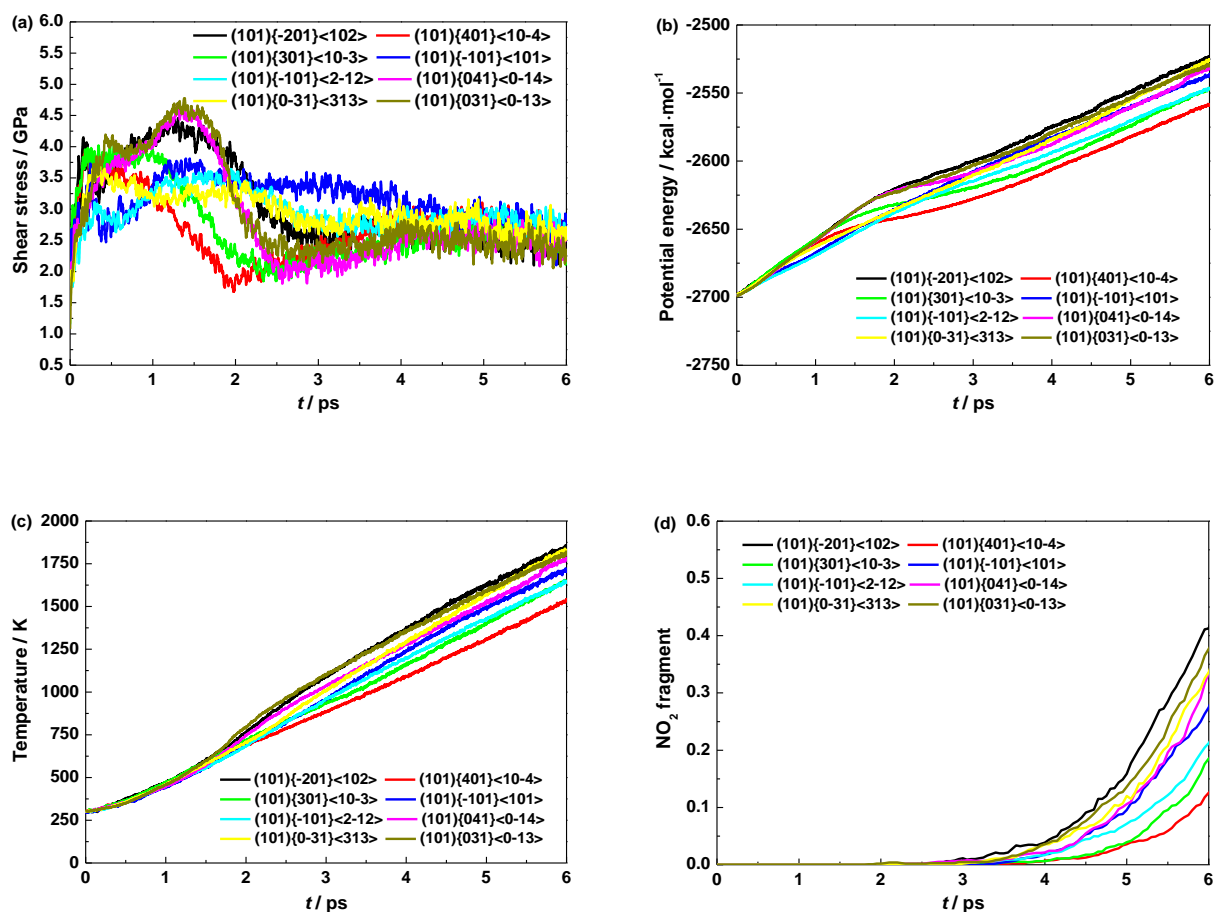
Fig. S6 Time evolutions of shear stress (a), potential energy per HMX molecule (b), temperature (c), and NO$_2$ fragment per HMX molecule (d) for the eight possible slip systems along shock direction normal to the (101) plane during shear simulations.
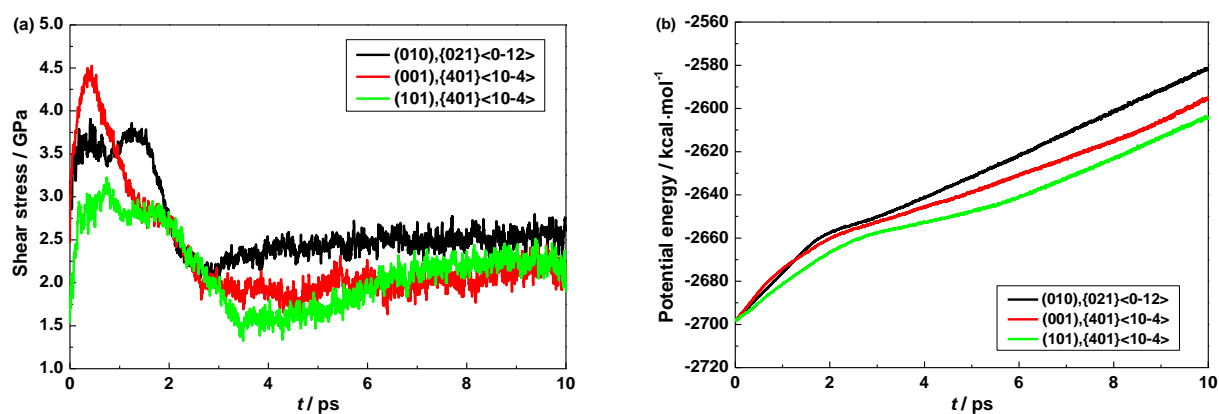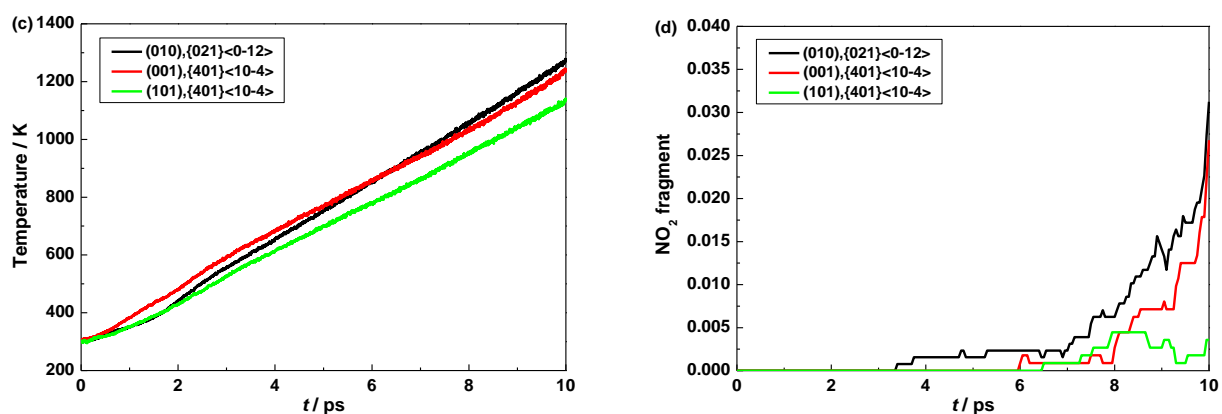
Fig. S7 Time evolutions of shear stress, potential energy per HMX molecule, temperature, and NO_2 product per HMX molecule for the (010), (001), and (101) shock planes during shear simulations at shear rate 0.25 ps^{-1}
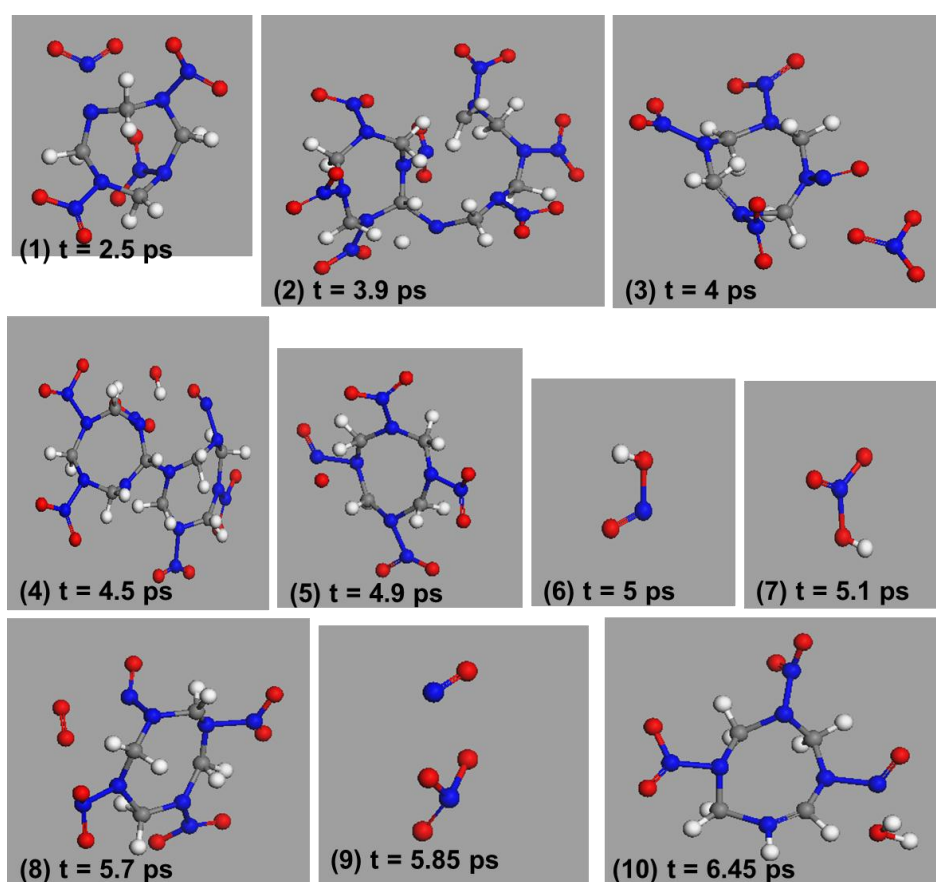

Fig. S8 The snapshots of reaction products at the first time of their appearances from the MD trajectories for the (010) shock plane. $C_4H_8O_8N_8$ (297) → $C_4H_8O_6N_7$ (1283) + O_2N (1284); (2) $C_4H_8O_6N_7$ (1281) + $C_4H_8O_8N_8$ (1245) → $C_8H_{15}O_{14}N_{15}$ (1349) + H (1350); (3) $C_4H_8O_{10}N_9$ (1344) → O_3N (1362) + $C_4H_8O_7N_8$ (1361); (4) $C_8H_{16}O_{12}N_{14}$ (1427) → $C_8H_{15}O_{11}N_{14}$ (1522) + HO (1523); (5) $C_4H_8O_8N_8$ (707) → $C_4H_8O_7N_8$ (1680) + O (1681); (6) O_2N (1444) + H (1718) → HO_2N (1740); (7) H (1459) + O_3N (1653) → HO_3N (1792); (8) $C_4H_8O_9N_8$ (2275) → O_2 (2334) + $C_4H_8O_7N_8$ (2333); (9) O_4N_2 (2157) → ON (2532) + O_3N (2533); (10) $C_4H_{10}O_6N_7$ (3315) → H_2O (3402) + $C_4H_8O_5N_7$ (3401). The numbers in brackets are molecule ID.
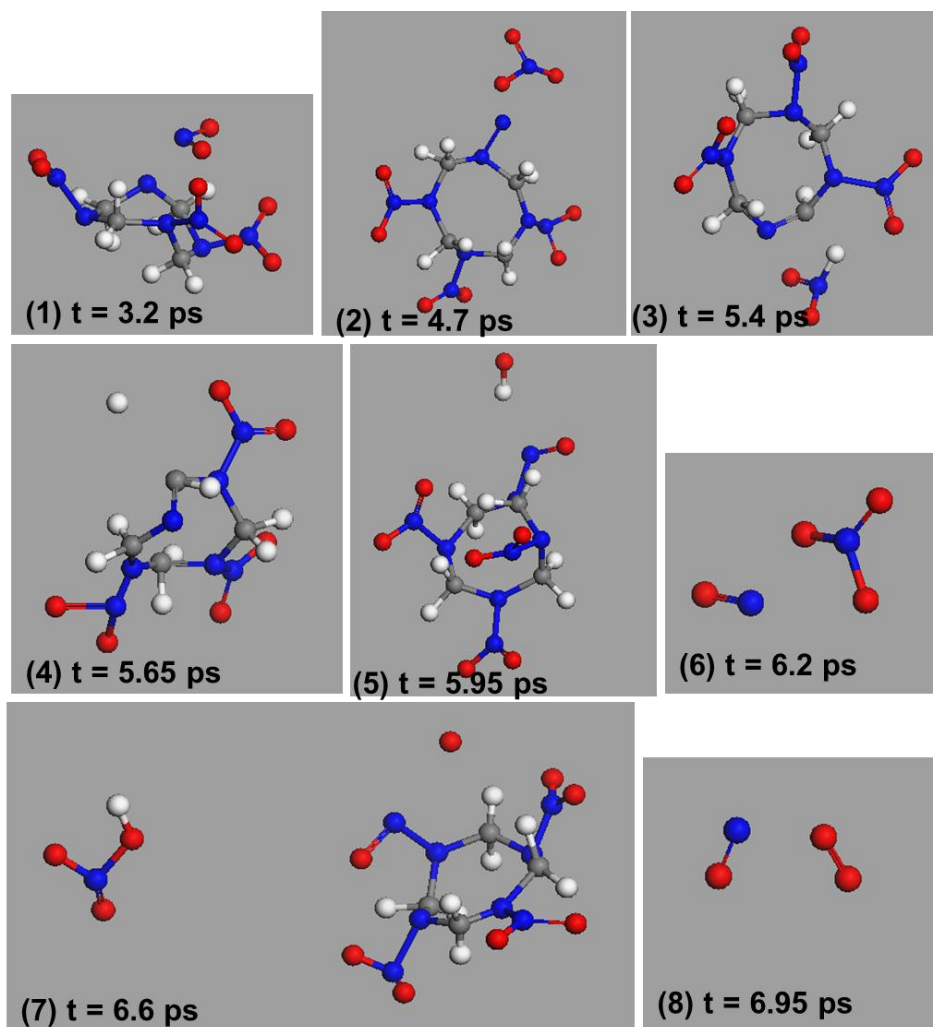
Fig. S9 The snapshots of reaction products at the first time of their appearances from the MD trajectories for the (101) shock plane. (1) $C_4H_8O_8N_8$ (474) → $C_4H_8O_6N_7$ (1121) + O_2N (1122); (2) $C_4H_8O_9N_9$ (1149) → $C_4H_8O_6N_8$ (1168) + O_3N (1169); (3) $C_4H_8O_8N_8$ (1272) → $C_4H_7O_6N_7$ (1290) + HO_2N (1291); (4) $C_4H_8O_6N_7$ (1302) → $C_4H_7O_6N_7$ (1388) + H (1389); (5) $C_4H_9O_8N_8$ (1493) → $C_4H_8O_7N_8$ (1519) + HO (1520); (6) O_4N_2 (1490) → ON (1669) + O_3N (1670); (7) $C_4H_8O_8N_8$ (1108) → $C_4H_8O_7N_8$ (2136) + O (2137), O_2N (1152) + HO (1520) → HO_3N (2084); (8) O_3N (2374) → O_2 (2435) + ON (2434). The numbers in brackets are molecule ID.
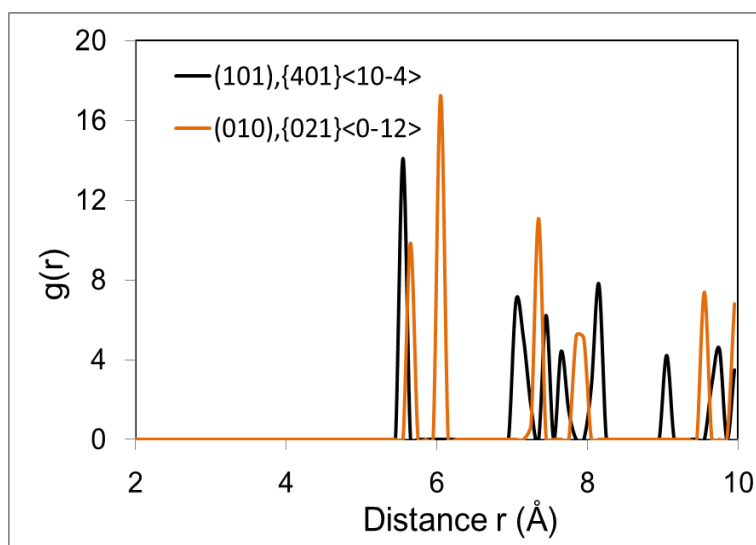

Fig. S10 The radical distribution function g(r) based on the molecular center of mass for the (010) and (101) shocked systems after energy minimization

7