Electronic Supplementary Information (ESI)

Anisotropic Shock Sensitivity in Single Crystal *δ*-Cyclotetramethylene Tetranitramine: A Reactive Molecular Dynamics Study

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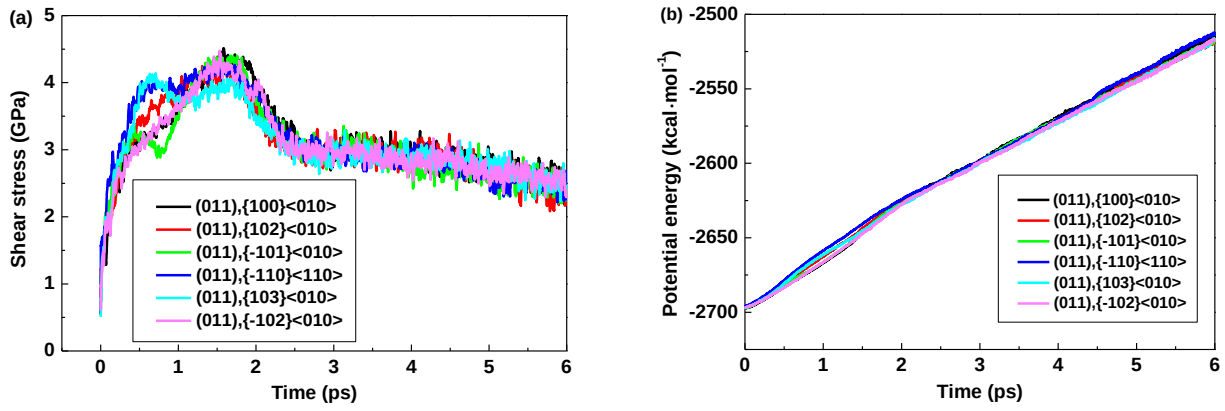
Table S1 The averaged full stress tensors for the seven compressed systems after NVT-MD relaxation (unit: GPa)

Shock plane	P	P_{xx}	P_{yy}	P_{zz}	P_{xy}	P_{xz}	P_{yz}
(110)	10.133	11.364	9.812	9.223	-0.069	-0.116	-0.008
(011)	9.550	9.380	9.740	9.531	0.605	-0.251	0.055
(010)	9.678	8.752	10.447	9.834	0.828	-0.006	0.004
(100)	9.619	10.681	8.918	9.258	-0.230	0.131	-0.074
(001)	8.954	8.041	8.052	10.769	-0.033	0.082	-0.065
(101)	9.673	10.789	8.884	9.347	0.521	-0.150	-0.401
(111)	9.778	10.612	9.987	8.735	-0.514	0.081	-0.228

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



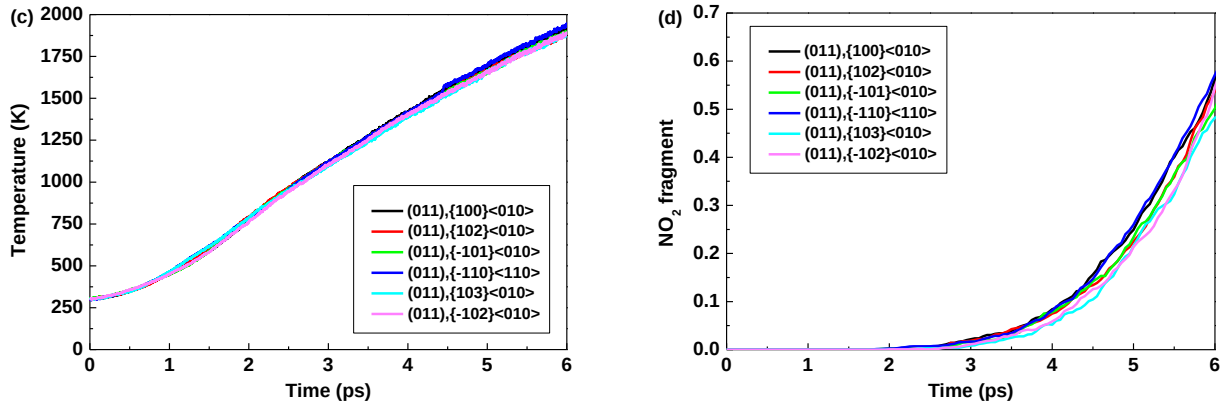


Fig. S1 Time evolutions of shear stress, potential energy per HMX molecule, temperature, and NO_2 product per HMX molecule for the four possible slip systems along shock direction normal to the (011) plane during shear simulations

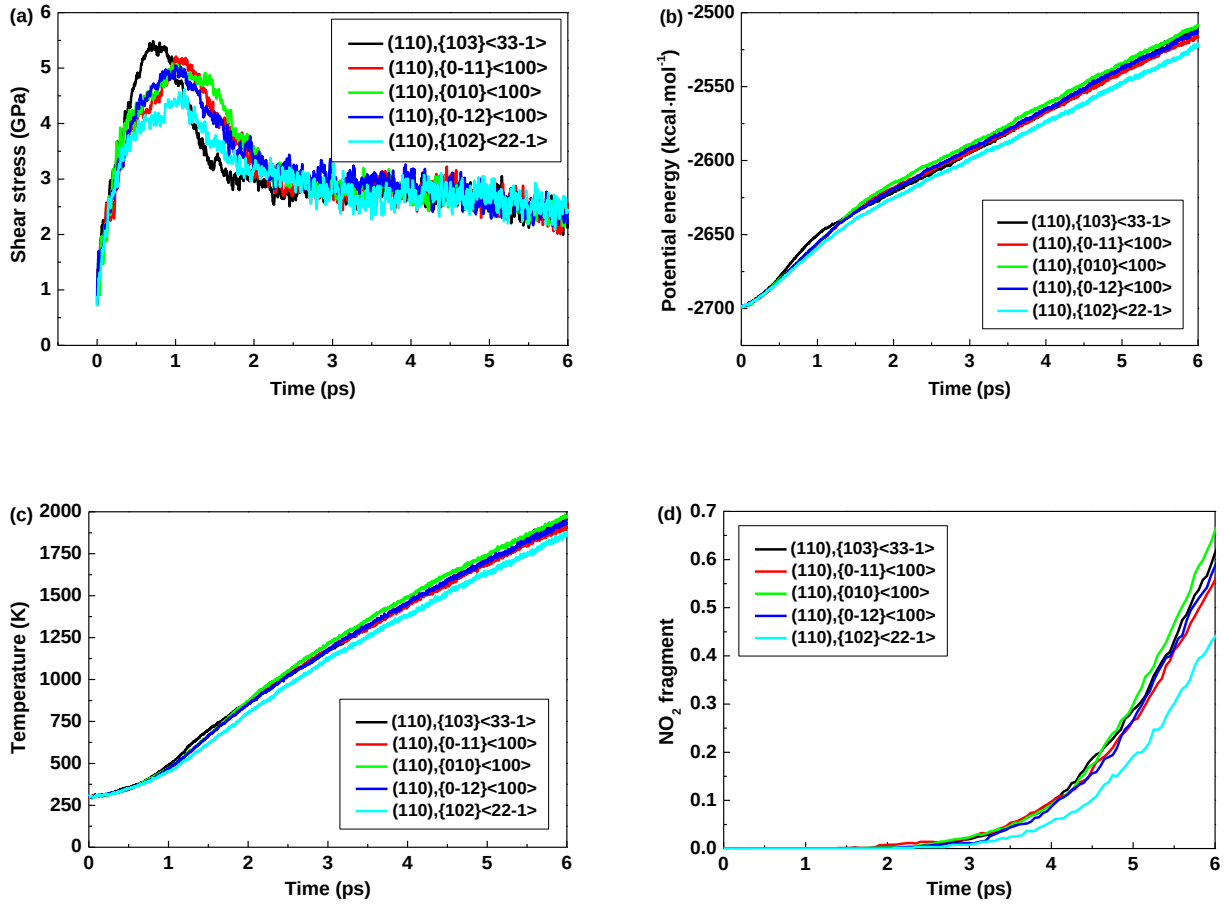


Fig. S2 Time evolutions of shear stress, potential energy per HMX molecule, temperature, and NO2 product per HMX molecule for the four possible slip systems along shock direction normal to the (110) plane during shear simulations

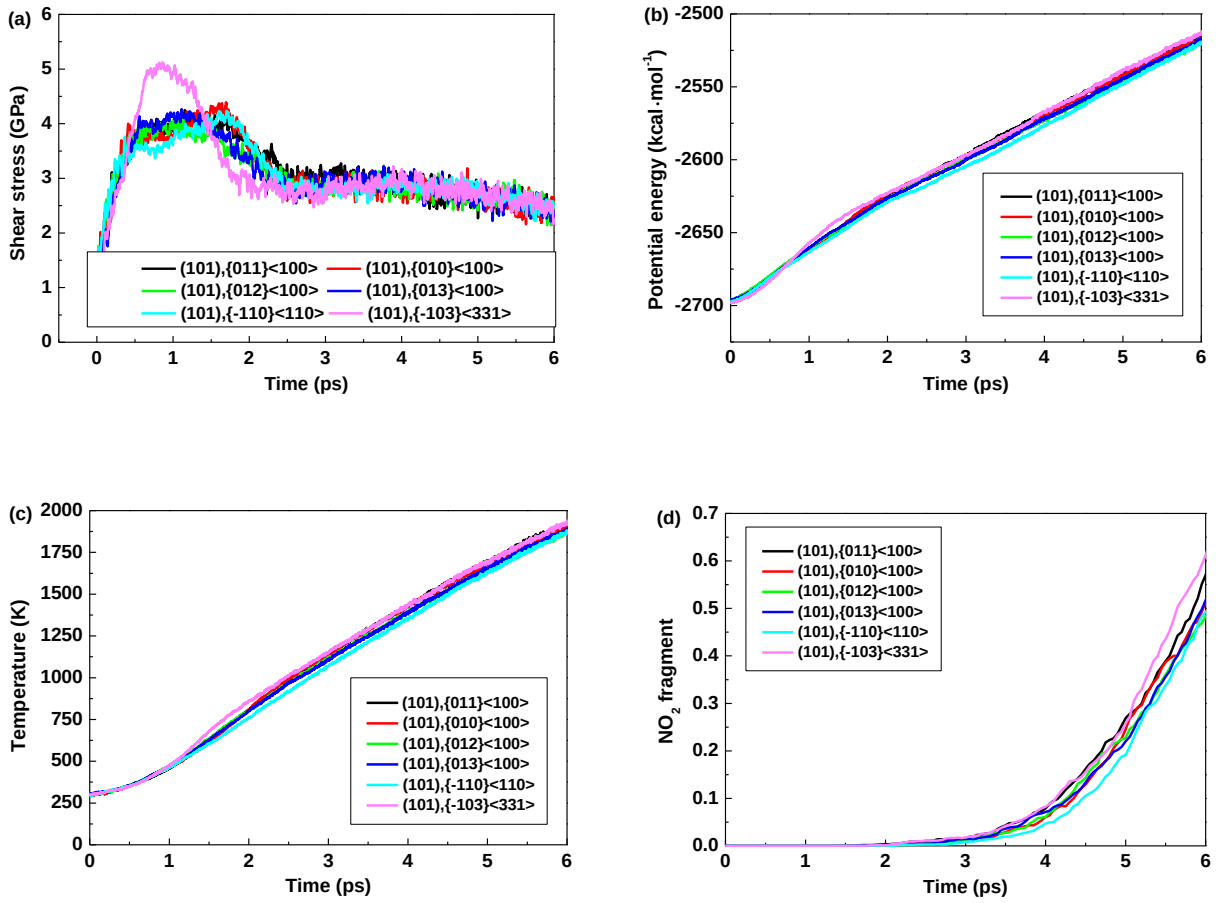
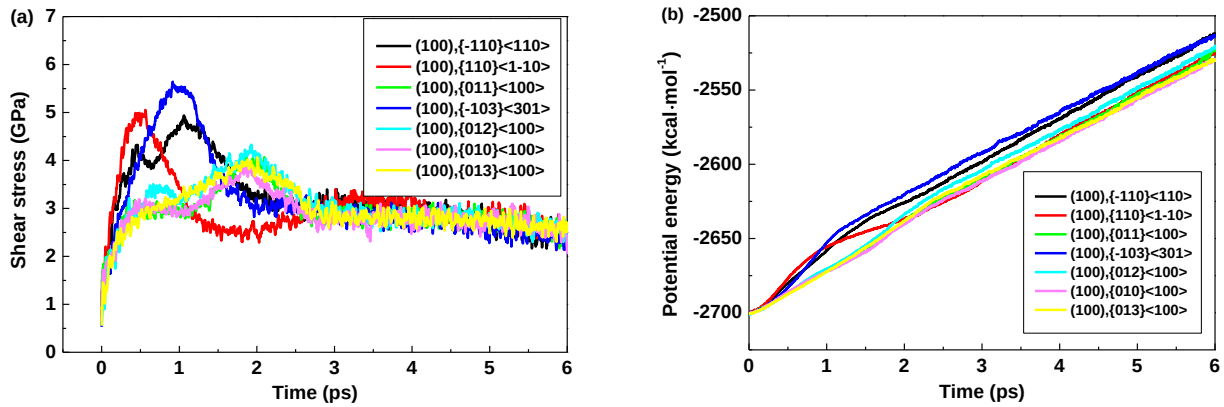


Fig. S3 Time evolutions of shear stress, potential energy per HMX molecule, temperature, and NO_2 product per HMX molecule for the four possible slip systems along shock direction normal to the (101) plane during shear simulations



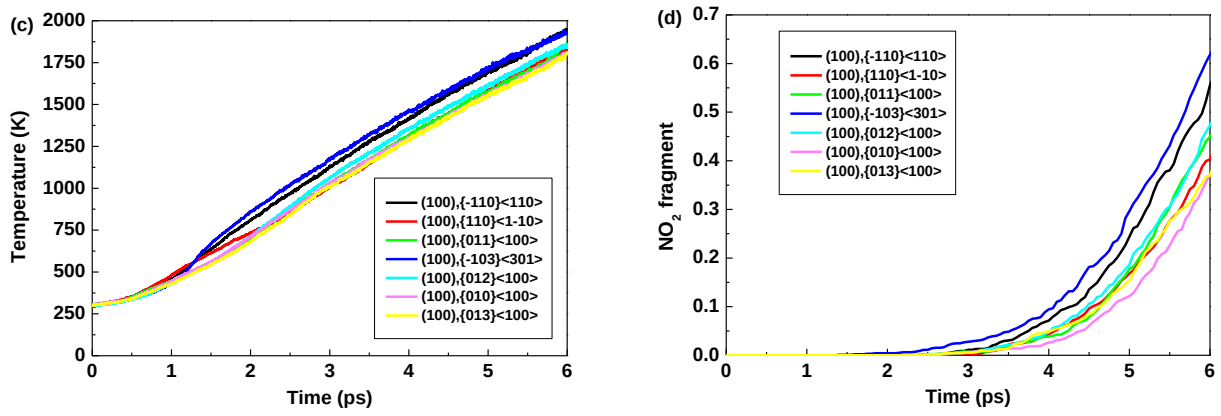


Fig. S4 Time evolutions of shear stress, potential energy per HMX molecule, temperature, and NO_2 product per HMX molecule for the four possible slip systems along shock direction normal to the (100) plane during shear simulations

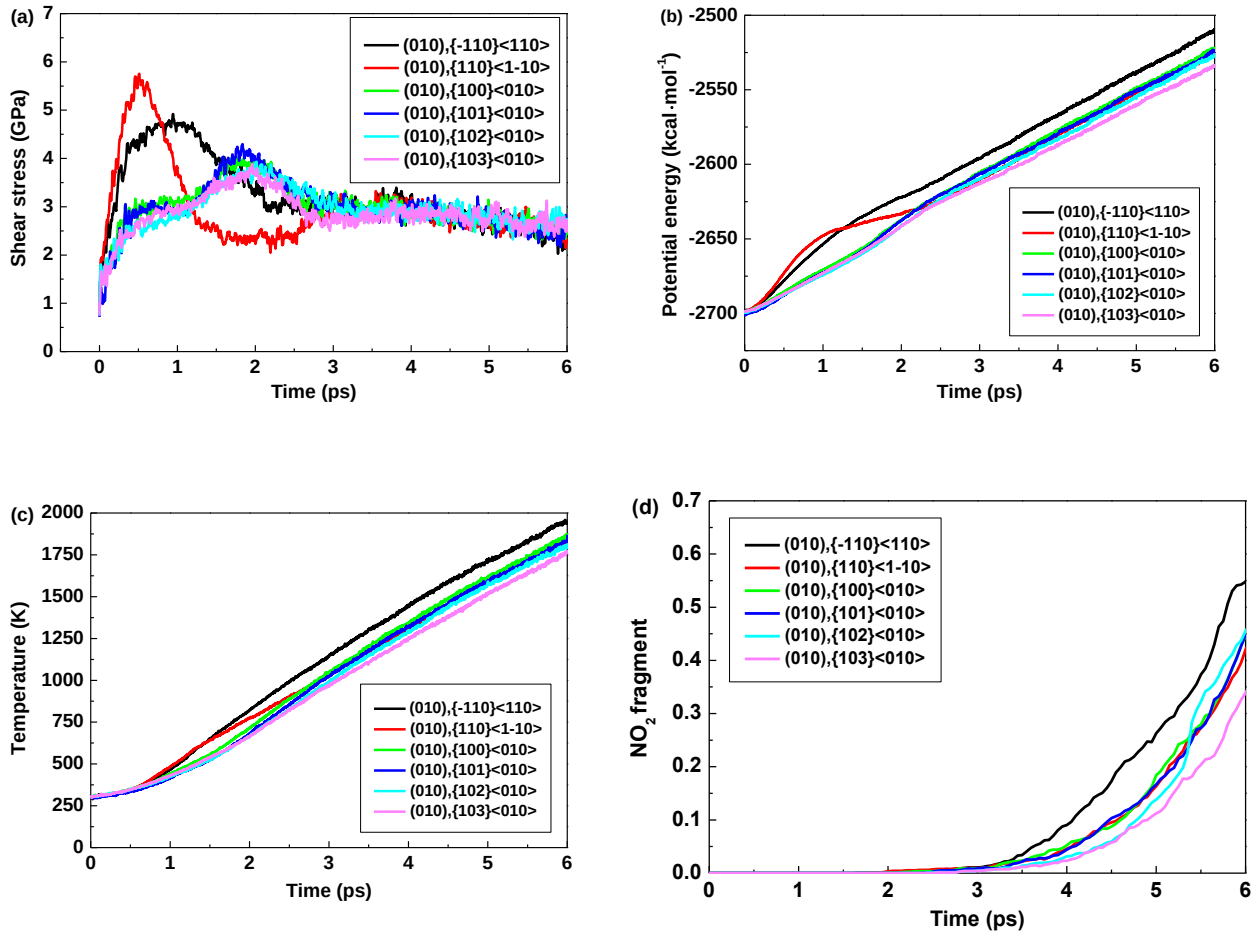


Fig. S5 Time evolutions of shear stress, potential energy per HMX molecule, temperature, and NO_2 product per HMX molecule for the four possible slip systems along shock direction normal to the (010) plane during shear simulations

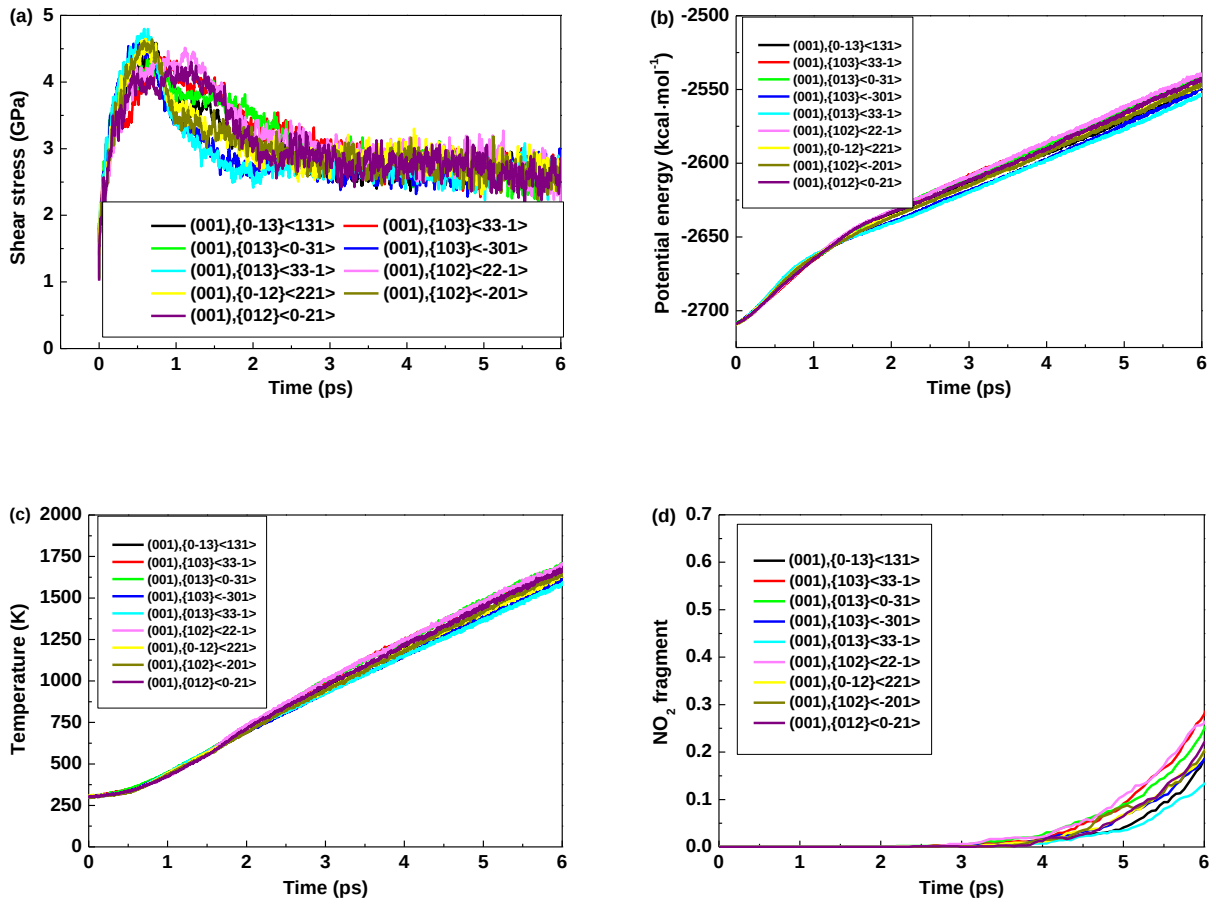
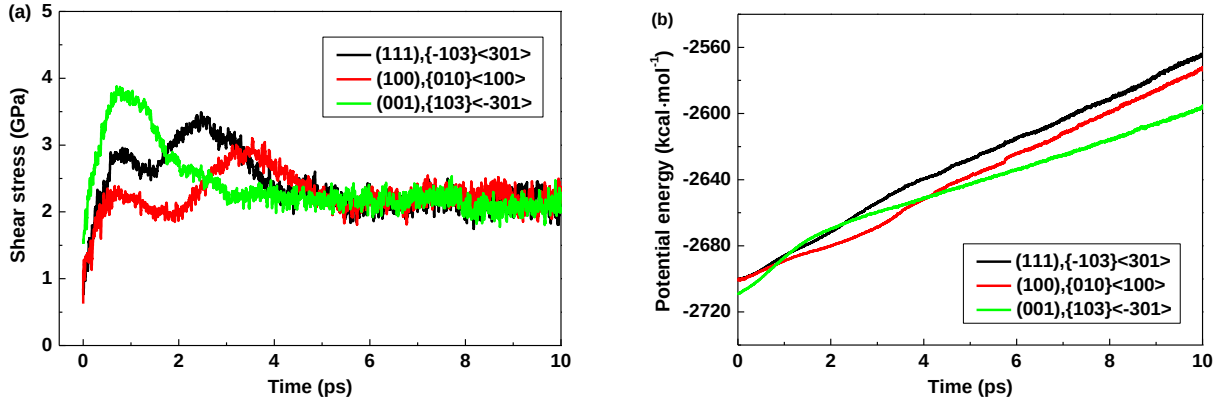


Fig. S6 Time evolutions of shear stress, potential energy per HMX molecule, temperature, and NO_2 product per HMX molecule for the four possible slip systems along shock direction normal to the (001) plane during shear simulations



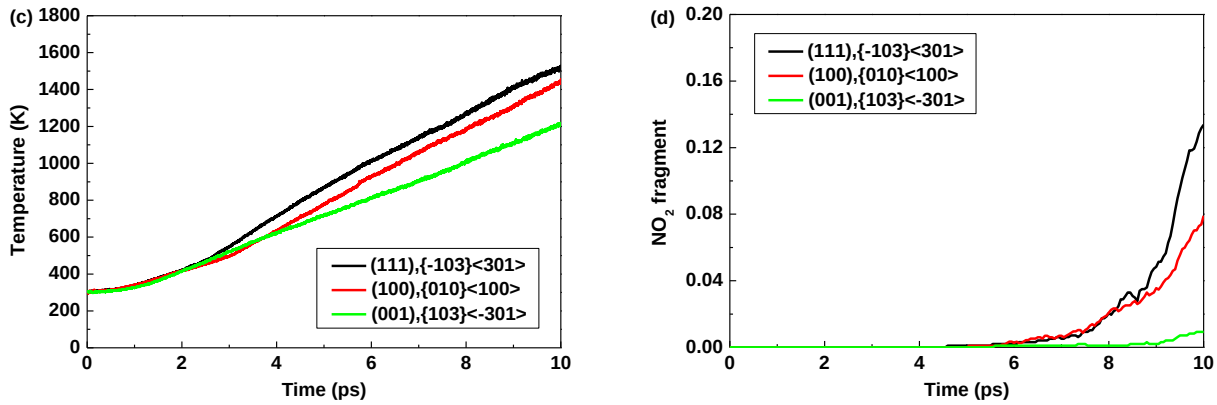


Fig. S7 Time evolutions of shear stress, potential energy per HMX molecule, temperature, and NO_2 product per HMX molecule for the (111), (100), and (001) shock planes during shear simulations at shear rate 0.25 ps^{-1}