Supplementary Information (SI)

Impact-Induced Hotspot Formation and Sensitivity Ranking in Energetic Crystals Revealed by Deep Potential Molecular Dynamics

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In the supplementary materials, we present:

1. Explicit_atomic_impactor_impact.in
2. **Figure S1** EOS curves for the eight EMs studied in this work.
3. **Figure S2** Total normalized energy drift curves during the impact simulations under NVE conditions.
4. **Figure S3** Spatial distributions of stress (a) and temperature (b) in the larger simulation cell (5 nm × 5 nm × 12 nm) under an impact velocity of 700 m s^{-1}.
5. **Figure S4** Evolution of (a) sample temperature, (b) strain, (c) decomposition ratio, and (d) stress between Size 1 (5 nm × 5 nm × 6 nm) and Size 2 (5 nm × 5 nm × 12 nm) under an impact velocity of 700 m s^{-1}.
6. **Figure S5** Evolution of (a) sample temperature, (b) strain, (c) decomposition ratio, and (d) stress between the porous aggregate model consisting of eight 2-nm RDX nanoparticles (Model 1, 2 nm × 8) and the single-crystal model (Model 2, 5 nm × 5 nm × 6 nm) under an impact velocity of 700 m s^{-1}.
7. **Figure S6** Spatial distributions of (a) stress and (b) temperature in the porous aggregate model composed of eight 2-nm RDX nanoparticles (Model 1, 5 nm × 5 nm × 5 nm) under an impact velocity of 700 m s^{-1}.

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1. Explicit_atomic_impactor_impact.in

```
# Usage: as explicit_atomic_impactor_impact.in and run with lmp
# ------------------- variables -------------------
variable fname              string    RDX_700ms
variable SPEED_mps          equal     -700.0                   # m/s, negative -> towards -z
variable speed_Aps          equal     v_SPEED_mps*1.0e-2 # convert to Å/ps (metal)
variable dt                 equal     0.0002
variable loadstep           equal     100000
# ------------------- system setup -------------------
units               metal
dimension           3
boundary            p p fs                  # periodic x,y; shrinkwrap/float z (open top)
atom_style          atomic
neighbor            2.0 bin
neigh_modify        delay 0 every 1 check yes
# ------------------- read sample -------------------
read_data           RDX_impactor_co.data
group flyer id 7939:113946
group sample     subtract all flyer
fix wall_z sample wall/reflect zlo EDGE
pair_style deepmd CHNO-iter-128-20240716-compress.pb
pair_coeff * *
# ------------------- thermo / timestep -------------------
timestep ${dt}
thermo 500
thermo_style custom step temp pe ke etotal press lx ly lz
# ------------------- minimization -------------------
min_style sd
minimize 1.0e-8 1.0e-10 1000 10000
```

```
reset_timestep 0
# ------------------- rigid -------------------
velocity sample create 300.0 12345 mom yes rot yes
fix fly_rigid flyer rigid/nve single force * off off on torque * off off off
velocity flyer set 0.0 0.0 ${speed_Aps} units box
fix sample_nve sample nve
# ------------------- computes for monitoring -------------------
compute zmax_sample sample reduce max z
compute zmin_sample sample reduce min z
run 0
variable zmax0 equal c_zmax_sample
variable zmin0 equal c_zmin_sample
variable Lz0 equal "v_zmax0 - v_zmin0"
variable time equal time
variable temp equal temp
compute sample_temp sample temp
variable sample_T equal c_sample_temp
variable pe equal pe
variable ke equal ke
variable etotal equal etotal
compute sample_pe sample pe/atom
compute sample_ke sample ke/atom
compute sample_pe_total sample reduce sum c_sample_pe
compute sample_ke_total sample reduce sum c_sample_ke
variable sample_PE equal c_sample_pe_total
variable sample_KE equal c_sample_ke_total
variable sample_Etotal equal "v_sample_PE + v_sample_KE"
compute         KE all ke/atom
variable        KB equal 8.625e-5
```

```
variable TEMP atom c_KE/1.5/${KB}
compute disp all displace/atom
compute 1 all centroid/stress/atom NULL
compute v all voronoi/atom
variable stressxx atom c_1[1]/c_v[1]/10000
variable stressyy atom c_1[2]/c_v[1]/10000
variable stresszz atom c_1[3]/c_v[1]/10000
variable stressxy atom c_1[1]/c_v[1]/10000
variable stressyz atom c_1[2]/c_v[1]/10000
variable stressxz atom c_1[3]/c_v[1]/10000
variable sx equal "-pxx/10000"
variable sy equal "-pyy/10000"
variable sz equal "-pzz/10000"
variable sxy equal "-pxy/10000"
variable syz equal "-pyz/10000"
variable sxz equal "-pxz/10000"
variable Lz0 equal ${Lz0}
compute zmax_now sample reduce max z
variable depth equal "v_Lz0 - c_zmax_now"
variable strain equal "v_depth / v_Lz0"
compute zmin_flyer flyer reduce min z
variable com_flyer equal c_zmin_flyer
variable vel_fly_z equal vcm(flyer,z)
variable outfreq equal 500
fix out_all all print ${outfreq} "${time} ${temp} ${sample_T} ${strain} ${depth} ${vel_fly_z} ${sx} ${sy} ${sz} ${sxy} ${syz} ${sxz} ${vonMises} ${pe} ${ke} ${etotal} ${sample_PE} ${sample_KE} ${sample_Etotal}" file ${fname}-impact-load.txt screen no
restart 50000 ${fname}-impact-*.restart
dump traj all custom 500 ${fname}-impact.dump id type element x y z vx vy vz fx fy fz
```

```
v_TEMP c_disp[*] v_stressxx v_stressyy v_stresszz v_stressxy v_stressxz v_stressyz
dump_modify traj element C H N O
dump traj_sample sample custom 100 ${fname}-impact_sample.dump id type element x y z
vx vy vz fx fy fz v_TEMP c_disp[*] v_stressxx v_stressyy v_stresszz v_stressxy v_stressxz
v_stressyz
dump_modify traj_sample element C H N O
run    ${loadstep}
```

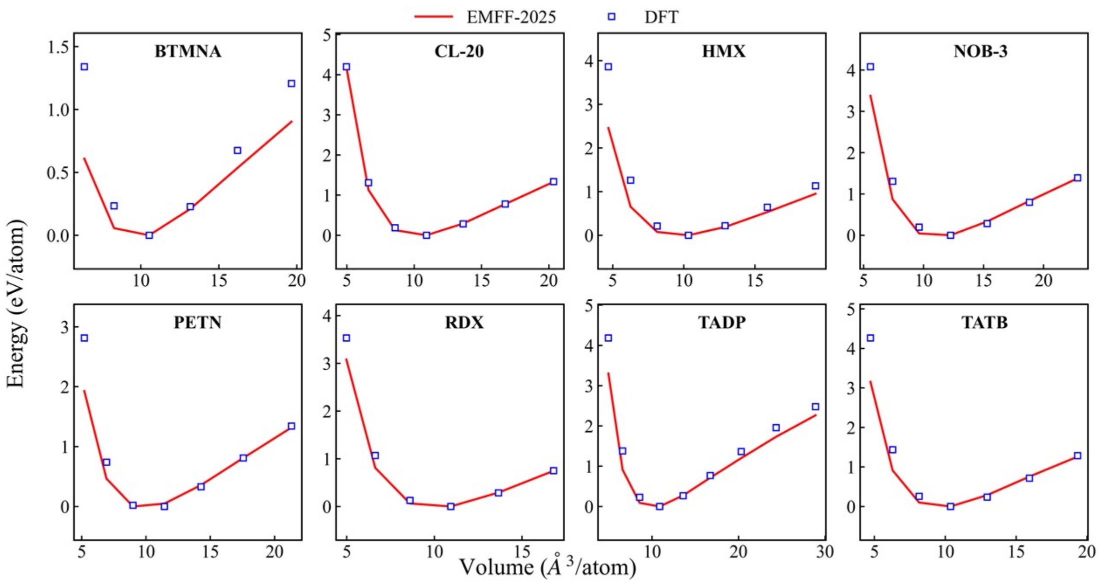

Figure S1 EOS curves for the eight EMs studied in this work.

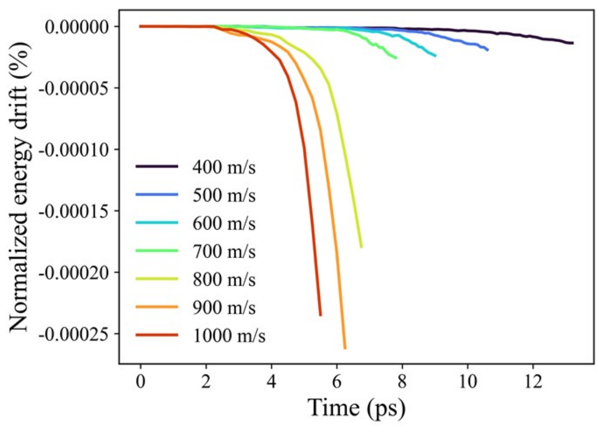

Figure S2 Total normalized energy drift curves during the impact simulations under NVE conditions.

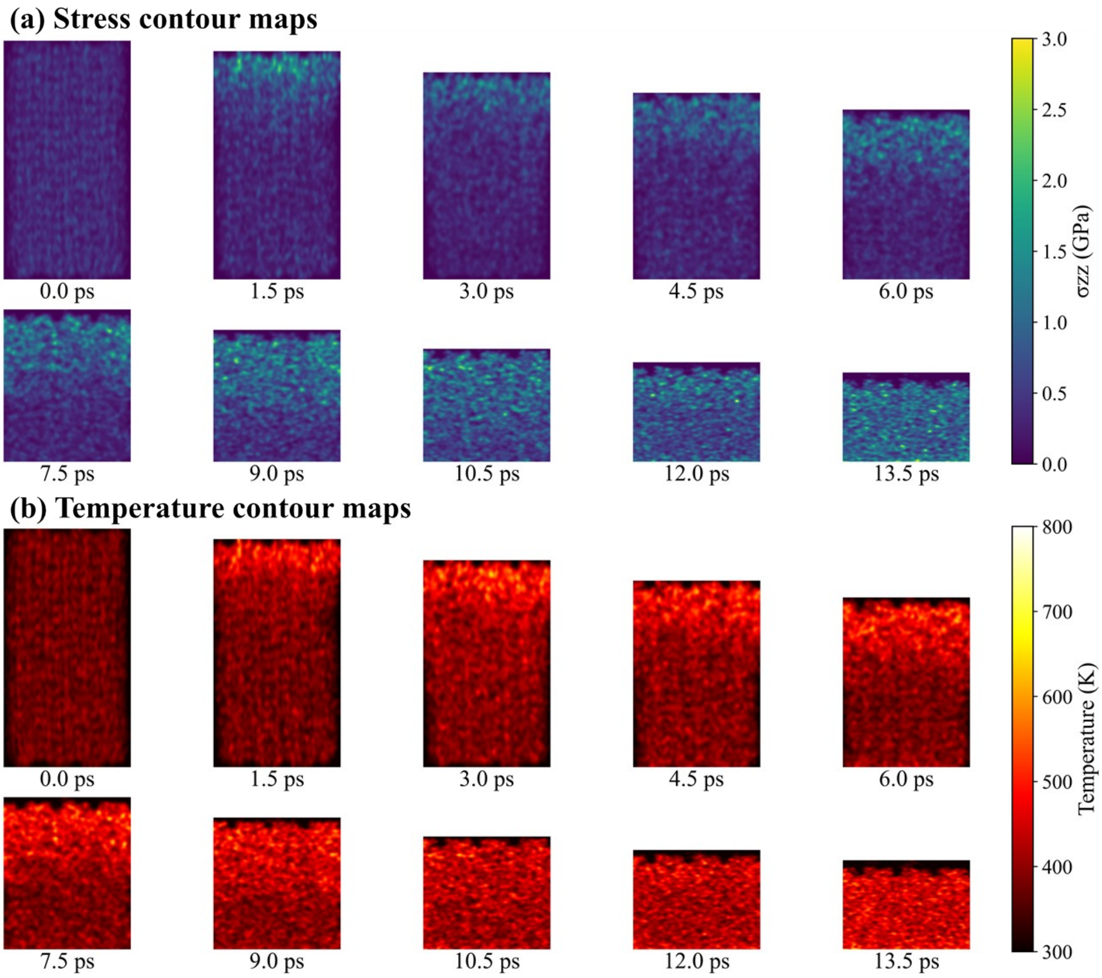

Figure S3 Spatial distributions of stress (a) and temperature (b) in the larger simulation cell (5 nm × 5 nm × 12 nm) under an impact velocity of 700 m s^{-1}.

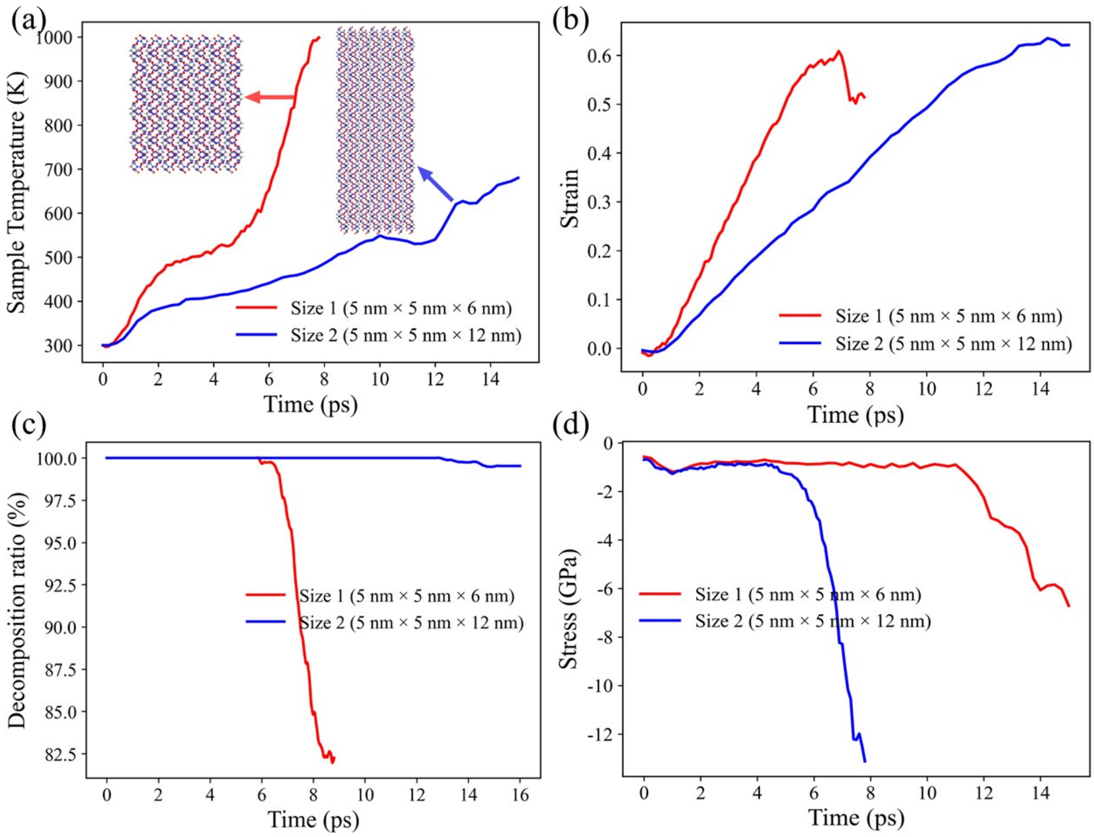

Figure S4 Evolution of (a) sample temperature, (b) strain, (c) decomposition ratio, and (d) stress between Size 1 (5 nm × 5 nm × 6 nm) and Size 2 (5 nm × 5 nm × 12 nm) under an impact velocity of 700 m s^{-1}.

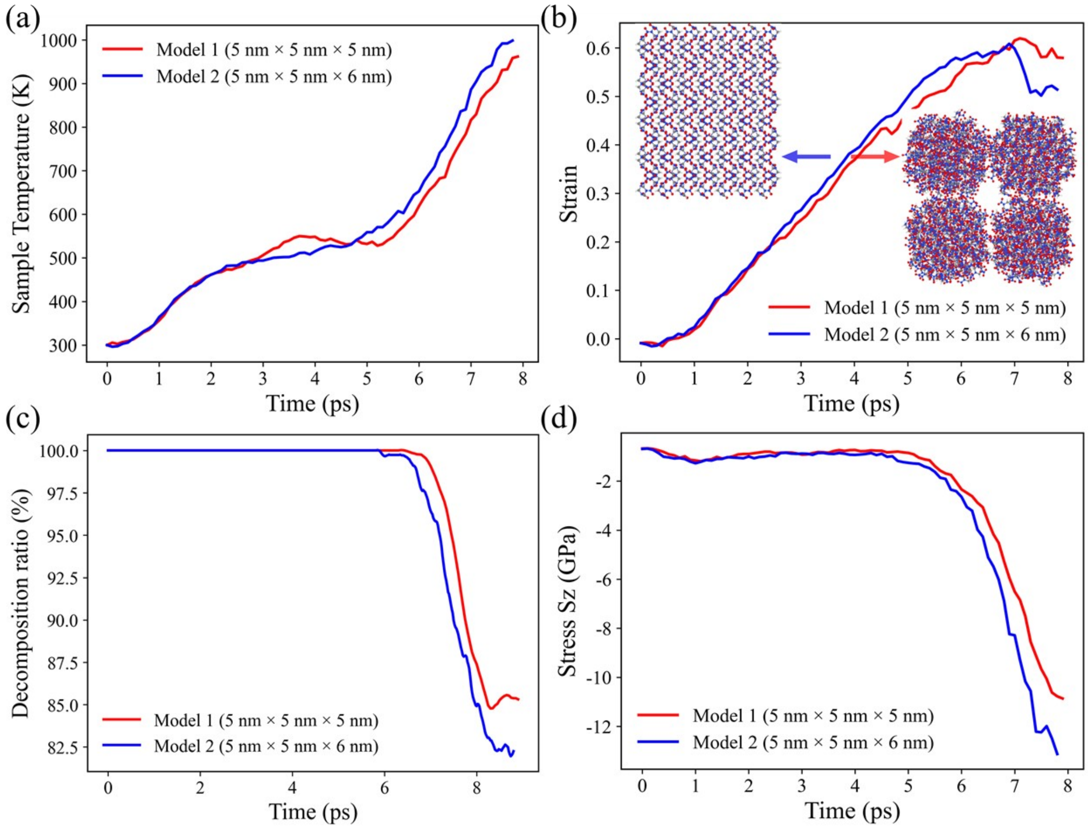

Figure S5 Evolution of (a) sample temperature, (b) strain, (c) decomposition ratio, and (d) stress between the porous aggregate model consisting of eight 2-nm RDX nanoparticles (Model 1, 5 nm × 5 nm × 5 nm) and the single-crystal model (Model 2, 5 nm × 5 nm × 6 nm) under an impact velocity of 700 m s^{-1}.

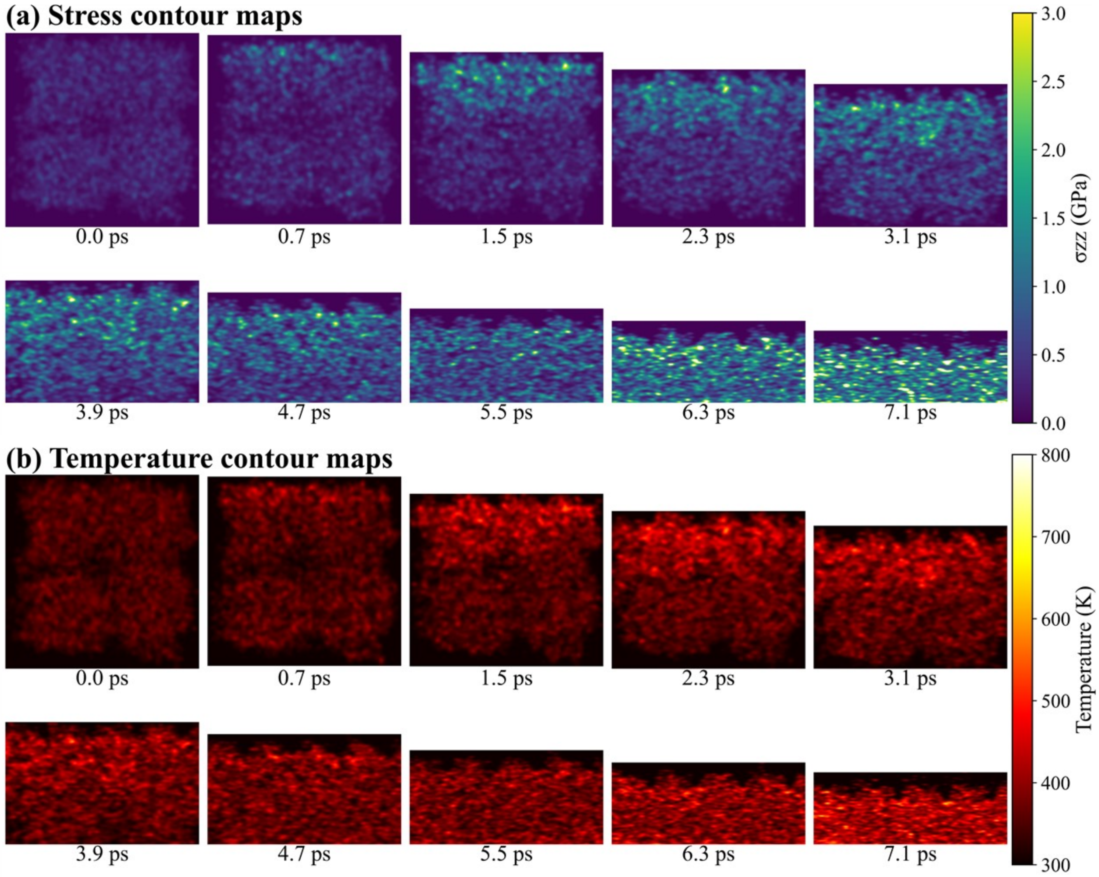

Figure S6 Spatial distributions of (a) stress and (b) temperature in the porous aggregate model composed of eight 2-nm RDX nanoparticles (Model 1, 2 nm × 8) under an impact velocity of 700 m s^{-1}.

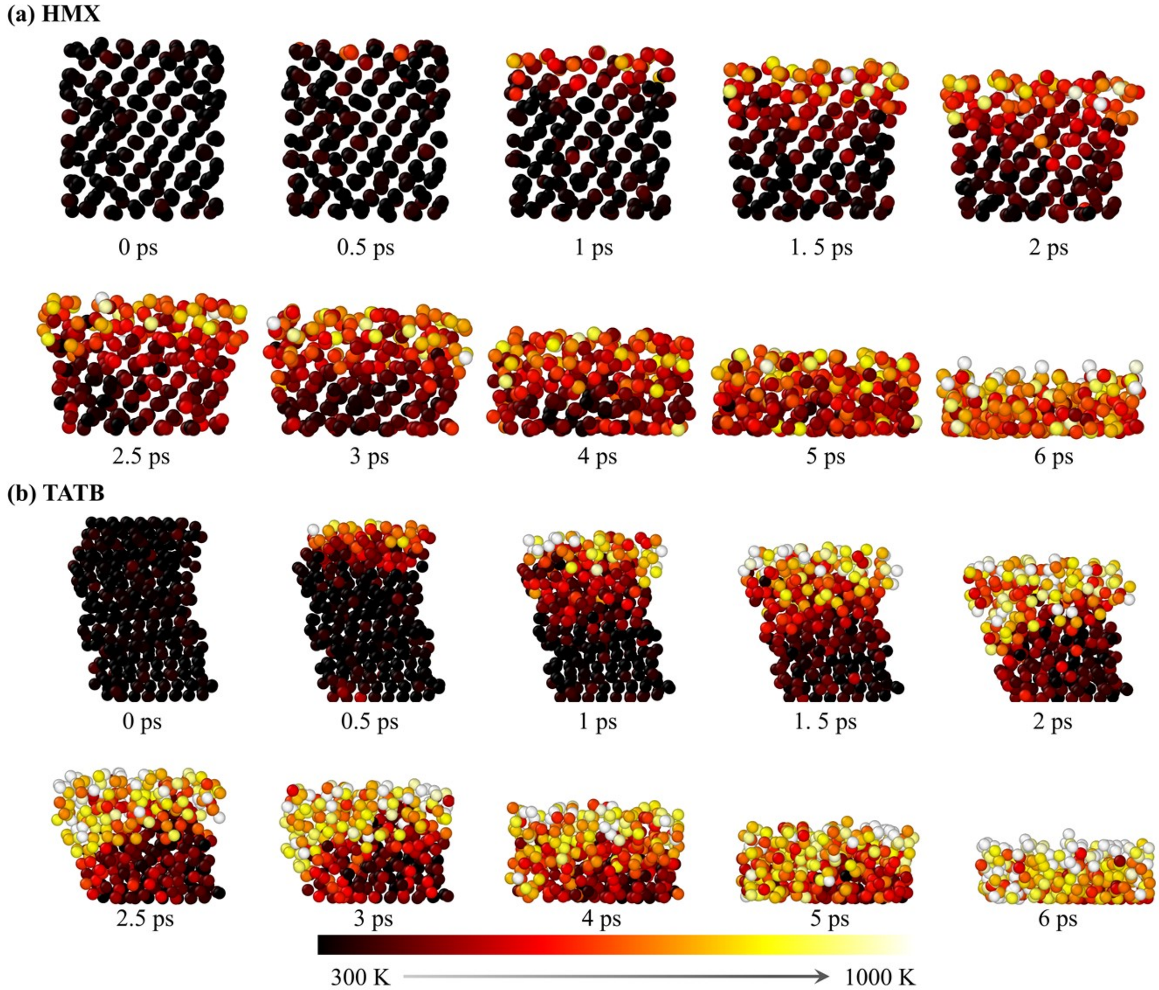

Figure S7 Structured temperature maps for HMX and TATB.

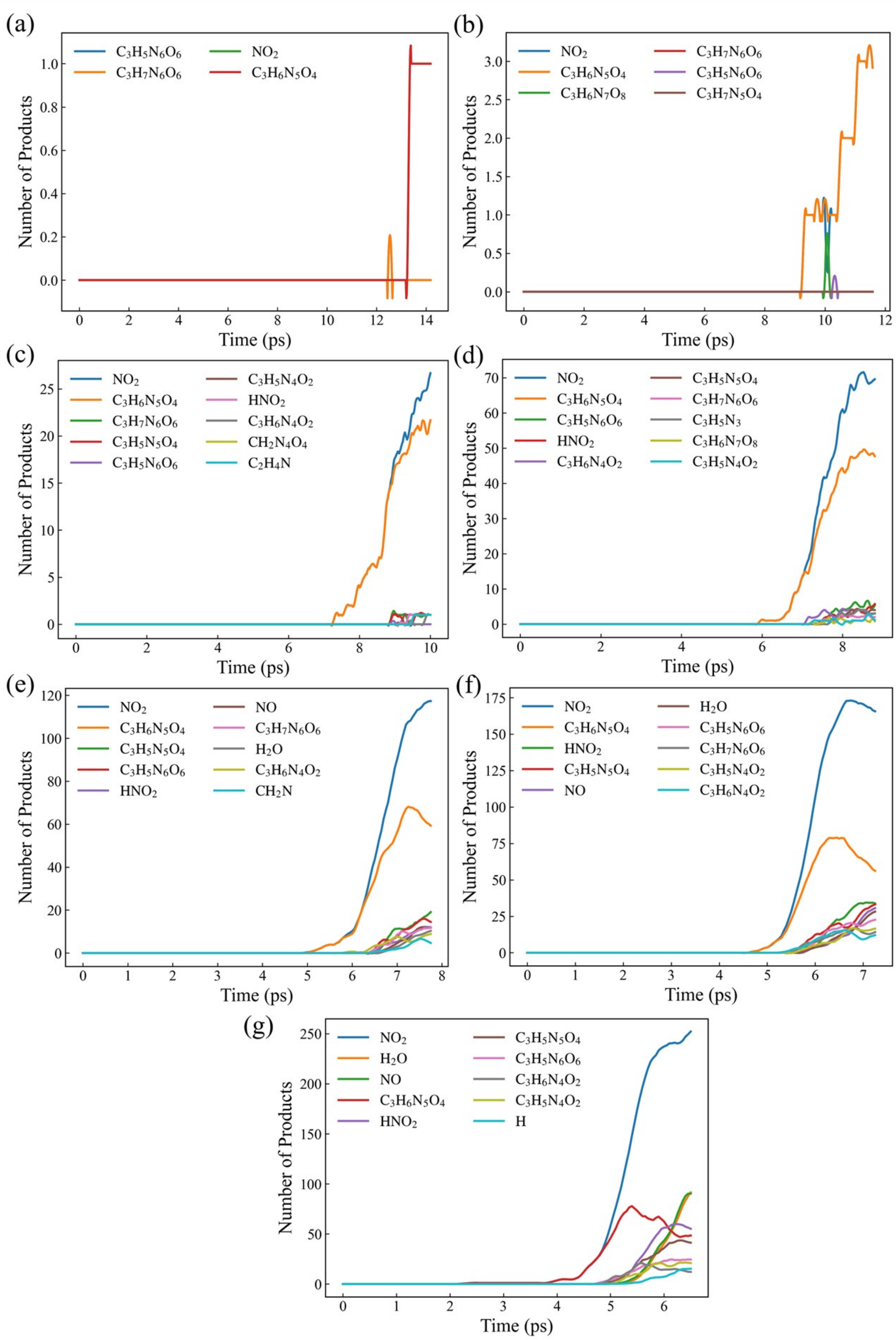

Figure S8 Products evolution of RDX under different impact velocities. (a) 400 m/s, (b) 500 m/s, (c) 600 m/s, (d) 700 m/s, (e) 800 m/s, (f) 900 m/s, (g) 1000 m/s,

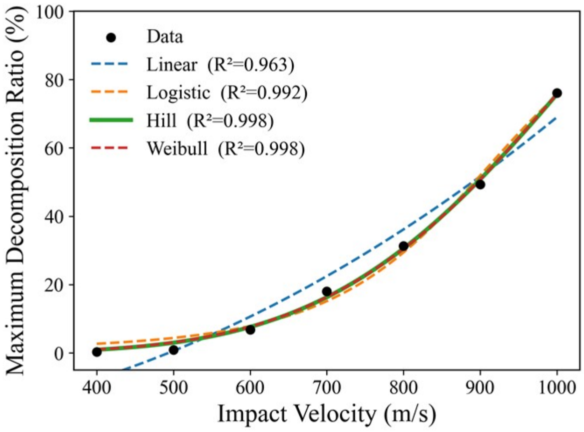

Figure S9 Fitting of the relationship between the final decomposition fraction and impact velocity using Logistic, Hill, and Weibull functions.

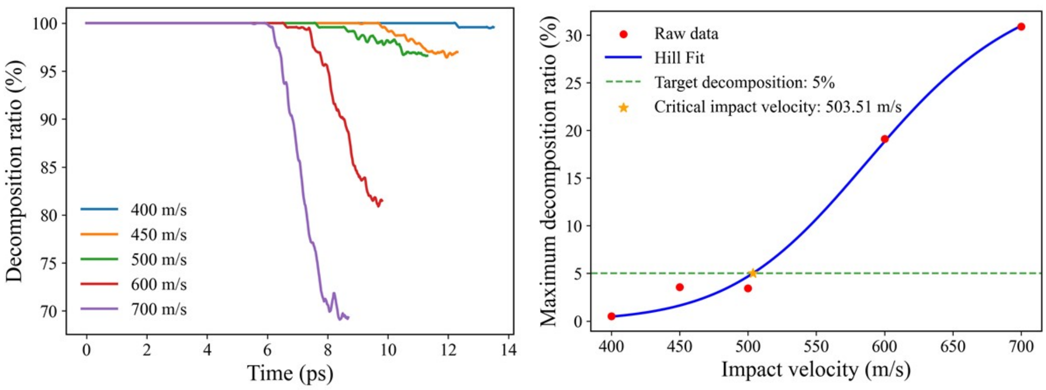

Figure S10 Decomposition fraction evolutions and critical velocity fittings of CL-20.

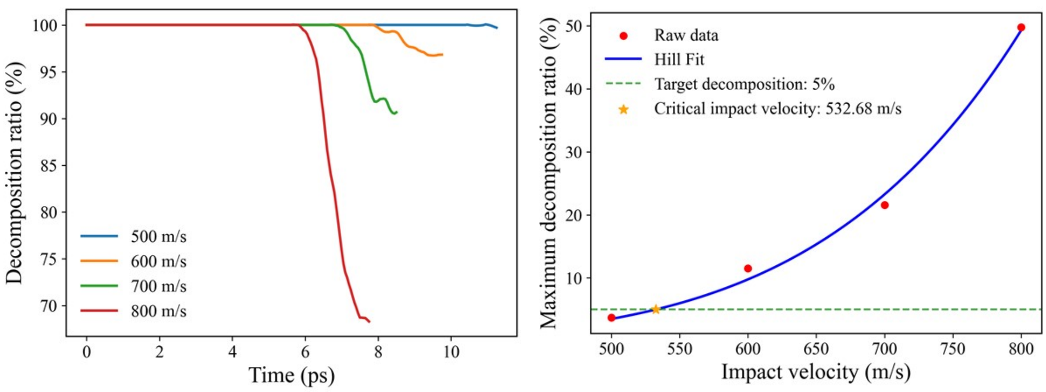

Figure S11 Decomposition fraction evolutions and critical velocity fittings of HMX.

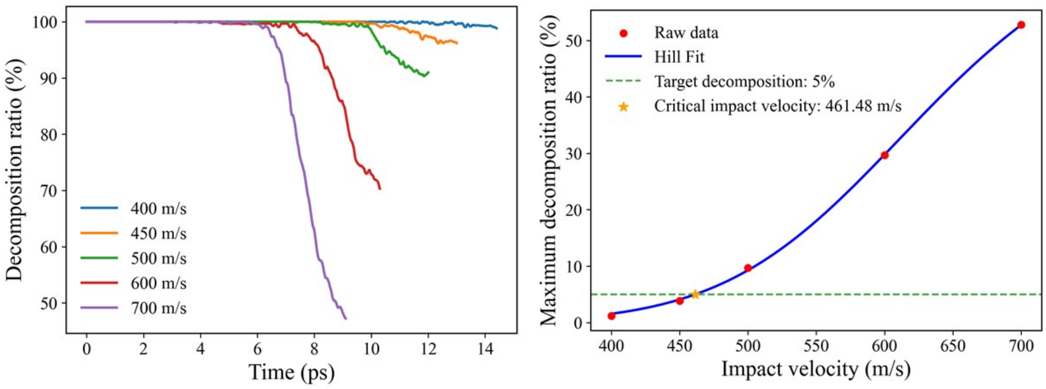

Figure S12 Decomposition fraction evolutions and critical velocity fittings of PETN.

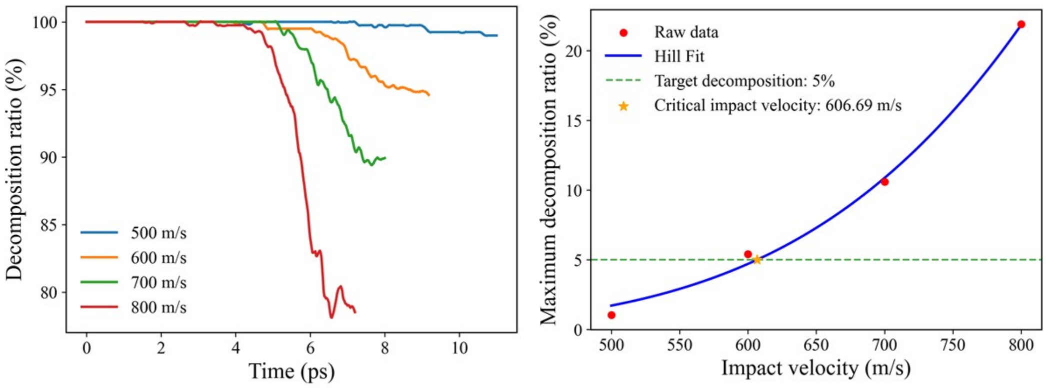

Figure S13 Decomposition fraction evolutions and critical velocity fittings of BTMNA.

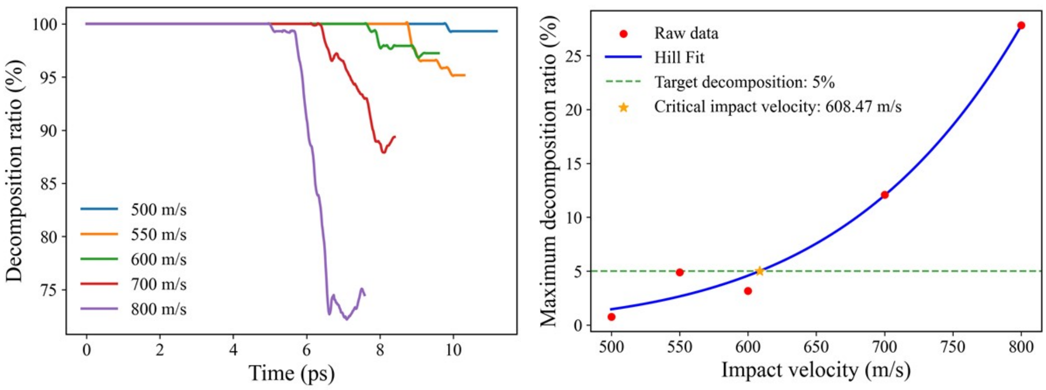

Figure S14 Decomposition fraction evolutions and critical velocity fittings of NOB-3.

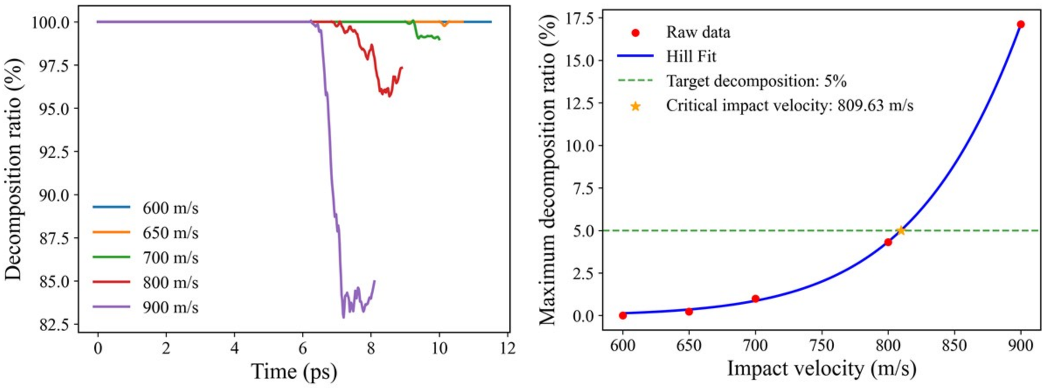

Figure S15 Decomposition fraction evolutions and critical velocity fittings of TADP.

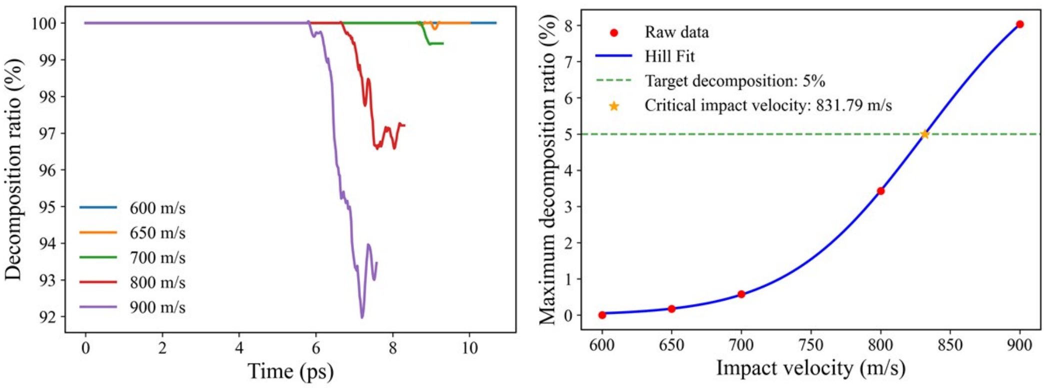

Figure S16 Decomposition fraction evolutions and critical velocity fittings of TATB.

Table S1 Experimental impact sensitivities (E_{50}) and the corresponding critical impact velocities obtained from MD simulations for eight EMs.

Material	Experimental impact sensitivity, E_{50} (J)	Critical impact velocity (m/s)
PETN	3.5	461.48
CL-20	4.0	503.51
HMX	7.4	532.68
RDX	7.5	552.79
BTMNA	30.0	606.69
NOB-3	32.0	608.47
TADP	>60.0	809.63
TATB	120.0	831.79

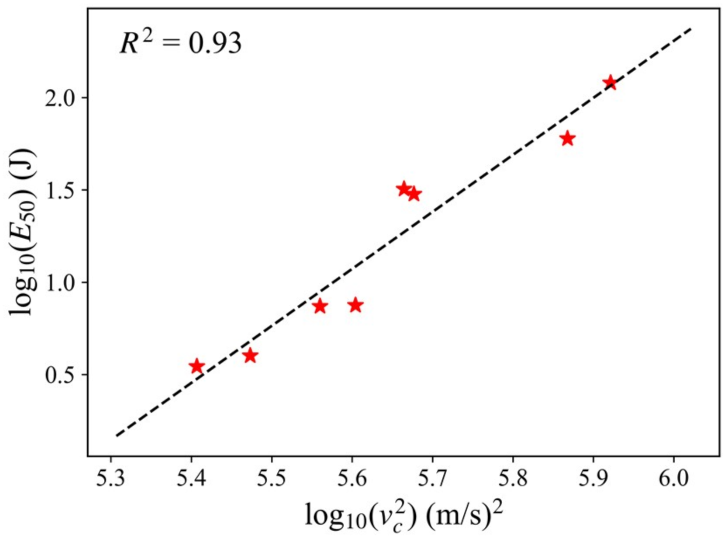

Figure S17 Correlation between simulation-derived critical impact velocity determined by 10% decomposition ratio and experimental impact sensitivity of EMs.

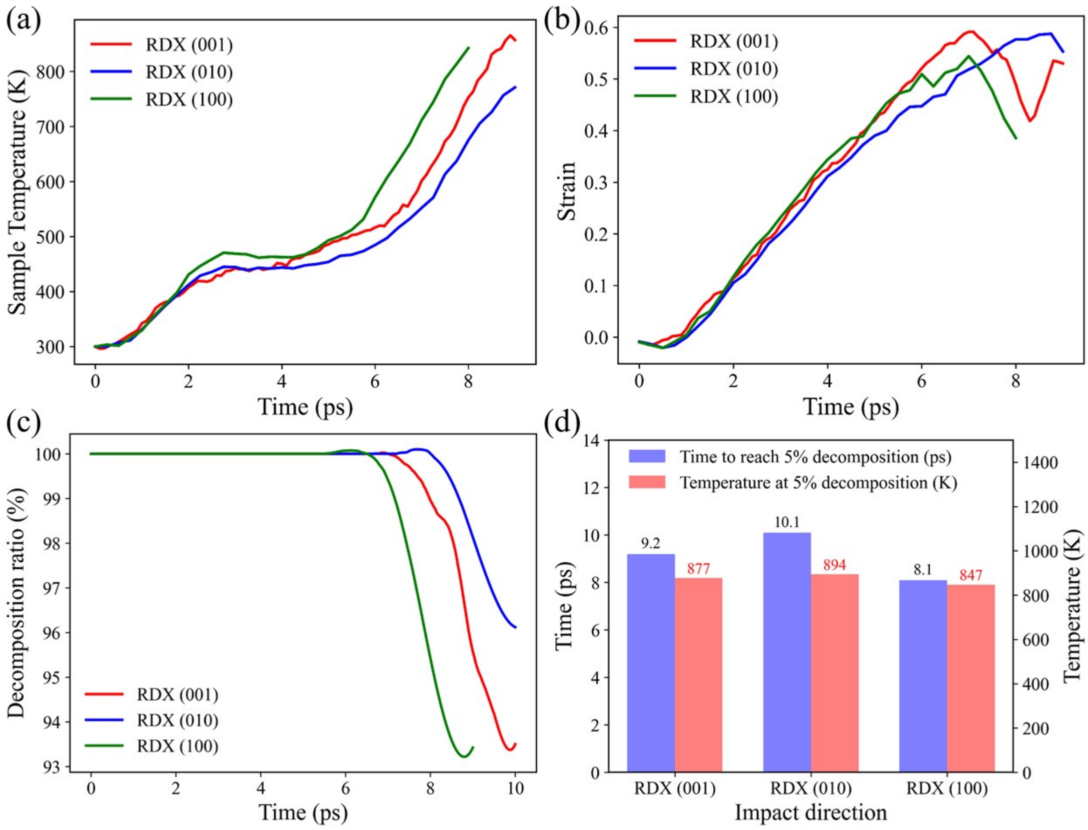

Figure S18 Orientation dependence of RDX under an impact velocity of 600 m s^{-1}. Evolution of (a) Sample temperature, (b) strain, (c) decomposition ratio, and (d) the time and temperature corresponding to a decomposition ratio of 5% for the (001), (010), and (100) surfaces.

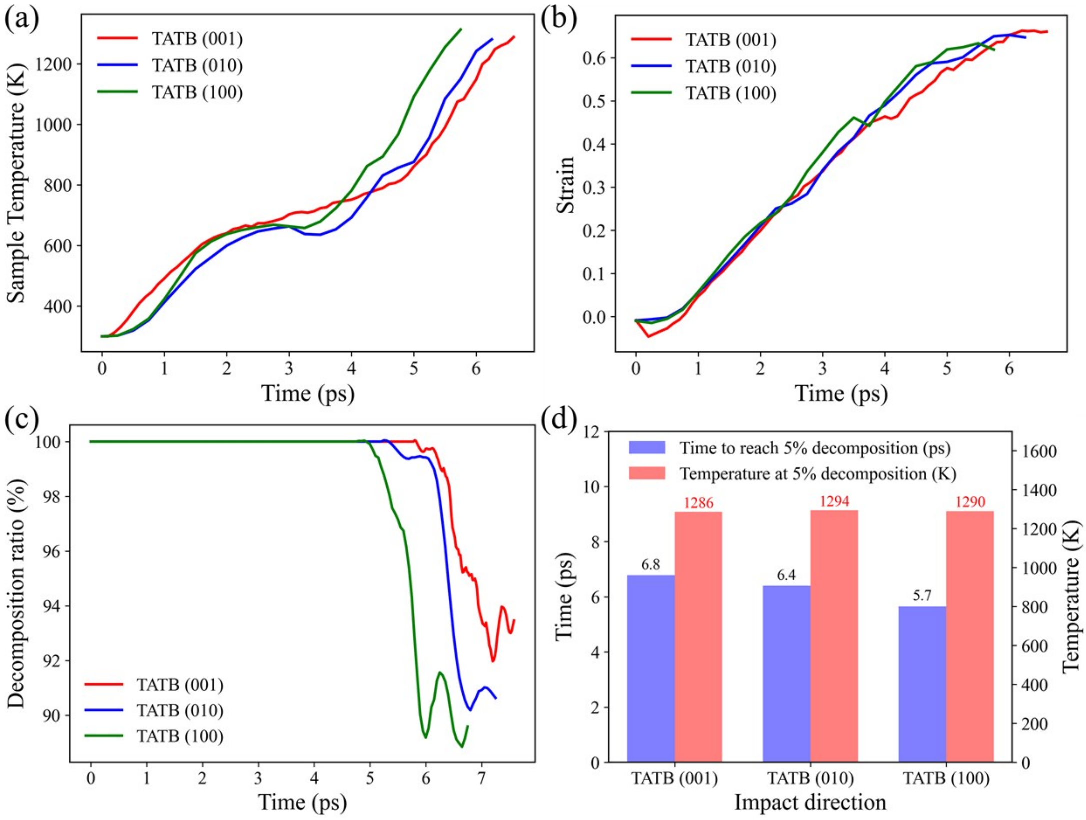

Figure S19 Orientation dependence of TATB under an impact velocity of 900 m s^{-1}. Evolution of (a) Sample temperature, (b) strain, (c) decomposition ratio, and (d) the time and temperature corresponding to a decomposition ratio of 5% for the (001), (010), and (100) surfaces.