

Supplementary Information

Hot Spot Formation and Initial Chemical Reaction of PETN Containing Nanoscale Spherical Void Under Highly Shocked Loading

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S1. The method of subtracting the center-of-mass velocity.

The local velocity $\langle u \rangle_i$ is defined in terms of its own center-of-mass velocity and those of its neighbor molecules velocities u_j , and is given by:

$$\langle u \rangle_i = \frac{\sum_j w(r_{ij})u_j}{\sum_j w(r_{ij})}$$

The local intermolecular temperature T_i is given by:

$$\frac{3}{2}k\langle T \rangle_i^{inter} = \frac{\frac{1}{2} \sum_j M_j w(r_{ij}) u_j |u_j - \langle u \rangle_i|^2}{\sum_j w(r_{ij})}$$

Where k is Boltzmann's constant, M_j is the total mass of the molecule.

The intermolecular temperature is given by:

$$\frac{3}{2}N_i^{at}kT_i^{inter} = \frac{1}{2} \sum_{j=1}^{N_i^{at}} m_j (u_j - u_i^{cm})^2$$

Where N_i^{at} is the number of degrees of freedom, u_j is the velocity of atom j , u_i^{cm} is the center of mass velocity.

S2.

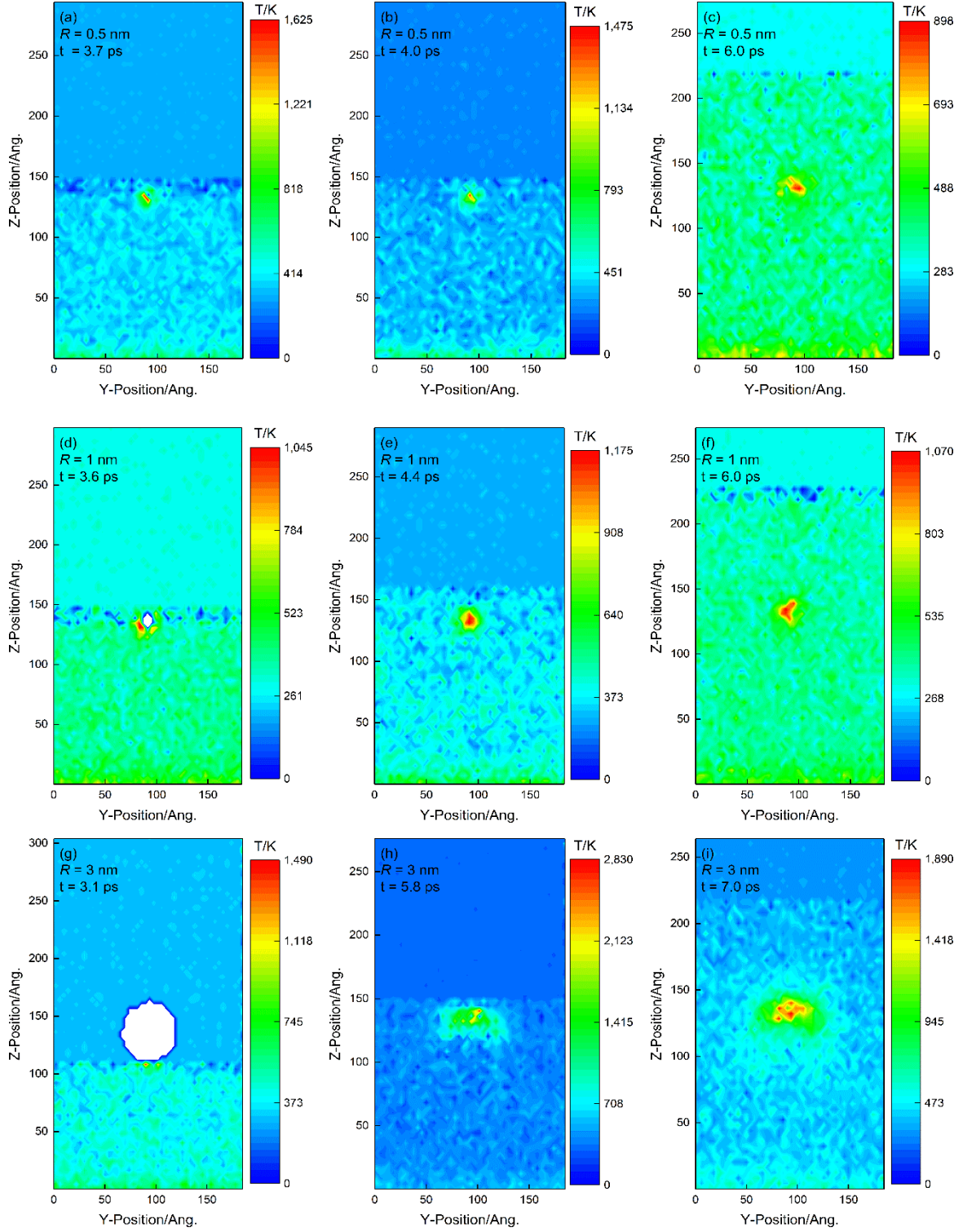


Fig. S1. The spatial-temporal temperature distribution of the void collapse for the case of U_p

$= 1 \text{ km} \cdot \text{s}^{-1}$. (a), (b), (c) correspond to the cavity radius $R = 0.5 \text{ nm}$; (d), (e), (f) correspond to the cavity radius $R = 1 \text{ nm}$; (g), (h), (i) correspond to the cavity radius $R = 3 \text{ nm}$.

S3.

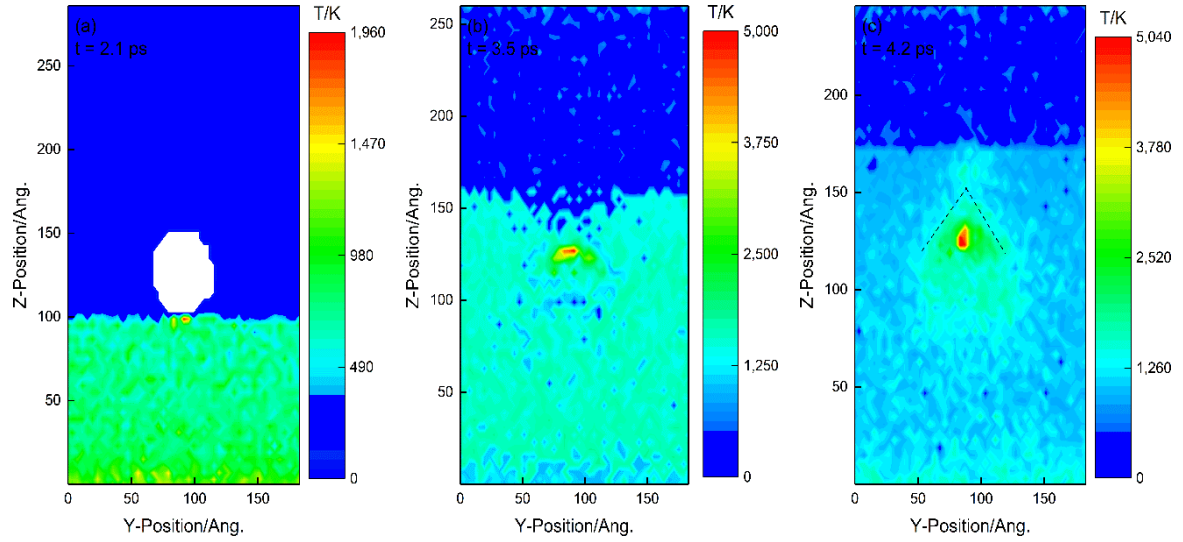


Fig. S2. The spatial-temporal temperature distribution of the hot spot formation process for the case of $U_p = 1 \text{ km} \cdot \text{s}^{-1}$, $R = 3 \text{ nm}$.

S4.

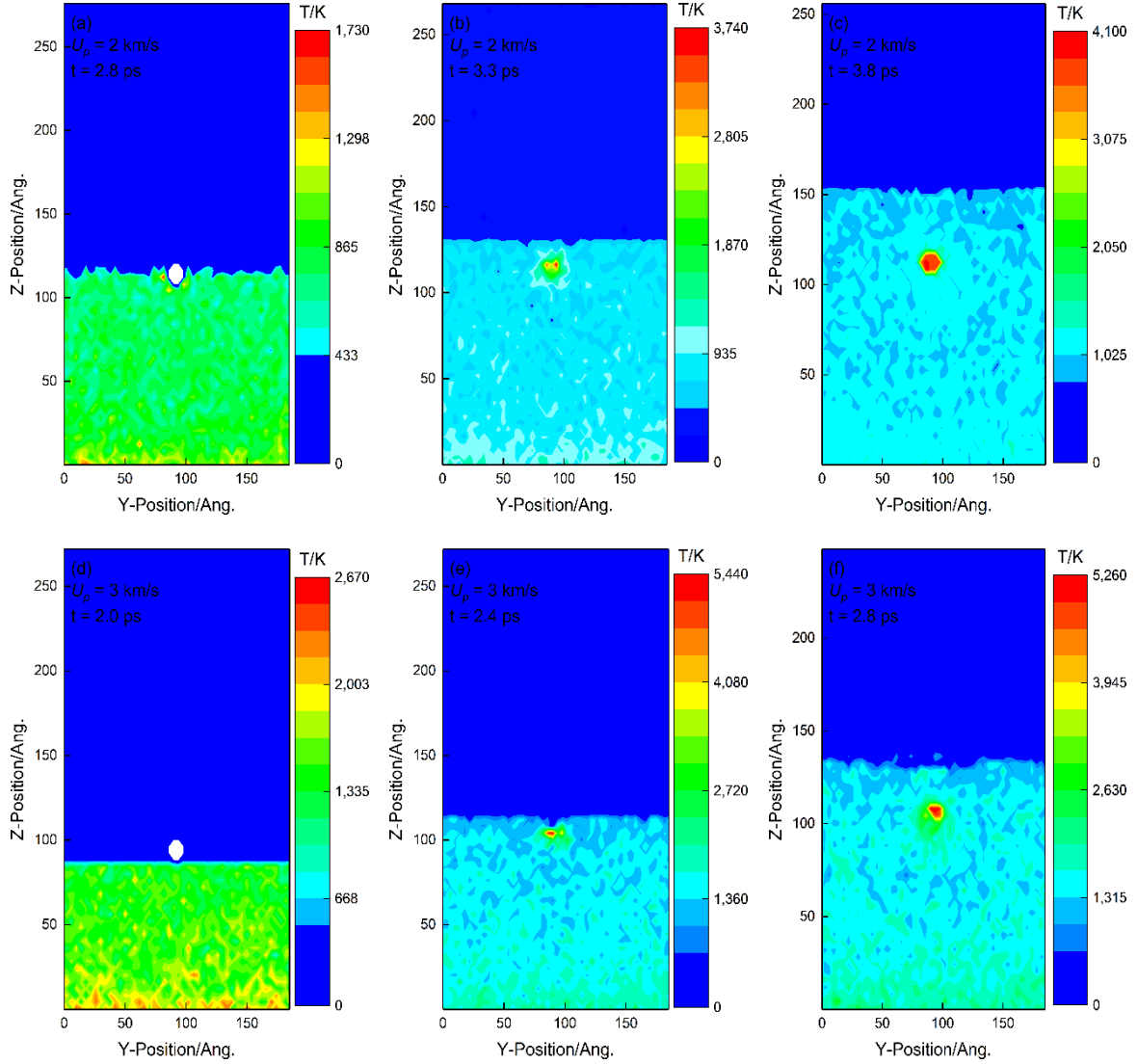


Fig. S3. Hot spot formation process for PETN system with cavity radius $R = 1 \text{ nm}$ at $U_p = 2 \text{ km}\cdot\text{s}^{-1}$, $U_p = 3 \text{ km}\cdot\text{s}^{-1}$. (a), (b), (c) correspond to $U_p = 2 \text{ km}\cdot\text{s}^{-1}$; (d), (e), (f) correspond to $U_p = 3 \text{ km}\cdot\text{s}^{-1}$.