Supplementary material

The unusual effect of paraffin wax on thermal decomposition of cyclotetramethylenetetranitramine

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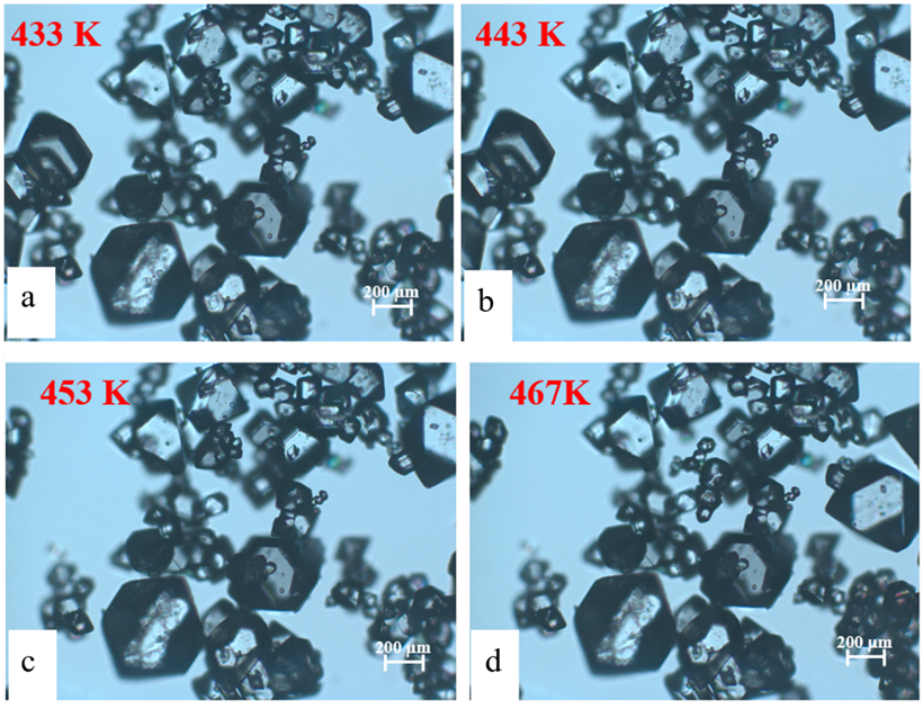

Fig. S1 Micrographs of HMX taken with an *in situ* optical microscope

The surface energy of PW and HMX

A ZL-2 automatic tensiometer was used to measure the surface tension of PW. The standard test solution contained water and glycerol. The surface energy, including the polarity and dispersion components, was calculated using geometric equations and the Owen-Kaelble-Chan equation.

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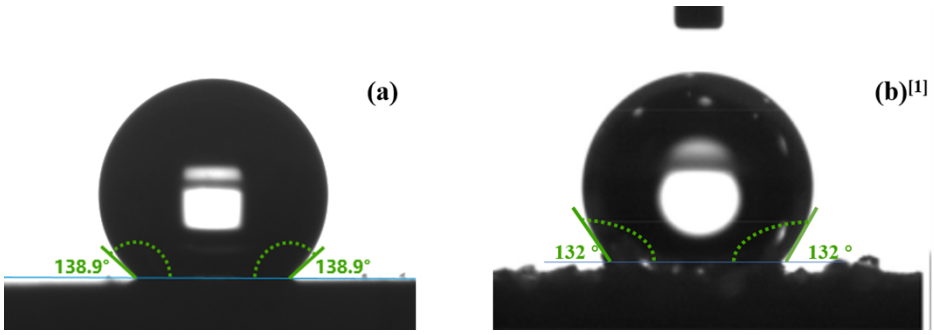

Fig. S2 Contact angles of (a) PW and (b) [1]HMX measured with water (HMX contact angle was cited from the literature)

Table S1 The surface energy of PW and HMX

Sample	Surface energy (mN/m)		
	γ^p	γ^d	γ
HMX	6.67	44.63	51.30
PW	0.16	0.39	6.55

Note: γ^p and γ^d represent the polarity and dispersion components, respectively, while γ represents surface energy.

Table S2 Decomposition parameters of HMX and PW/HMX

Sample	T_0 (K)	T_i (K)	P_i (MPa)	dP/dt_{max} (MPa min^{-1})	P_{max} (MPa)
HMX	449.7	511.5	0.15	2.54	2.17
PW/HMX	484.8	510.5	0.19	0.95	1.21

Note: T_0 is the initial decomposition temperature, T_i is the temperature at ignition, P_i is the pressure at ignition, P_{max} is the maximum pressure, and dP/dt_{max} is the maximum pressure growth rate.

Dynamic simulations

The ARC data model dynamics analysis was based on three assumptions.

The first assumption was made for the model-based method: (i) the reaction consists of several

elementary reaction steps; (ii) the reaction rate of each step can be described by a kinetic equation depending on the concentration of the initial reactant (e_j), the concentration of the product (p_j), the pre-exponential factor (A_j) and the activation energy (E_j) which is specific only for this step. The equation is the following:

$$ReactionRate_j = -A_J f_j(e_j, P_j) exp\left(-\frac{E_i}{RT}\right) \quad (1)$$

Each step has its own reaction type described by the function $f_j(e_j, P_j)$.

The second assumption was made for the model-based analysis: (i) the kinetic parameters are constant during the reaction for every step, including the activation energy, the pre-exponential factor, and the order of reaction; (ii) the reaction type is constant during the reaction.

The third assumption was also made for the model-based analysis: (i) the total thermoanalytical signal is the sum of the signals of each reaction step; (ii) the signal of each step is calculated as the reaction rate multiplied by the total effect of a given step (e.g., the total enthalpy change or total mass loss).

Data fitting can be carried out by the Kinetics NEO software.

The kinetic parameters of HMX and PW/HMX were fitted according to Eq. 1, as shown in the following figure:

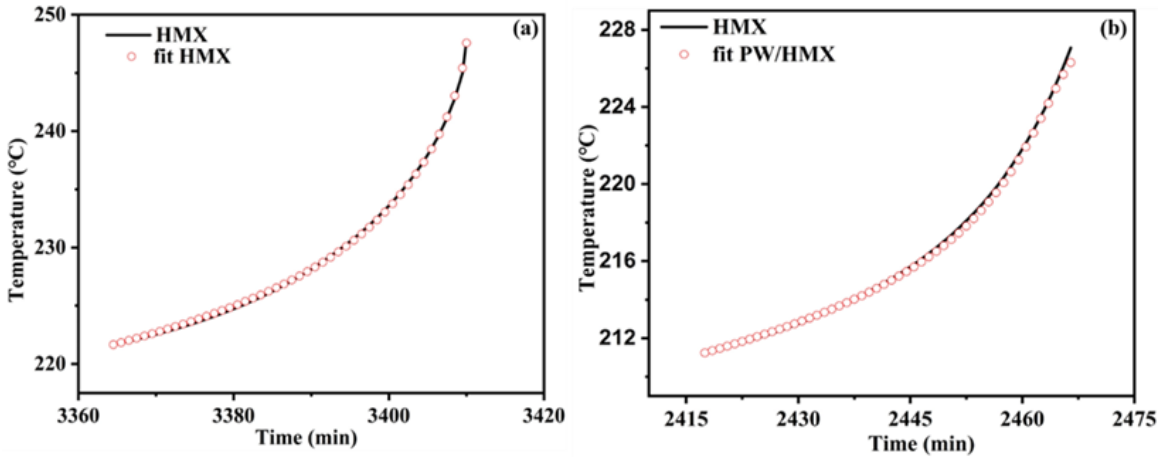

Fig. S3 The reconstructed adiabatic decomposition curves based on kinetic parameters for (a) HMX

and (b) PW/HMX.

Reference

[1] T. Liu, C. Geng, B. Zheng, S. Li, Encapsulation of cyclotetramethylenetetranitramine (hmx) by electrostatically self-assembled graphene oxide for desensitization, Propell. Explos. Pyrot. 42 (9) (2017) 1057-1065.