Twin Induced Sensitivity Enhancement of HMX versus Shock: A Molecular Reactive Force Field Simulation

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S1 Modeling

(a)

\( u=13.51 \ \text{Å}, \ v=11.05 \ \text{Å}, \ \theta = 90^\circ \)

(b)

thickness is 20 times of the lattice fractional \( u=13.51 \ \text{Å}, \ v=11.05 \ \text{Å}, \)

\[ a=13.51 \ \text{Å}, \ b=11.05 \ \text{Å}, \ c=69.53 \ \text{Å}, \ \alpha = \beta = \gamma = 90^\circ \]

(c)

\[ a=13.51 \ \text{Å}, \ b=11.05 \ \text{Å}, \ c=69.53 \ \text{Å}, \ \alpha = \beta = \gamma = 90^\circ \]

(d)

\[ a=13.51 \ \text{Å}, \ b=11.05 \ \text{Å}, \ c=139.06 \ \text{Å}, \ \alpha = \beta = \gamma = 90^\circ \]

(e)

\[ a=13.51 \ \text{Å}, \ b=11.05 \ \text{Å}, \ c=139.06 \ \text{Å}, \ \alpha = \beta = \gamma = 90^\circ \]

(f)

\[ a=27.05 \ \text{Å}, \ b=22.10 \ \text{Å}, \ c=139.06 \ \text{Å}, \ \alpha = \beta = \gamma = 90^\circ \]

Figure s1. Modeling for twinned HMX. (a) Slice HMX crystal along its (101) face, (b) a slice with 20 times of thickness of unit fractional, (c) a cell established in terms of (b), (d) the mirror of (c), (e) a twinned HMX built by combining (c) and (d), and (f) is a super cell of (e).

(a) twinned HMX  (b) non-twinned HMX

Figure s2. Optical imagines of HMX crystals adopted from ref 1.
The model of TH was built (Figure s1) in terms of the experimental observation of the most common “cross” twins usually growing in the (101) face of β-HMX crystals (Figure s2). We sliced a β-HMX crystal along its (101) face (Figure s1(a)) to get the twinning interface. Next, a slice with 20 times of thickness of unit fractional (Figure s1(b)) was obtained. We established a cell according to the slice (Figure s1(c)) and its mirror (Figure s1(d)), and combined them to a cell with twinning interface along (001) face (Figure s1(e)). Enlarging the cell by increasing it’s a and b axes once, a super cell of the TH containing 320 HMX molecules, namely 8960 atoms, was gotten for following simulations.

S2 Validation of ReaxFF_lg to this work

ReaxFF is a first-principles-based force field, and the bond strength and bond length calculated by ReaxFF can adjust appropriately in response to variations of the local chemical environment. The bond cleavage and formation can be accurately described during the chemical reactions. ReaxFF_lg is an improved version which is extended by the term of London dispersion using low gradient model to improve the description of large distances interaction between molecules, leading to an excellent agreement between equilibrium crystals volumes and experiment.

The validity of ReaxFF_lg has also been reexamined in this work. 10ps NPT simulations at 300K and atmospheric pressure using ReaxFF_lg were implemented to obtain the initial configurations of PH or TH. Upon the initial configurations, 20ps NVT (300K-2500K) and 50ps shock wave compression simulations were conducted, respectively. The results of NPT simulations showed that both the lattice parameters of PH and TH reduce about 1.2 % on average, namely there is only a 3.5 % volume or density error compared with the experimental values, indicating that ReaxFF_lg can appropriately describe the physical processes of HMX. The initial and final chemical species of our thermal and shock compression simulations and the Hugoniot curve derived
from our shock compression simulations also confirmed that ReaxFF_lg can also appropriately
describe the physical and chemical behaviors of HMX under high temperatures and strong shock
wave compression.

S3 Snapshots of typical Molecular clusters formed at the primary stage against shock

Figure s3. Formation of typical molecular clusters in the earlier stage after shock loading for 7-10
km/s.

Reference