Atomistic simulation of detonation initiation by ultra-short impact

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Abstract. We present results of the classical molecular dynamics simulation of detonation initiation in simple AB model of a high explosive compressed by ultra-short shock wave (SW). The simplified reactive empirical bond order potential (REBO) defines interatomic forces in the AB model explosive made up of diatomic AB molecules. Simulation of ultra-short piston-driven compression of AB explosive with duration of picoseconds represents an indirect initiation via a thin metal foil irradiated by a femtosecond laser pulse. We studied transition of SW to a detonation wave (DW), including evolution of calculated pressure profile in a sample. A run distance to detonation of such AB explosive film, which is required for detonation initiation, was obtained. Variation of loading time and piston velocity gives a 2D region of transition from SW to DW. The influence of pores on detonation initiation threshold is discussed.

1. Introduction

Nowadays an available femtosecond laser intensity is sufficient for generation of an ultra-short shock wave (SW) in metals with a peak pressure up to hundreds of gigapascals. Concurrent progress of high-precision laser diagnostics in the visible and X-ray ranges with picoseconds-time and nanometer-size precisions [1–3] makes possible the experimental research of the condensed matter response to such the ultra-short compression/unloading. On the other hand a study of wave evolution in thin films in micrometer scale can be simulated directly with molecular dynamics (MD) method, which gives us an opportunity to trace hundred-millions atoms motion in nanosecond time-scale simulations. Experimental studies of only non-reactive materials under action of ultra-short laser irradiation have been done so far [1–3]. MD simulation of ultra-short SW propagation was still performed in non-reactive materials [4].

Last two decades many MD simulations of detonation wave propagation were performed [5–12], since the first reactive interatomic potential was developed [13]. Formation of hotspot was found in MD simulations of explosives with pores, where a collapse of pores facilitates transition to detonation. [14–16] Here we report MD simulation results on detonation initiation by ultra-short loading of a simple AB model of explosive, and an effect of pore on the threshold impact parameters of detonation initiation.

2. Simulation results

Interatomic forces and chemical reactions in the explosive are represented by AB model [5,12] using a simplified REBO potential [12]. The binding energy of N atoms in original AB model is...
time is 67 ps. Free bounds of the sample in \( x \)-direction are spaced at 25 nm from MD box boundaries, where absorption boundary conditions are employed. In transverse \( y \)- and \( z \)-directions the sample has dimensions \( L_y = 50 \text{ nm} \) and \( L_z = 8 \text{ nm} \), respectively, with imposed periodic boundary conditions.

2.2. Planar detonation initiation

Analysis of evolution of calculated pressure profile in a sample gives a run distance to detonation front formation, if a transition time from a ultra-short shock wave (SW) with velocity \( u_s \) to a detonation wave (DW) is less than a propagation time \( L_x/u_s \). Because the shock velocity \( u_s = 5.9 \text{ km/s} \) in AB material for the piston velocity \( u_p = 2.85 \text{ km/s} \), the maximal propagation time is 67 ps. Free bounds of the sample in \( x \)-direction are spaced at 25 nm from MD box boundaries, where absorption boundary conditions are employed. In transverse \( y \)- and \( z \)-directions the sample has dimensions \( L_y = 50 \text{ nm} \) and \( L_z = 8 \text{ nm} \), respectively, with imposed periodic boundary conditions.

The sample’s size \( L_x = 400 \text{ nm} \) along direction of loading is enough for the detonation front formation, if a transition time from a ultra-short shock wave (SW) with velocity \( u_s \) to a detonation wave (DW) is less than a propagation time \( L_x/u_s \). Because the shock velocity \( u_s = 5.9 \text{ km/s} \) in AB material for the piston velocity \( u_p = 2.85 \text{ km/s} \), the maximal propagation time is 67 ps. Free bounds of the sample in \( x \)-direction are spaced at 25 nm from MD box boundaries, where absorption boundary conditions are employed. In transverse \( y \)- and \( z \)-directions the sample has dimensions \( L_y = 50 \text{ nm} \) and \( L_z = 8 \text{ nm} \), respectively, with imposed periodic boundary conditions.

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2.2. Planar detonation initiation

Analysis of evolution of calculated pressure profile in a sample gives a run distance to detonation of AB explosive film (Fig. 1), which is required for transition from SW to DW. Such transition happens at distance 50 nm from the left side of the sample when the loading piston was removed. Due to fast combustion on the left side of sample the pressure increases on rear-side of loading pulse profile, even though a rarefaction unloading wave starts there. The pressure bump moves faster than the leading front of the loading pulse. The bump becomes steeper and reaches the leading front resulting in large increase of pressure up to 40 GPa, which is high enough to ignite AB material almost immediately at the leading front.

The transition time takes 8.4 ps after impact. The maximal achieved pressure in von Neumann (vN) peak is 57 GPa, which is about twice higher than the pressure of 23 GPa in the loading pulse. With further propagation of formed DW the peak pressure decreases gradually toward a value of 40 GPa corresponding to the vN peak in self-supported CJ detonation wave. The time required to achieve the CJ regime is about 10 ps after detonation initiation.
Figure 1. Evolution of profiles at SW-to-DW transition. Detonation in AB explosive was initiated by a piston with velocity $v_p = 2.85$ km/s with loading time $t_p = 4$ ps. The initiated DW shown by a red-colored profile first has a too high von Neumann pressure peak, which then decreases gradually toward a value corresponding to the self-supported CJ detonation wave. The run distance to detonation of explosive film indicated by the pressure maximum in red-colored profiles approximately 50 nm for given loading conditions.

Figure 2. Detonation initiation propagation/failure curve [17] of piston loading parameters gives 2D regions in plane $(t_p, v_p)$ on the left figure (a) and plane $(t_p, E_p)$ on the right figure (b). To determinate transition from SW to DW in “gray zone” additional calculations are needed. Black dash-and-dot lines represent an estimate of maximal piston velocity $v_{p0} \approx 2.77$ km/s, for which detonation cannot be generated by ultra-short pulse loading during several picoseconds. For comparison the red dotted lines represent isobars $P \approx 27.9$ GPa for a piston velocity $v_p = 3.5$ km/s, calculated for unburned AB material under compression.

Determination of the loading piston parameters, when SW is able to turn into DW, requires series of simulations with different pairs of impact parameters $(v_p, t_p)$ using scenario described in previous subsection. As a result we got 2D region of impact parameters $(v_p, t_p)$, which are shown on the Fig. 2a. The point $(P, V)$ on Hugoniot corresponding to picoseconds initiation of combustion for a given AB explosive makes it possible to estimate the highest speed of piston $v_{p0}$ for which detonation cannot be generated by ultra-short pulse loading. From data [12] we obtain an estimate of piston speed of $v_{p0} \approx 2.77$ km/s, which is in agreement with our simulation results. To determine input energies a full energy increase per loading were calculated (shown on the Fig. 2b). On the other hand an input energy calculated in unburned AB material compressed to constant $P \approx 27.9$ GPa by a piston with velocity $v_p = 3.5$ km/s displays an excess of input energy over the minimal energy required for the shock-to-detonation transition.
Figure 3. Pairs of maps with the pressure $P$ and potential energy $E_{pot}$ of atoms averaged in 2D mesh with about $\approx 120$ atoms/pixel. The coupled $P - E_{pot}$ snapshots in the $xy$–plane of SW propagation are shown for times increasing from the left to the right. Local high pressure distributions regions in the sample at moment $t = 7.8$ ps are resulted from a composition of the loading shock pulse and an expanding SW formed from a pore’s collapse. Directions of SW propagation are shown by blue arrows on the second pair of snapshots. Arrows on the third pair show directions of the most intensive products formation at the moment $t = 10$ ps. There are approximately equal angles between two SWs and the loading SW propagation direction, which are together initiating a transition to detonation. Parameters of the presented simulation: $d = 30$ nm, pore’s radius $r = 5$ nm, $t_p = 4$ ps, $v_p = 2.8$ km/s.

2.3. Pore effect
Several MD simulation studies of effect cylindrical [16], spherical [15] or rectangle [18] pores (voids) in sustained shock-induced detonation showed that a nanometer-scale pore is able to influence on the detonation initiation threshold in explosives. We placed a single nanometer-scale cylindrical pore with radius $r$, which was included into the sample at tens nanometers distance $d$ from the free boundary of sample. We see a qualitative effect of the pore on the detonation initiation threshold by the ultra-short loading. The velocity threshold for transition to detonation decreases for fixed loading duration of $t_p = 4$ ps. In such a case the initiation of self-sustained detonation occurred for the piston velocities in the range $v_p: 2.75 – 2.78$ km/s, while for perfect crystal it was $v_p: 2.8 – 2.82$ km/s. We think that the found decrease of detonation threshold results from the composition of initial shock and an additional expanding SW generated from the pore’s collapse. Such wave composition produces high-pressure areas localized in places where two shock wave combines as shown in Fig.3.

3. Summary and conclusions
Large-scale MD simulation of detonation initiation in an unbounded thin film of condense-phase model explosive by ultra-short piston loadings is performed. Removing of piston from model in the end of impact makes sample’s boundary free, which leads to generation of an unloading wave, similar to what happens after irradiation of metal film by a femtosecond laser pulse.

Variation of piston velocity and loading time gives a 2D region of $(t_p, v_p)$ parameters where transition of SW to detonation wave is observed, $(t_p, E_p)$ initiation parameters corresponded to $(t_p, v_p)$ give a minimal energy required for detonation, if the piston has a constant velocity during loading. Analysis of thermodynamic and chemical profiles evolution is performed. We marked out characteristics of the transition from SW to DW: run distance to detonation (by maximum of pressure amplitude) of such AB explosive film, which is required for transition from SW to detonation wave for given loading, time to transition from SW to DW; reaction zone length in the formed detonation wave; maximal achieved pressure in vN peak.
We studied a qualitative influence of a cylindrical pore on detonation initiation by variation of the cylinder radius and the distance from the cylinder centre to the free surface of sample. Placement of the pore close enough ($d = 30$ nm) to the loading entry plane (free surface of sample) facilitated transition from ultra-short SW to DW as compared with initiation in a perfect crystal of AB explosive.

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