Mesoscopic simulation of laser initiation in pentaerythritol tetranitrate

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Abstract. A numerical simulation of laser initiation in a pentaerythritol tetranitrate is presented. A contact smoothed particle hydrodynamics modeling with an explicit simplified-geometry of the microstructure is defined. A sequence of spheres in simple cubic and face-centred cubic lattices is considered. Different types of PETN crystal particles compression by high-enthalpy products expansion are simulated in the hydrodynamic approach. The compactification of spheres and formation of a shock wave in a porous material is observed. Compactification of spherical particles stops the flow of hot products and shock wave is able to override the reaction front propagation. The simulation demonstrates a shock-driven mechanism in the detonation initiation processes.

1. Introduction
The use of a laser to initiate high explosives is a promising direction for the development of safety during blasting operations. A pentaerythritol tetranitrate (PETN) with different values of dispersion and porosity is used in most of the experimental studies. So in [1] it was shown that a neodymium laser with a wavelength of 1.06 \mu m and a duration of several nanoseconds was able to initiate a porous heating element, but even at the maximum energy value, issued by the installation, it was not possible to set fire to explosives with an open surface. It leads to the fact that for further understanding of what occurs when initiating combustion and detonation of explosives, as well as improvements in laser systems, it is necessary to simulate at the microscopic level.

2. Simulation techniques
A porosity of PETN is described with a pressed material equation of state and explicit simplified geometry of micrometer size spheres [2]. A sequence of spheres forms a primitive cubic cell (pcc) or face-centered cubic cell (fcc) lattices. Lattices fcc and pcc are shown in figure 1 and 3. A two-phase Jones-Wilkins-Lee equation of state [3,4] describes a pressed pentaerythritol tetranitrate (PETN) in the simulation. The equation-of-state uses temperature and pressure equilibrium of reactants and products conditions for partially decomposed material description. The simulation is conducted with a contact smoothed particle hydrodynamics (SPH) parallel code [5,6]. This method is natural for microstructure definition and tracking SPH particles in a complex geometry of a couple of shock and reaction front.
Deflagration wave propagation simulation is defined with the reaction diffusion artificial model [7]. This model is applied in the simulation of turbulent flames in supernovae. The model is applicable in cases of several orders lesser width of reaction zone than deflagration propagation length.

This model is used for inferring a hydrodynamics propagation velocity, which is defined by the adjustable diffusion coefficient and reaction rate depends on the size of SPH particles (or cell size).

The diffusion of mass fraction of products added to the SPH code and correspondent decomposition rate is defined. This model creates the front with a width of the given number of SPH particles. The model is founded on the reaction-diffusion equation for reactants mass fraction. The reaction rate is a step-like function, and the diffusion coefficient has a fixed value for given velocity and particle size. In that case, an analytical solution of constant velocity propagation exists. The value of diffusion coefficient $C$ and decomposition rate $k$ are calculated from the analytical solution in [7]

$$k = D_l \beta \Delta r \sqrt{\lambda_0}; \quad C = D_l \sqrt{\rho_0} \ l (\beta \Delta r),$$

where $D_l$ - a normal flame speed, $\Delta r$ - the size of SPH particle. Other parameters are free to be prescribed and define the width and form of the reaction front. In the simulation $\lambda_0=0.1$ is a mass fraction at which decomposition rate switches on. The parameter $\beta = 4$ increase leads to the wider reaction zone. In the SPH method, to save symmetry of mass fraction diffusion between SPH particles with indexes $i$ and $j$, an average size of particles couple is used $\Delta r = 0.5 (D_i + D_j)$ in (1), where $D_i, D_j$ are sizes of SPH particles. The mass fraction flow from particle $i$ to $j$ is approximated in finite differences by

$$\frac{d \lambda_i}{dt} = \sum_j \frac{m_j W^j}{\rho_i \rho_j h} \frac{\lambda_j - \lambda_i}{|\vec{r}_j - \vec{r}_i|},$$

\[ (2) \]
where \( m_j \) is a mass of particle \( j \), \( \rho_i, \rho_j \) are correspondent densities, \( \vec{r}_i, \vec{r}_j \) are radius-vectors, \( \lambda_i, \lambda_j \) are mass fractions of products, \( h \) is a smoothing length and \( W'_{ij} \) is a gradient of smoothing kernel from particle \( i \) to \( j \). The velocity of a normal flame speed is assumed to be fitted to the given dependence of reaction propagation front of combustion in PETN at high pressures [8]. The observed front propagation velocity is fitted to the equation \( D_l [\text{ms}^{-1}] = 50 P^{0.5465} [\text{GPa}] \). In the simulation, a pressure-dependent value of \( D_l \) is used in the reaction-diffusion model for qualitative characterization of deflagration propagation velocity dependence on pressure.

3. Simulation results and discussion
Consider a system consisting of several layers of spherical explosive crystals of the same size, located in the fcc and pcc lattice sites. On the left border, there is a fully reacted heating element with ambient density for the equation of state of reactants [4]. A rigid wall boundary condition is imposed on the left side of the computational box. On the opposite side, there is a vacuum boundary condition. On all other boundaries periodic boundary conditions are imposed. The computational box is a rectangular domain with transversal sizes of 10·10 (2/\( \sqrt{3} \)) \( \mu \text{m} \). There are eight periods in the [111] of fcc lattice direction. The direction of the lattice replication is collinear to the shock wave propagation direction. Each sphere has a 2.3 \( \mu \text{m} \) radius. In figure 2, there are density, pressure, and reactants mass fraction in a non-reactive and reactive material simulation. Distributions are shown for the moment of time \( t=14.71 \) ns.

![Figure 2](image_url)

**Figure 2.** A distribution of pressure, density and mass fraction of products in a close-packed system of spheres, where shock wave produced by products. In the left part of figure a non-reacting simulation is shown, while reactive case is shown on the right.

A simple cubic pack of PETN spheres in contact with two neighbouring is shown in figure 3. A sequence of 44 spheres is a set where spheres have a radius of 5 \( \mu \text{m} \) each.

Initially, products are defined as a rectangular sample on the left from these spheres with a length of 100 \( \mu \text{m} \) in the direction of shock propagation. Expansion of products leads to the compactification of spheres and develops a shock wave in a pressed material. Reactions are observed as products inflow to the packed sequence of spheres. Shock propagates similarly in both simulations for fcc packing with the difference of shock amplitude increase in the reactive PETN. The diffusive mechanism of reaction seed in the model [7] leads to the shock wave which propagates independently.
In the simulation with pcc packing of spheres, products pass ahead of the shock front. The reactions start in front of shock, therefore reactive, and shock waves are bonded. The structure of this wave has a complex geometry and involves several balls behind the leading front, where decomposition of the explosive material is observed.

**Figure 3.** Distribution of pressure, density and mass fraction of products in simulation of PETN spheres which are packed in primitive cubic cell (pcc). Initially, the shock wave is induced by pressure in products on the left part of the computational domain (the figure shows only products near the contact with PETN). The reactive front and the shock front are bonded and pressure increases with time due to the decomposition processes.

4. Conclusions

Expanding explosive products begin to compact the first layers of explosive crystals, which prevent further penetration of the products and cause a chemical reactions in deeper layers. The diffusion burning model allows maintaining a burning front. As time goes by, more and more explosive crystals form an impenetrable “plug,” which indicates a short zone of convective combustion [9].

According to the results of the calculation, it is clear that the explosive compaction wave moves forward leaving behind the combustion front which corresponds to the existing ideas about wave formation detonation in solid explosives on the shock front [10].

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