Simulation of melting and vaporization of metals at hypervelocity impact

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Abstract. Simulations of experiments on shock-induced melting, fragmentation and vaporization in aluminum and zinc targets are presented. A titanium impactor moves at a velocity of 10.4 km/s and causes melting of these materials in a shock wave. Under rarefaction thermodynamic path crosses the liquid–vapor coexistence boundary and enters into metastable liquid region. Liquid in a metastable state may undergo either liquid–vapor phase separation or mechanical fragmentation. Homogeneous nucleation theory and mechanical fragmentation criterion of Grady are taken into account to control the kinetics of these processes in our model. The first effect dominates in the vicinity of the critical point, the second one — at lower temperatures. Analysis of phase transitions and kinetics of phase separation is performed using thermodynamically complete equation of state with allowance for stable and metastable regions for all materials under consideration.

1. Introduction
The dynamics of impact loading depends basically on material properties and impact velocity. Effects of shock-induced melting in metals come into play at impact velocities of the order of 6 km/s. Partial or full vaporization is possible at higher speeds and thus higher shock-wave pressures. These phenomena were studied experimentally and theoretically in [1-4].

2. Method
Numerical analysis is performed based on a multi-material high-order Godunov method in a purely Eulerian form [5,6]. This approach for modeling of strong shock waves in problems involving multiple condensed phases was proposed in [5]. Multiple phases are modeled by constructing an effective single phase in which the density, specific energy, and elastic properties are given by self-consistent averages of the individual phase properties [5]. For the interface reconstruction procedure, which is an essential step in multi-material Eulerian hydrodynamics, a second-order volume-of-fluid method is used [7].

For completeness of the model we apply a semi-empirical multi-phase equation of state (EOS) accounting for melting and evaporation effects. The free energy is used as a thermodynamic potential and has a form \( F(\rho, T) = F_c(\rho) + F_a(\rho, T) + F_e(\rho, T) \), composed of three terms, which describe an elastic part of interaction at \( T = 0 \) K (\( F_c \)) as well as thermal contribution of atoms (\( F_a \)) and electrons (\( F_e \)). Here, \( \rho \) is the material density, \( T \) is temperature. Analytical form of \( F \) items has different expressions for the solid and liquid phases [8]. The tables of pressure and specific internal energy over...
a density-temperature mesh are calculated taking into account changes of these thermodynamic parameters during the solid-liquid, liquid-gas and solid-gas phase transitions and possible metastable states of matter at both positive and negative pressures [9].

The EOS used for aluminum, zinc and titanium satisfy experimental data on both room-temperature and shock-wave compressions, as well as on adiabatic expansion for a wide range of densities and temperatures including measured temperatures and phase transition heats at melting and evaporation points under normal pressure. Calculated parameters of the critical point (CP) of the liquid-gas phase transition are as follows: $P_{cr}=0.3988$ GPa, $T_{cr}=6.595$ kK, $\rho_{cr}=0.6979$ g/cm$^3$ for aluminum; $P_{cr}=0.3560$ GPa, $T_{cr}=3.261$ kK, $\rho_{cr}=2.342$ g/cm$^3$ for zinc; $P_{cr}=0.4775$ GPa, $T_{cr}=8.658$ kK, $\rho_{cr}=1.128$ g/cm$^3$ for titanium. They agree with earlier evaluations [10].

Analysis of isentropic expansion of highly compressed matter can be performed using the phase diagram of each substance under consideration. In figure 1 we demonstrate for aluminum several isentropes, which cross binodal at different densities.

It is known that physics involved into an expansion process depends on the position of material state on the phase diagram. When isentrope goes above CP the direct atomization occurs under rarefaction (see isentrope 1 in figure 1). The more complex situation takes place when the thermodynamic path crosses the liquid-vapor equilibrium curve (binodal) and penetrates into the metastable liquid region (see figure 1, isentropes 2-4). The lifetime of this metastable state is limited by increase of instabilities and the substance undergoes either phase explosion (explosive boiling) with the formation of a liquid-gas mixture or mechanical spallation (cavitation) into liquid droplets. It is known that the first effect is typically observed in the vicinity of CP, whereas the second one dominates in metastable liquid region at lower temperatures, where the energy is less or of the order of the evaporation threshold. In our model, when the liquid branch of the binodal curve is crossed and the matter transits to a metastable liquid state, we include a particular treatment for each of the following two competitive effects. First one (i) is the thermal decomposition; a criterion of the metastable liquid lifetime is used based on the theory of homogeneous nucleation [11,12]. Second effect (ii) is the process of mechanical fragmentation; a failure criterion of Grady is applied [13]. Both criteria are based upon the lifetime estimation of a metastable state and require the knowledge of the surface tension. The application of these criteria are described in [14], the necessary parameters for the surface tension dependence on temperature can be found in [15].

3. Results
A titanium flier of 0.9 mm thick travels at 10.4 km/s and interacts with Al target of 1.0 mm thick. These initial data correspond to parameters achieved in [4]. In figure 2 one can see the thermodynamic path of aluminum target layer (initially located in the middle section of the target) after the collision with the projectile. The fast compression in a shock wave (the time of shock propagation through the numerical cell is of $t \sim [10$ km/s]$^{-1} \times 10^{-7}$ mm$=1$ ns) results in melting, when the Hugoniot curve crosses the melting zone, see the segment $AB$ in figure 2. Then the shock wave moves through the target, reaches the free surface and reflects as a rarefaction wave. Melted and strongly compressed material of the target stays in this state until the leading fan of the rarefaction wave reaches this point. After that an adiabatic expansion starts and thermodynamic trajectory crosses the liquid branch of the binodal ($BC$ path in figure 2). From this moment the lifetime of metastable liquid is governed by the kinetics-based criteria described in [14]. It is seen that the mechanical fragmentation mechanism dominates for present thermodynamic path and after fragmentation (turning point $C$ in figure 2) the trajectory relaxes to the zero pressure ($CD$ path in figure 2). This interpretation is confirmed by experimental results [3], where the shock threshold for vaporization of Al was determined to be about $P \sim 230$ GPa. The shock-induced pressure (that at point $B$ in figure 2) in our simulation was observed to be around $P \sim 210$ GPa that is below the threshold value and thus we should not expect a noticeable vaporization of Al material in a rarefaction wave.
Figure 1. Phase diagram of aluminum. States: $g$ — gas, $l$ — liquid, $s$ — solid, $l+hg$ — liquid-gas mixture, $s+hg$ — solid-gas mixture, $s+hl$ — melting region, $(g)$ — metastable gas, $(l)$ — metastable liquid, $(s)$ — metastable solid, $(s+hl)$ — metastable solid-liquid mixture. Solid lines are the phase boundaries; the critical point (CP), liquid-gas binodal (bn) and spinodal (sp) are signed. Dash-dot lines correspond to isentropes 1-4 (1 — above the critical point, 2 — with thermal phase separation process, 3 and 4 — with mechanical fragmentation); arrows along the isentropes show the time direction under expansion. Dashed lines mean isobars of $P=-2$ and $-5$ GPa.

Figure 2. Thermodynamic path (dash-dot line) of the target (Al) during Ti-with-Al collision consisting of three parts: $AB$ — fast compression, $BC$ — material expansion under pressure release, $CD$ — relaxation after fragmentation. Arrows along the thermodynamic path show the time direction in the process. Solid lines correspond to the phase boundaries; the rest of notations are as in figure 1.

Figure 3. Thermodynamic path of the impactor (Ti) during collision of Ti with Al. Notation is analogous to figure 2.

Figure 4. Density distribution in Ti-Al simulation for different time delays after impact, $t=0$, 0.2, 0.5 and 1 $\mu$s.
We also plot the thermodynamic path on the phase diagram for the middle section of the impactor (figure 3). It is seen that adiabatic expansion of the projectile material ends with mechanical fragmentation (cavitation) of the material in metastable liquid phase (point $C$ in figure 3). Then material shrinks back until the pressure is zero (segment $CD$ in figure 3).

The fragmentation dynamics in Ti-Al interaction is shown in figure 4 for different time delays after collision. Already by the time of $t=0.2 \, \mu s$ both impactor and target materials are in the liquid state. Intensive tensile waves pass through the samples resulting in fragmentation (see the density profile at $t=0.5 \, \mu s$ in figure 4). Finally, the debris cloud expansion is accompanied by increasing of the gaps between the spalls (compare the profiles of $t=0.5$ and 1 $\mu s$ in figure 4). Such formation of the plate-like debris of aluminum target was previously observed in experiment [3].

The similar simulation with zinc targets 0.5 mm thick shows that Zn can be partially vaporized in hypervelocity impact with the same thickness and velocity of Ti impactor, 0.9 mm and 10.4 km/s correspondingly. Previous experimental studies on shock-induced vaporization of aluminum and zinc [2,4] demonstrate that the kinetics of vaporization is controlled by the ratio $E/E_v$, where $E$ is the specific internal energy in a material, $E_v$ is the specific energy of evaporation. It was found in [2] that full vaporization of zinc under rarefaction occurs at the shock pressure $P \approx 550$ GPa. These pressure values are not achieved in the present simulation. Nevertheless we observe that a formation of liquid-gas mixture upon release of zinc takes place at shock pressure $P \approx 316$ GPa.

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