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Simulation of shock-induced fragmentation and vaporization in metals

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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 the thermodynamic path crosses the liquid–vapor coexistence boundary and enters into a metastable liquid region. Liquid in a metastable state may undergo either liquid–vapor phase separation or mechanical fragmentation. Homogeneous nucleation theory and the 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 separations is performed using a thermodynamically complete equation of state with stable and metastable states for all materials under consideration.

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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 Refs. [1–10].

The purpose of this work is to investigate numerically the dynamics of isentropic expansion of metastable liquid and possible interplay of mechanical and thermal effects of material decomposition. An impact of titanium plate with a velocity of 10.4 km/s on aluminum and zinc targets is simulated. To describe media properties and phase transitions we use semi-empirical thermodynamically complete multi-phase equation of state (EOS) in a tabular form for all metals under consideration.

2. Method

2.1. Numerical model

Numerical analysis is performed based on a multi-material high-order Godunov method in a purely Eulerian form [11,12]. This approach for modeling of strong shock waves in problems involving multiple condensed phases was proposed in Ref. [11]. 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 [11]. For the interface reconstruction procedure, which is an essential step in multi-material Eulerian hydrodynamics, a second-order volume-of-fluid method is used [13].

2.2. Equation of state

For completeness of the model we apply a semi-empirical multiphase 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, ρ is the material density, T is the temperature. Analytical form of F items has different expressions for the solid and liquid phases [14]. 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 [15,16].

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: $P_{\rm cr} = 0.3988$ GPa, $T_{\rm cr} = 6.595$ kK, $\rho_{\rm cr} = 0.6978$ g/cm³ for aluminum; $P_{\rm cr} = 0.3560$ GPa, $T_{\rm cr} = 3.261$ kK, $\rho_{\rm cr} = 2.342$ g/cm³ for zinc; $P_{\rm cr} = 0.4775$ GPa, $T_{\rm cr} = 8.658$ kK, and $\rho_{\rm cr} = 1.128$ g/cm³ for titanium. They agree with earlier evaluations [17].

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2.3. Metastable liquid phase treatment

Analysis of isentropic expansion of highly compressed matter can be performed using the phase diagram of each substance under consideration. In Fig. 1 we demonstrate several isentropes in aluminum which cross binodal at different densities. It is known that the physics involved in an expansion process depends on the position of the material state in the phase diagram. When the isentrope goes above the CP the direct atomization occurs on rarefaction (see isentrope 1 in Fig. 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 Fig. 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 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 the CP, whereas the second one dominates in the metastable 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 into a metastable liquid state, we include a particular treatment for each of the following two competitive effects. The first (i) is the thermal decomposition; a criterion of the metastable liquid lifetime is used based on the theory of homogeneous nucleation [18,19]. The second effect (ii) is the process of mechanical fragmentation; a failure criterion of Grady is applied [20].

In the first case (i), we estimate the metastable liquid lifetime as

$$\tau_{\text{nucl}} = (CnV)^{-1} \times \exp(W/k_BT), \tag{1}$$

where $C = 10^{10} \text{ s}^{-1}$ is the kinetic coefficient [21], *n* is the concentration, *V* is the volume under consideration (the volume of a numerical cell in our case), $W = 16\pi\sigma^3/\Delta P^2$ is the work required on a formation of the critical-size gas bubble in the liquid phase, k_B is the Boltzmann constant, ΔP is the difference between the saturated vapor pressure at the same temperature, which are known from



Fig. 1. Phase diagram of Al. States: g - gas, l - liquid, s - solid, l+g - liquid-gas mixture, s + g - solid-gas mixture, s + l - melting region, (g) - metastable gas, (l) - metastable liquid, (s) - metastable solid, (s + l) - metastable solid-liquid mixture. Solid lines are the phase boundaries; the critical point (*CP*), liquid-gas binodal (*bn*), and spinodal (*sp*) are signed. Dot-dashed 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 <math>P = -2 and -5 GPa.

EOS, and the current pressure of substance. The temperature dependence of the surface tension σ is described in the form [18, 19]

$$\sigma = \sigma_0 (1 - T/T_{\rm cr})^{1.25}, \tag{2}$$

Where T_{cr} is the temperature in CP, and σ_0 is the surface tension at the melting temperature; $\sigma_0 = 860$, 767, and 1400 g/s² for aluminum, zinc, and titanium, respectively [22]. When the lifetime τ_{nucl} in the volume of interest *V* is expired, the metastable *one-phase* liquid separates into stable *two-phase* liquid–vapor mixture. This phase separation process is accompanied by abrupt changes of thermodynamic parameters such as pressure, temperature, sound speed, compressibility, heat capacity, etc. (point C_2 on isentrope 2 in Fig. 1). The EOS with metastable phase states is therefore no longer relevant in this volume, so that we continue to calculate the thermodynamic properties by using the EOS without metastable states.

To account for the second effect (ii), a fragmentation criterion of Grady [20] is used for the liquid phase with the spall strength and the time to fracture in the form

$$P_{\rm spal} = \left(6\sigma\dot{\varepsilon}\rho^2c^3\right)^{1/3},\tag{3}$$

$$\tau_{\rm spal} = \left(6\sigma/\rho\dot{\varepsilon}^2 c^3\right)^{1/3},\tag{4}$$

where $\dot{\epsilon}$ is the strain rate, and *c* is the sound speed. When the pressure of matter drops below the negative value $-P_{\rm spal}$, and the duration of this event is longer than the time $\tau_{\rm spal}$, a criterion of fragmentation is satisfied, and thus the confluence of the voids occurs and new free surfaces can appear in the material. To describe this phenomenon numerically we let a "destroyed" substance shrink back until the pressure comes to zero value (through the segments C_3B_3 and C_4B_4 of isentropes 3 and 4 in Fig. 1). The difference between old and new volumes we compensate by introducing a vacuum fraction into a numerical cell. Both thermal and mechanical criteria described above are used simultaneously and each of them can prevail in a given computational cell depending on the substance location on the phase diagram.

3. Results and discussion

3.1. Aluminum target

A titanium flier of 0.9 mm thickness travels at 10.4 km/s and interacts with an aluminum target of 1.0 mm thickness. These initial data correspond to parameters achieved in experiments of Chhabildas et al. [10]. In Fig. 2 one can see the thermodynamic path of the 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 given by $t \sim [10 \text{ km}/$ $s]^{-1} \times 10^{-2} \text{ mm} = 1 \text{ ns}$) results in melting, when the Hugoniot curve crosses the melting zone, see the segment AB in Fig. 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 the thermodynamic trajectory crosses the liquid branch of the binodal (BC path in Fig. 2). From this moment the lifetime of the metastable liquid is governed by the kinetics-based criteria described above. It is seen that the mechanical fragmentation mechanism dominates for the present thermodynamic path and after fragmentation (turning point C in Fig. 2) the trajectory relaxes to the zero pressure (CD path in Fig. 2). This interpretation is confirmed by experimental results

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Fig. 2. Thermodynamic path (dot-dashed 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. Dashed line is calculated principal Hugoniot of Al. Solid lines correspond to the phase boundaries; the rest of notations are the same as in Fig. 1.

[9], where the shock threshold for vaporization of aluminum was determined to be about $P \sim 230$ GPa. The shock-induced pressure (pressure at point *B* in Fig. 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.

We also plot the thermodynamic path on the phase diagram for the middle section of the impactor (Fig. 3). It is seen that adiabatic expansion of the projectile material ends by mechanical fragmentation (cavitation) of the material in a metastable liquid phase (point *C* in Fig. 3). The material then shrinks back until the pressure is zero (segment *CD* in Fig. 3).

The fragmentation dynamics in Ti–Al interaction is shown in Fig. 4 for different time delays after collision. Already by the time of



Fig. 3. Thermodynamic path of the impactor (Ti) during collision of Ti with Al. Notation is analogue to Fig. 2.



Fig. 4. Density distribution in Ti–Al simulation for different time delays after impact, $t = 0, 0.2, 0.5, and 1 \mu s$.

 $t = 0.2 \ \mu$ 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 Fig. 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 μ s in Fig. 4). Such formation of the plate-like debris of the aluminum target was previously observed in experiment [9].

3.2. Zinc target

For this simulation a titanium impactor of 0.9 mm thickness travels at 10.4 km/s and interacts with zinc target of 0.5 mm thickness. In Fig. 5 one can see the thermodynamic path of the zinc target after the collision with the projectile. The higher impedance of zinc with respect to aluminum is the reason why higher pressure (316 GPa) is achieved on compression in this experiment. Thus, on rarefaction, the thermodynamic trajectories cross the binodal closer to CP. In Fig. 5 the adiabatic expansion of zinc (segment *BC*)



Fig. 5. Thermodynamic path of the target (Zn) during collision of Ti with Zn. Notation is analogue to Fig. 2. Slow expansion process of two-phase liquid–gas mixture is also presented as the segment *DE*.

crosses the binodal in the vicinity of the CP. In this case the thermal mechanism of homogeneous nucleation prevails over mechanical fragmentation. Formation of the gas nuclei gives rise to the meta-stable liquid phase separation on the two-phase liquid–vapor mixture. This process is accompanied by abrupt increase of pressure from negative to positive value and fast decrease of the sound speed. Then the zinc target expands as a two-phase mixture (segment *DE* in Fig. 5). In the present simulation we do not distinguish the individual liquid droplets in the liquid–vapor state. We control only the mean density of the mixture knowing however the individual thermodynamic properties for each of the components.

In Ti–Zn interaction the temperature in the impactor after compression is higher than in the case of Ti–Al. It means that thermodynamic path under rarefaction penetrates into the metastable liquid region closer to the CP. We observe in this case that material of the projectile is also partially vaporized (Fig. 6, expansion segment *CD*). An abrupt jump of temperature in the vicinity of the liquid spinodal corresponds to the moment of phase explosion in considered point of the flier.

One can see in Fig. 7, that some layers of the target material are already turned into the liquid–gas mixture by the time moment 0.5 μ s. We see that the target material expansion results in conversion of the liquid droplets from the liquid–gas region into a gas fraction. The relative fraction of liquid and gas components depends on the time instant after the collision. It is seen in Fig. 7 that the impactor debris cloud contains long-lived individual liquid droplets (the temperature $T \sim 6$ kK and density $\rho \sim 3$ g/cm³ which correspond to the point of intersection of binodal and isentrope) separated by the liquid–vapor mixture, the mean density of which decreases in time.

3.3. Comparison with experiment

It has been found that numerical results are quite sensitive to the mesh size in the regions of unsmooth flow (zones of spallation). An acceptable convergence of the solution is observed when the grid cell has size 10 μ m. Further refinement results in negligible introduction of clarity in drops size. The presented results were obtained on the grid size 10 μ m for each cell. Some remarks ought to be done about comparison with available experimental findings. In this work we ignore the fact of possible data spread in



Fig. 6. Thermodynamic path of the impactor (Ti) during collision of Ti with Zn. Notation is analogue to Fig. 2.



Fig. 7. Density distribution in Ti–Zn simulation for different time delays after impact, $t = 0, 0.2, 0.5, and 1 \mu s$.

experiments caused by the internal structure of prepared samples such as manufacturing conditions, grain size in a sample, inclusions of admixture. We expect that these parameters make a negligible contribution into the entire picture of the process at chosen velocities of impact. The results of simulation of shock-induced fragmentation and vaporization were obtained in 1D-geometry and thus may be used for the interpretation of experiment [10] only on small time delay after the impact. Previous experimental studies on shock-induced vaporization of aluminum and zinc [7,8,10] demonstrate that the kinetics of vaporization are 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 Ref. [8] that full vaporization of zinc under rarefaction from the shock pressure occurs at $P \sim 550$ GPa. These pressure values are not achieved in the present simulation. Nevertheless we observe that partial evaporation with formation of the liquid-gas mixture upon release of zinc takes place at shock pressure $P \sim 316$ GPa. Further analysis should be done based on the information of witness plate free surface response [8,10] to verify the used criteria of spallation and vaporization.

4. Conclusions

In this study, simulations of shock-induced fragmentation and vaporization processes were carried out. Analysis of possible evolution of target and impactor materials is based on application of semi-empirical multi-phase equation of sates with metastable states and phase boundaries. The thermodynamic path of substance through the metastable liquid region is governed by two competitive mechanisms: homogeneous nucleation and mechanical fragmentation. These time-dependent mechanisms play an important role in formation of the debris cloud and its properties upon long-term release. In simulation the liquid–gas balance in the cloud is sensitive to the parameters of the models of nucleation and spallation. Experimental findings with a witness plate will be used for verification and adjustment of these models.

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References

- [11] Miller GH, Puckett EG. A high-order Godunov method for multiple condensed
- Al'tshuler LV, Bakanova AA, Bushman AV, Dudoladov IP, Zubarev VN. Evaporation [1] of shock-compressed lead in release waves. Sov Phys JETP 1977;46:980-3.
- [2] Al'tshuler LV, Bushman AV, Zhernokletov MV, Zubarev VN, Leont'yev AA, Fortov VE. Unloading isentropes and the equation of state of metals at high energy densities. Sov Phys JETP 1980;51:373–83.
- Bakanova AA, Dudoladov IP, Zhernokletov MV, Zubarev VN, Simakov GV. [3] Vaporization of shock-compressed metals on expansion. J Appl Mech Tech Phys 1983;24:204-9.
- Bushman AV, Fortov VE. Wide-range equations of state for matter under [4] extreme conditions. Sov Tech Rev B Therm Phys 1987;1:219–336. Asay JR, Trucano TG, Chhabildas LC. Time-resolved measurements of shock-
- [5] induced pressure profiles. In: Schmidt SC, Holmes NC, editors. Shock waves in condensed matter - 1987. Amsterdam: Elsevier Science; 1988. p. 159-62.
- Asay JR, Trucano TG. Studies of density distributions in one-dimensional shock-[6] induced debris clouds. Int J Impact Eng 1990;10:35-50.
- Wise JL, Kerley GI, Trucano TG. Shock-vaporization studies on zinc and porous carbon. In: Schmidt SC, Dick RD, Forbes JW, Tasker DG, editors. Shock compression [7] of condensed matter - 1991. Amsterdam: Elsevier Science; 1992. p. 61-4.
- Brannon RM, Chhabildas LC. Experimental and numerical investigation of [8] shock-induced full vaporization of zinc. Int J Impact Eng 1995;17:109-20.
- Chhabildas LC, Reinhart WD, Thornhill TF, Bessette GC, Saul WV, Lawrence RJ, [9] et al. Debris generation and propagation phenomenology from hypervelocity
- impacts on aluminum from 6 to 11 km/s. Int J Impact Eng 2003;29:185–202. [10] Chhabildas LC, Reinhart WD, Thornhill TF, Brown JL. Shock-induced vaporization in metals. Int J Impact Eng 2006;33:158-68.

- phases. J Comput Phys 1996;128:134-64. Povarnitsyn ME, Khishchenko KV, Levashov PR. Hypervelocity impact
- modeling with different equations of state. Int J Impact Eng 2006;33:625-33. Pilliod JE, Puckett EG. Second-order accurate volume-of-fluid algorithms for [13]
- tracking material interfaces. J Comput Phys 2004;199:465–502. [14] Khishchenko KV. Equation of state for tungsten at high temperatures and pressures. In: Fortov VE, editor. Physics of extreme states of matter - 2005.
- Chernogolovka: IPCP RAS; 2005. p. 170–2. in Russian. [15] Khishchenko KV, Tkachenko SI, Levashov PR, Lomonosov IV, Vorob'ev VS. Metastable states of liquid tungsten under subsecond wire explosion. Int J
- Thermophys 2002;23:1359-67. [16] Oreshkin VI, Baksht RB, Ratakhin NA, Shishlov AV, Khishchenko KV, Levashov PR, et al. Wire explosion in vacuum: simulation of a striation
- appearance. Phys Plasmas 2004;11:4771-6. [17] Lomonosov IV, Fortov VE, Khishchenko KV, Levashov PR. Phase diagrams and thermodynamic properties of metals at high pressures, high temperatures. In: Furnish MD, Thadhani NN, Horie Y, editors. Shock compression of condensed matter – 2001. New York: AIP; 2002. p. 111–4.
- [18] Frenkel J. Kinetic theory of liquids. Oxford: Clarendon Press; 1946.
- [19] Skripov VP. Metastable liquids. New York: Wiley; 1974.
- Grady DE. The spall strength of condensed matter. J Mech Phys Solids [20] 1988:36:353-83.
- [21] Tkachenko SI, Vorob'ev VS, Malyshenko SP. The nucleation mechanism of wire explosion. J Phys D Appl Phys 2004;37:495-500.
- [22] Semenchenko VK. Surface phenomena in metals and alloys. New York: Pergamon; 1961.