Shock-induced ejecta from a layer of spherical particles. Part I: SPH meso-scale simulation

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Abstract. According to the data obtained by the Photonic Doppler Velocimetry (PDV) shock wave propagation through a layer of bulked metallic particles produces dust ejecta consisting of fragments with various velocities. While velocity distribution of dust particles can be measured by the PDV, the spatial mass distribution and size distribution of the fragments are hard to derive from the PDV experimental data.

To study the mechanism of ejecting and composition of ejected material, direct simulation of experimental conditions is performed with the massive-parallel SPH code. We find that the cumulative jets are produced by the collisions of neighbor spheres accelerated by a shock wave. Those of jets which are able to reach free boundary, leave the layer and decay with formation of many fragments.

The data we acquire via direct numerical simulation of the described process is used as initial data for further investigation of dust motion in the air with the finite differences method.

1. Introduction

When a layer of bulked metallic micron-size spherical particles is shock-loaded by pressures of from 60 to 100 GPa, a formation of the dust ejecta consisting of fragments with various velocities is observed [1]. Analysis of processes that lead to dust jetting and distribution of dust fragments by sizes and velocities is an unresolved problem up to now.

The spectrograms of particle velocities in the dust ejecta are one of the few sources of information available for analysis. The time evolution of PDV spectrograms enables us, based on the law of particle slowing-down in the air, to estimate the characteristic size of ejecting particles. There is an approach to solving the inverse problem of reconstruction of the ejected mass distribution with Doppler shift measurements [2, 3]. The inverse problem solution offers rough estimation of the size distribution of the fragments, but it does not demonstrate profound understanding of the physical processes that occur in a layer of spherical particles during shock wave propagation and release on the surface.

One can use, for example, optical registration of particles that detach from the layer when a shock wave hits its free surface. Numerical simulation either involves complex models of heterogeneous medium that operate averaged parameters of the layer (as it is shown in Part II),
or completely corresponds to real pattern of the layer observed. The latter enables us to obtain sizes of the dust particles directly, without any averaging or simplifying, but appears to be time-consuming. Precise choice of an appropriate simulation method in combination with effective computational resource allocation can make a solution to be possible.

CSPH&VD, our massive-parallel software which implements SPH method with incorporated Riemann problem solution [4], allows us to simulate the experiment [1] with different packings of spheres.

Part I of the present work presents the simulation results which demonstrate the mechanism of dust ejecta in experimental conditions [1].

2. From experimental conditions to numerical simulation

Figure 1 demonstrates the scheme of experiment [1]. A 100 mm diameter high-explosive plane wave generator was used to generate a shock wave in a set of transmitters (consisting of a 1 mm thick plate of denal, which is a heavy tungsten alloy, and a 5 mm thick copper plate). The denal plate was machined with 8 notches. One of the notches was left empty for the transmitter free surface velocity measurement. The others were either filled with spheres with calibrated diameter (1 or 9 µm diameter golden spheres) or were containing a grooved plate.

![Figure 1. Experimental setup [1].](image1)

It is known from the experiment that after the shock wave broke through the free boundary of the layer, generated fragments (or the denal transmitter surface if considering the empty notch) were accelerated up to 4000 m/s (up to 1550 m/s for the empty notch) for less than 30 ns. The acceleration could not be resolved by PDV diagnostic used in the experiment.

3. Numerical simulation setting

Our simulation setting was slightly different from the experimental conditions. The scheme of the computational area is presented in figure 2.

In order to reproduce denal plate interaction with a bulked spheres layer, it was represented by a tungsten sample with periodical boundary conditions at y and z axes. We used pure tungsten instead of denal, because denal was a registered trademark for several tungsten heavy alloys and particular composition used in the experiment was left unknown. Thickness of the plate was 1.2 of height of the spheres layer and the length was estimated to be enough to avoid influence of the reflected rarefaction wave from the other side of the plate.
4. Numerical simulation technique

4.1. Modeling method

In order to solve the problem, the classic SPH method [5] was modified. The modification (CSPH) incorporates Riemann problem solution [6].

First of all, interparticle contact surface is introduced, which is similar to contact surface in a Riemann problem. Let us consider ORST coordinate system, which is associated with two particles in contact, \( i \) and \( j \). Let an OR axis point in \( \vec{r}_j - \vec{r}_i \) direction, where \( \vec{r}_i \) is a vector of a position of particle \( i \). An interparticle contact surface is in the middle between particles \( i \) and \( j \), normal to OR direction. We denote conditions of media to the left and to the right from the contact plane in direction of OR axis with \( (\cdot)^R \) superscript sign, so, for example, we have a Riemann problem for velocities \( v_i^R = \vec{v}_i \cdot \vec{e}_{ji} \) and \( v_j^R = \vec{v}_j \cdot \vec{e}_{ji} \). We denote the Riemann problem solution between particles \( i \) and \( j \) on OR axis with a \( (\cdot)^R \) superscript. Then CSPH approximations of mass and impulse conservation laws take the following forms:

\[
\frac{d\rho_i}{dt} = \frac{2}{\rho_i} \sum_j \frac{m_j}{\rho_j} (v_{ij}^R - v_{ij}^0) \frac{\partial W_{ij}}{\partial r_{ij}},
\]

\[
\frac{dv_{ij}^R}{dt} = \frac{2}{\rho_i} \sum_j \frac{m_j}{\rho_j} \sigma_{ij}^* \frac{\partial W_{ij}}{\partial r_{ij}}.
\]

Here \( \sigma_{ij}^* \) is the Riemann problem solution for a tension vector on the contact plane after an inverse coordinates transform from ORST to Oxyz.

Unlike [6], our code uses the conservative form of energy conservation law:

\[
\frac{(e_i + \vec{e}_{ij}^0/2)}{dt} = -\frac{1}{\rho_i} \sum_j \frac{m_j}{\rho_j} \sigma_{ij}^* \cdot \vec{v}_{ij} \frac{\partial W_{ij}}{\partial r_{ij}},
\]

where \( e_i + \vec{e}_{ij}^0/2 \) is a full energy in particle \( i \). The Riemann problem solution for velocity \( \vec{v}_{ij}^R \) and tension \( \sigma_{ij}^* \) are represented in the same coordinate system. To solve the Riemann problem the Dukowicz Riemann solver [7] is used in our code.

We consider a variable smoothing length, which is specified as \( h_i = d_i = \sqrt{m_i / \rho_i} \), assuming it to be equal to a length of cube side, where the cube is occupied by an SPH particle. Shape of an SPH particle is undetermined, so the assumption does not conflict with SPH theory. In order to assure conservation properties of particle interaction we need either to set \( h_{ij} = (h_i + h_j)/2 \) and then evaluate SPH sum assuming \( W_{ij} = W_{ij}(|\vec{r}_{ij}|, h_{ij}) \), or to set an SPH kernel to be equal to \( W_{ij} = (W(|\vec{r}_{ij}|, h_i) + W(|\vec{r}_{ij}|, h_j))/2 \). We choose the first way without explanation. An interaction length depends on the chosen smoothing length, and in general \( W(|\vec{r}_{ij}|, h_{ij}) > 0 \) if \( |\vec{r}_{ij}| < k h_{ij} \). We use the Wendland C^2 kernel with \( \kappa = 1/(2\sqrt{15}) \approx 1.94 \) [8, 9].

4.2. Equation of state

Equation system (1)–(3) is enclosed by the equation of state (EoS) in Mie—Gruneisen form:

\[
p - p_r = \Gamma_0 \rho (e - e_r).
\]

Here \( e \) is the internal energy of medium, calculated from energy conservation law (3), \( \Gamma_0 \)—Gruneisen parameter, \( p_r(\rho) \) and \( e_r(\rho) \) are the reference pressure and the internal energy curves, respectively.

The Shock Hugoniot curve \( p_H(\rho) \) is used as reference pressure if density is higher than an initial density; elastic curves are used if density is lower than initial one:

\[
p_r = \begin{cases} p_H, & \rho > \rho_0 \\ p_C, & \rho \leq \rho_0 \end{cases}, \quad e_r = \begin{cases} e_H, & \rho > \rho_0 \\ e_C, & \rho \leq \rho_0 \end{cases},
\]

where \( \rho_0 \) is the initial density; \( e_H, \rho > \rho_0 \) and \( e_C, \rho \leq \rho_0 \) are the internal energies of the medium in the initial state and in the final state, respectively.
where $p_H = C^2_a(V_0 - V) / [V_0 - s_a(V_0 - V)]^2$, $e_H = p_H(V_0 - V)/2$, $p_C = K(V_0 - V)/V_0$, $e_C = p_C(V_0 - V)/2$, $V = 1/\rho$, $K$ is an isothermal bulk modulus.

Elasto-plastic behavior of material follows Hooke’s law (with constant shear modulus $G$) and von Mises yield criterion. Yield strength $Y$ is considered constant.

Table 1 provides all the necessary parameters for our simulation.

| Material  | $\rho_0$, kg/m$^3$ | $\Gamma_0$ | $c_a$, m/s | $s_a$ | $K$, GPa | $G$, GPa | $Y$, MPa | $T_m$, K |
|-----------|---------------------|-------------|------------|-------|----------|----------|----------|---------|
| Gold      | 19.32 · 10$^3$      | 1.05        | 3.07 · 10$^3$ | 1.540 | 166.4    | 28.5     | 40       | 1339    |
| Tungsten  | 19.6 · 10$^3$       | 1.17        | 4.029 · 10$^3$ | 1.237 | 300.0    | 155.0    | 2400     | 3693    |

4.3. Solid—liquid phase transition

The preliminary modeling showed that experimental conditions [1] lead to pressures and temperatures that guarantee melting of materials. In order to conduct correct modeling of a phase transition phenomenon we added some code modifications. We used the following phase transition condition in form of Simon—Glatzel equation for gold [10]: if temperature exceeds

$$T > T_m \left(1 + \frac{P}{16.1}\right)^{0.57},$$

then the metal is considered melt. Pressure in equation (5) is measured in GPa. For tungsten we have the following condition [11]:

$$T > T_m + m_c \left(1 - \frac{\rho_0}{\rho}\right),$$

where $m_c = 5000$ K is a Kennedy’s constant.

If the conditions (5), (6) are not satisfied, respective materials are considered to be in solid state.

4.4. Initial packing of particles

Three-dimensional modeling of the shock wave propagation through a random metallic spheres pack requires development of a specific algorithm of packing of spheres in limited computational area with periodical boundary conditions (BC). Meanwhile the exact experimental golden spheres packing upon the denal transmitter is unknown (additional “shaking” may lead to packing density increase and may influence results of experiments, as will be shown further). Therefore two types of regular packing were used in our simulations: plain cubic and face-centered cubic (dense) without irregular vacancies. Considering the direction of shock wave propagation as $Ox$ axis and applying periodic BCs by $Oy$ and $Oz$, one can illustrate the packs by $Ox$ axis in the following form (see figure 3).

It is important to identify SPH particles not only by a material they represent, but also by their initial belonging to one or another golden sphere (or the denal transmitter). It helps to apply correct BCs between SPH particles in the golden spheres in contact.

Number of layers can be calculated from the provided information about mass that was ejected from the notches per unit area (88 and 71 g/cm$^3$ for spheres of 9 $\mu$m and 1 $\mu$m respectively). We used 10 layers of 9 $\mu$m diameter spheres for cubic packing and 9 layers of 9 $\mu$m diameter spheres for dense packing; 70 layers of 1 $\mu$m diameter spheres for cubic packing and 60 layers of 1 $\mu$m diameter spheres for dense packing in our numerical experiments.
4.5. Boundary conditions between spheres

The contact slip condition (non-viscous contact) and the no merging condition are applied between solid spheres. It means that between SPH particles that belong to different bodies there is no tangential stress. Contact pressure for such particles cannot become negative.

Absence of tangential stress in the SPH formulation we use means that for $i$ and $j$ particle

$$\vec{v}^{RST}_{ij} = \begin{bmatrix} v^R_{ij} \\ v^S_j \\ v^T_j \end{bmatrix}^T,$$

(7)

$$\vec{\sigma}^{RST}_{ij} = \begin{bmatrix} \sigma^R_{ij} \\ 0 \\ 0 \end{bmatrix}^T,$$

(8)

if calculating for particle $i$; non-negative contact pressure reads as

$$\sigma^R_{ij} = \min(\sigma^R_{ij}, 0)$$

(9)

Liquid phase is always non-viscous, so all the contacting pairs of liquid SPH particles employ conditions (7), (8). Condition (9) should not be applied to liquids (liquid materials can merge).

5. Simulation results

We choose the experiment in which the free surface was accelerated to 1500 m/s (as measured in the notch with no insertion) and golden spheres were of 9 $\mu$m diameter for discussion of physical phenomena which take place in layer of spheres. Our choice is driven by a low number of layers of spheres that are necessary for simulation in this case: 9–10 layers in contrast with 60–70 for 1 $\mu$m diameter spheres for a given mass per unit area (88 mg/cm$^2$). It is obvious that if we use the same number of SPH particles per a single golden sphere for the two cases, computational expenses grows greatly, but solving the harder problem will not help us to shed light on the ejecta phenomenon in the experiment under discussion. Considering the chosen computation area shape (in figure 3) it is convenient to show results for the 9 $\mu$m diameter case (spheres layer is not “stretched” in computational area).

5.1. Dense spheres packing

Here we consider a case of constructing initial computational area as shown on figure 4.

The layer of spheres consists of $2.488 \cdot 10^6$ SPH particles. A single sphere is comprised by $70 \cdot 10^3$ SPH particles. As it was already mentioned, we also considered the transmitter plate which acted like an impactor in our simulation so the whole number of particles reached $6.412 \cdot 10^6$. The number of SPH particles was estimated after they were placed at nodes of body centered cubic cells of size equal to the minimal computational area size divided by 70.
Figure 4. Initial pattern of spheres placement for dense packing (at $t = 0$). Here and below figures are provided in 3D perspective, and different spheres are shown in different colors.

At an initial time the transmitter plate is hit into layers of spheres with the experimental free surface velocity of 1500 m/s. Figure 5 shows flow evolution till and including ejecta formation. As a result of the impact of adjoining spheres cumulative jets are formed that hit shielding layers (figure 5, (a)). As shock wave propagates, the compaction of spheres and formation of typical Richtmayer—Meshkov instability structures are observed (figure 5, (b, c)). The eddy structures consist of SPH particles originating from different golden spheres. After shock wave arrival to the free surface of packing freely escaping jets are formed (figure 5, (d)). The jets are comprised by SPH particles, originating from upper layers of packing.

Figure 5. 9 µm diameter dense packed spheres layout at different times.

At $t \approx 50$ ns separation of particles from the transmitter occurs. At $t \approx 105$ ns the packing have the layout as in figure 6.

By the time $t \approx 240$ ns relaxation of pressure field is observed in ejecta. Typical ejecta pattern is the same as in figure 6. Dust ejecta mass fraction is approximately 2% of initial mass of packing of spheres. Free surface of the compacted layer obtained velocity of 1600 m/s.

The results show that the flow pattern of the compacted spheres packing is determined by a cumulation phenomenon. The dust observed in experiments is in fact fragments of cumulative jets. Moreover, for the dense packing the fragments come from upper packing layers.
5.2. Plain cubic spheres packing

Let us consider the case of initial computational area constructed as shown on figure 7.

The spheres layer is comprised by $1.13 \times 10^6$ SPH particles. One sphere consists of $28 \times 10^3$ particles. Overall number of SPH particles is $4.77 \times 10^6$. The number was obtained after we placed them at nodes of body centered cubic cells (as in the previous case) of a size equal to minimal computational area size divided by 60.

Figure 8 shows evolution of packing while it undergoes shock wave loading by the transmitter plate. Figures show cumulative jets formation (figure 8, (a)). The jets have free space in upper layers and thus pass the free surface of the packing before the shock wave reaches upper layers of spheres (figure 8, (b)). Cumulative jets that form ejecta cloud consist of fragments of different (all) spheres layers, and also of the transmitter material. The moment of the shock wave arrival to the free surface of layers is shown in figure 8, (c).

Figure 9 shows jets that are observed in computational area some time after the shock wave breakage through the free surface. It is clear that the jet heads consist of the lower layers material and also from the transmitter plate material (tungsten in the simulation or denal, if interpreting the real experiments). Mass fraction of dust is 11% of overall ejecta mass. Tungsten mass fraction is $\approx 4\%$ of the dust mass.

The simulations of shock loading of smaller spheres show similar small-scale flow trend to the described above. As mentioned above, a number of spheres of 1 $\mu$m diameter is one order greater than it is necessary to use for 9 $\mu$m diameter spheres. It took 60 layers for dense packing and 70—for plain cubic. It was required to use $30.5 \times 10^6$ and $26 \times 10^6$ particles respectively to obtain appropriate number of particles per single sphere ($44 \times 10^3$ and $30 \times 10^3$, respectively). Total number of SPH particles comprising golden spheres reached $14.9 \times 10^6$ and $7.9 \times 10^6$, respectively. As in previous cases, number of SPH particles was calculated after they were initially placed in nodes of body centered cubic cells of size equal to minimal computational area size divided by 60.

Similar to the larger spheres case, the formation of the cumulative jets is observed for plain cubic pack of spheres of 1 $\mu$m diameter each. Fragments of all layers of the pack and of the transmitter plate are found in the jets. Dense packing produces less jetting compared to plain
$t = 12.4$ ns.  

$t = 30.7$ ns.  

$t = 42.2$ ns.

**Figure 8.** Spheres of a 9 $\mu$m diameter, plain cubic packing. Layout at different times.

**Figure 9.** Layer layout at $t = 120.0$ ns.

cubic pack: the jets include only upper layers of the sphere pack. We do not provide full illustrations of the flow in this case due to the computational area length-to-width large ratio. The local flow has the same layout as shown above for the system of 9 $\mu$m diameter spheres.

6. Conclusion

The simulation results of shock-loaded regular layer of spherical particles have been presented. Two regular types of lattice have been discussed: plain cubic and faced-centered cubic one. Original results have demonstrated that the ejecta formed when a shock wave reaches the free surface of bulked spheres consist of the fragments of the cumulative jets. These fragments originate from different layers of spheres and also from the transmitter plate. We have found that ejecta structure is highly dependent on the initial packing of spheres. In the case of real random packing the ejecta appears to consist of the fragments both of the spheric particles and the transmitter plate.

CSPH&VD$^3$, the software we develop, enables us to estimate the distribution of fragments by their masses and velocities. The modeling results could serve as a reliable base for mesh methods and, as it is shown in Part II, is also suitable for further simulations of evolution of dust ejecta in the air.

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