Shock-produced ejecta from tin: Comparative study by molecular dynamics and smoothed particle hydrodynamics methods

S A Dyachkov\textsuperscript{1,2,3}, A N Parshikov\textsuperscript{1,2} and V V Zhakhovsky\textsuperscript{1,2}

\textsuperscript{1} All-Russia Scientific Research Institute of Automatics, Sushchevskaya 22, Moscow 127055, Russia
\textsuperscript{2} Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
\textsuperscript{3} Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia

E-mail: serj.dyachkov@gmail.com

Abstract. Experimental methods of observation of early stage of shock-induced ejecta from metal surface with micrometer-sized perturbations are still limited in terms of following a complete sequence of processes having microscale dimensions and nanoscale times. Therefore, simulations by the smoothed particle hydrodynamics (SPH) and molecular dynamics (MD) methods can shed of light on details of micro-jet evolution. The size of simulated sample is too restricted in MD, but the simulations with large enough number of atoms can be scaled well to the sizes of realistic samples. To validate such scaling the comparative MD and SPH simulations of tin samples are performed. SPH simulation takes the realistic experimental sizes, while MD uses the proportionally scaled sizes of samples. It is shown that the velocity and mass distributions along the jets simulated by MD and SPH are in a good agreement. The observed difference in velocity of spikes between MD and experiments can be partially explained by a profound effect of surface tension on jets ejected from the small-scale samples.

1. Introduction

The machining of materials produces regular micrometer-sized surface perturbations. The microscopic cumulative jets can be generated from such surface under shock loading. It is too complicated task to resolve space-time evolution of such jets in experimental conditions. The involved process is also difficult to describe analytically due to nonlinearities which takes place for intense shocks and big perturbations. On the other hand the details of jet formation can be obtained via hydrodynamics and molecular dynamics methods.

The process is usually considered in terms of Richtmyer–Meshkov instability, when the shock wave passes through the perturbed interface with the amplitude $a$ and the wavelength $\lambda$ between two media A and B (figure 1). The instability growth shows itself as the spikes of medium A penetrate into medium B and the bubbles of B penetrate into A.

The linear model was developed by Richtmyer for fluids [1] based on the Rayleigh-Taylor instability. After that, in the work of Meshkov [2] the first experiments were described. The limiting case of the Richtmyer–Meshkov instability with Atwood number $A = (\rho_B - \rho_A)/(\rho_B + \rho_A) \simeq -1$ is used for the description of the jetting phenomena [3]. The linear models here can...
be used only at early times of the jet evolution. The nonlinear models which are fully reviewed in [4] are built on the basis of the results of hydrodynamic and molecular dynamic simulations as corrective coefficients to the linear model. The spike velocities obtained from such models are predicted with lower values, than it is in experiment. Nevertheless, the distribution of the mass along jet can be obtained only from simulations and experiments. The fragmentation process at the late times of jet evolution is another interesting problem, widely discussed in [5] using MD simulation. Presently, the linear size of a MD sample is limited by the order of 100 nm, depending on available computational resources. Because of the strong influence of the surface tension and fracture effects on atomic scales the simulated jet fragmentation cannot be easily scaled from the MD scale to the realistic micrometer sized samples. The validity of such scaling should be verified for various samples with different geometry.

In this work MD and SPH simulations of the jetting of tin are prepared with parameters similar to the used ones in [6]. SPH method is applicable in wide range of amplitudes of perturbations, but it has problems in deciding on a fracture model and lack of surface tension of molten metal. In contrast to SPH approach, thermodynamic and kinetic properties of material of interest in MD approach are defined with a potential of inter-atomic interaction. As a result the problems of SPH approach disappear, but the size of simulated sample is restricted much in MD. However, to be sure that hydrodynamic regime takes place in MD the large enough number of atoms should be used in simulation. Thus, the results of MD can be scaled to the size of real sample.

2. Simulation methods and parameters of samples
The jetting process is usually accompanied by dramatic deformation of material. It leads to the high strain rate phenomena, phase transitions and the formation of spatial inhomogeneity. These peculiarities should be taken into account while selecting the efficient method for calculations.

Simulations with Smoothed Particle Hydrodynamics (SPH) have an advantage among the grid algorithms. The Euler grid methods require contact and free surfaces to be handled accurately, because there are the main source of errors. The Lagrange grid methods should use special approaches for a grid transformation in the domain of jetting, which is fraught with high numerical diffusion of momentum and energy till the jet formation. So that the non-grid

**Figure 1.** The scheme of the jetting phenomena in terms of Richtmyer–Meshkov instability.
SPH method is optimal for the simulations of the jetting phenomena, rotational and shear flows of compressible media, fragmentation of material. In this work SPH non-grid code SPHERA-2D \cite{7, 8} is used for hydrodynamic simulations.

The existing MD codes are generally use two approaches for domain decomposition: static (LAMMPS, SPaSM) and dynamic (MD-MPD\textsuperscript{3} \cite{9}), where each domain is handled by a single processor core. Due to a spatial inhomogeneity some static domains may have low number of atoms and may be processed rapidly. However, the overall calculation time mostly depends on the processing of domains with high number of atoms. So that the high efficiency can be achieved by keeping an approximately equal number of atoms in the each domain. The code MD-MPD\textsuperscript{3} performs the adaptive decomposition of the material into material particles which are represented by Voronoi cells, which results in good load-balancing in simulation of samples with highly nonuniform time-dependent density distribution in computational box.

Thermodynamic and kinetic properties in MD approach are defined with a potential of interatomic interaction. The EAM potential cannot reproduce well characteristics of solid tin. But tin is fusible metal and in jetting phenomena simulations in most cases it becomes melt. Therefore, it is quite enough to have the potential for tin in liquid state, and it has been developed with this aim in view. It turned out that the shock hugoniot of liquid tin is well reproduced with this potential in comparison to experimental data. The calculated melting point $T = 450$ K agree well with the experimental one $T = 505$ K and the calculated surface tension of liquid tin $\sigma_{MD} = 0.590$ J/m$^2$ at $T = 683$ K is also in good correspondence with the experimental value $\sigma_{exp} = 0.525$ J/m$^2$.

The properties of tin, used in the SPH simulations are presented in table 1. The parameters $\rho_0$, $S_a$ and $C_a$ of equation of state were taken from MD simulations for keeping the full similarity of MD and SPH results.

The comparative MD and SPH simulations of tin samples are performed with geometric properties which are similar to the used ones in the experiments \cite{6}. In hydrodynamic simulations samples have the real experimental sizes $L_x \times L_y = 1650 \mu\text{m} \times 550 \mu\text{m}$ (~$10^5$ SPH particles), but for MD simulations we have to take nanoscaled samples with the sizes $L_x \times L_y \times L_z = 150 \text{nm} \times 50 \text{nm} \times 16 \text{nm}$ (~$5 \times 10^6$ atoms). The shock wave with an amplitude $P$ is initiated by an impact of a sample moving towards piston with velocity $v_p$. The following amplitudes of perturbations are selected for simulations: $ak = 0.25, 0.5, 1.0, 2.0$ for $P = 27$ GPa ($v_p = 930$ m/s) and $ak = 0.12, 0.35, 0.75, 1.5$ for $P = 22$ GPa ($v_p = 800$ m/s).

| Property                  | Value     |
|---------------------------|-----------|
| Initial density $\rho_0$, kg/m$^3$ | 7206      |
| Gruneisen parameter $\gamma_S$ | 1         |
| Shock hugoniot coefficient $S_a$ | 1.548     |
| Shock hugoniot coefficient $C_a$, m/s | 2366      |
| Bulk modulus $K$, GPa      | 58        |
| Yield strength, $Y_0$, MPa | 9         |

3. Velocity distributions

Only spike and bubble velocities were measured in the experiments with Laser Doppler Velocimetry (LDV) method \cite{6}. The velocities of spikes and bubbles are measured with relation to the velocity of the unperturbed interface $v_{fs}$.
In figure 2 MD and SPH results for the spike velocities are presented in comparison to the experiment. SPH data is in better agreement with the experiment. In addition, while increasing the amplitude of perturbations the error in definition of velocity diminishes to 15%.

In figure 3 MD and SPH results for the bubble velocities are presented in comparison to the experiment. The results do not correspond experimental data, but agreement with SPH is better in figure 3a, for big amplitudes of perturbations. However, nonmonotonic experimental dependency may be due to unaccounted errors.

The explanation of the spike velocity decreasing in MD simulations is in high influence of the surface tension on atomic scales. In figure 4 one can see the time evolution of the velocity profile for MD calculation with $P = 27$ GPa and $ak = 2$. The peak velocity here is about 2 km/s what perfectly match experimental result, and in further profiles the velocity decreasing due to forces of surface tension. Only at the shown time period which is less than half of totally calculated time the velocity has decreased in 200 m/s.

The effect of the surface tension is rather small for intense shocks and big amplitudes of perturbation.
Figure 4. Time-dependent velocity profiles in MD simulation of the tin sample with parameters $ak = 2.0$, $P = 27$ GPa. One can see the effect of surface tension: the velocity at the end of spike is going down while the blob grows at the end of it.

Figure 5. Comparison of the velocity profiles calculated with MD and SPH methods for the tin sample with parameters $ak = 2.0$, $P = 27$ GPa.

Figure 6. Reduced mass distribution along jet $m^*_jet = m_{jet}/m_{out}$ as a function of reduced coordinate $x^* = x/\lambda$ in MD and SPH simulations of the tin sample with parameters $ak = 2.0$, $P = 27$ GPa.

4. Mass distributions

Total ejected mass is calculated in relation to the bubble boundary. It is convenient to consider the jet mass from the beginning of the spike to some coordinate $x$ along the jet:

$$m_{jet}(x) = \int_{x_{sp}}^{x} \sigma(x) \, dx,$$

where $\sigma(x)$ – linear density of the jet. From here the total mass is $m_{jet} = m_{jet}(x_b)$. The example of mass distribution along the jet is given in figure 6 which shows a good correspondence between MD and SPH simulations.

The additional mass in MD appears in the bulb, and then it grows along the jet in accordance with SPH. At the end of the jet near the bubble the mass also grows in a different way.

In figure 7 the reduced masses $m^* = m_{jet}/m_{out}$ are compared for all simulations during this work. Here is $m_{out}$ – the mass of material, which was removed from the surface after machining. The results agree well, again, for the more intense shock and for the bigger perturbations of the surface.
Figure 7. Reduced jet masses calculated for tin samples with the shock pressure of 22 GPa (a) and 27 GPa (b) as the function of the perturbation amplitude in MD and SPH simulations.

5. Conclusion
In spite of the number of atoms in the MD simulations was enough big for hydrodynamic regime, the high influence of the surface tension which guides evolution of nanoscale jet shape, may lead to discrepancies between MD and SPH simulations, especially for weak shocks and small surface perturbations. While jet is being formed and surface tension has lack of time to affect jet motion, the velocity of spike in MD is very close to the experimental results. The problem may be partially resolved with the increasing of the sizes of samples what diminishes the curvature of surface and the surface tension.

The spike velocities and ejecta masses obtained in MD and SPH simulations are in good agreement. Small differences also may be disappear with the bigger number of particles in samples. Such effects will be accounted in the future research with tin and other materials. The investigation of the phenomena with more complex 3D surface perturbations and the fragmentation of jet at the late times are also interesting problems for the future research.

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