Investigation of the dynamic fragmentation of shock-induced sheets of liquid metal using large-scale molecular dynamics simulations

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When a metal with a roughened free surface is shock-loaded, the reflection of the shockwave onto the free surface causes the ejection and the development of instabilities. In the particular case where the metal directly melts under shock or shock-release and if the roughness consists of two-dimensional (2D) grooves, the instabilities take the form of 2D sheets of liquid metal. The sheets stretch, and they finally break up, forming fragments (ejecta) of various sizes. This phenomenon, called micro-jetting, pays ongoing attention since it can be a source of inhibition in application like inertial confinement fusion.

In order to investigate in detail micro-jetting, we perform large scale molecular dynamics (MD) simulations. Such simulations are indeed at the good scale to capture the physics of fragmentation [1-3]; we show that they exhibit striking similarities with experiments, although the length and time scales involved are 3 or 4 orders of magnitude smaller than the ones of experiments. A three-dimensional tin crystal with a sinusoidal free surface roughness is set in contact with a vacuum (see Fig. 1). It contains up to 700×10^6 atoms, and it is shock loaded above its fusion point.

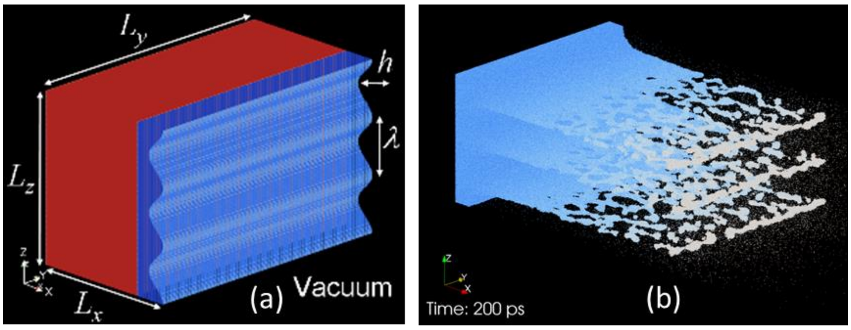

Fig. 1 (a) Description of the generic system simulated and (b) oblique view of the system 200 ps after reflection of the shockwave onto the surface defect

The simulations show that the resulting particle size distributions obey a power law dependence in the small size limit, and obey an exponential form in the large size limit. These two components are the signature of two distinct basic mechanisms of fragmentation. The power law dependence results from the fragmentation of the sheets in a 2D web-like structure of ligaments of liquid metal; the exponential distribution results from a secondary fragmentation process of the largest ligaments previously generated, following a one-dimensional Poisson statistics.

We perform also MD simulations to investigate the fragmentation of static sheets of liquid metal. We show that both dynamic and static regimes of fragmentation are similar when the sheets are stretched with expansion rates below typically 1×10^7 s^{-1}.

[1] O. Durand and L. Soulard, J. Appl. Phys. **111**, 044901 (2012)
[2] O. Durand and L. Soulard, J. Appl. Phys. **114**, 194902 (2013)
[3] O. Durand and L. Soulard, J. Appl. Phys. **120**, 045306 (2016)