# MULTISCALE MODELING OF DYNAMIC TENSILE FRACTURE OF METAL MELTS

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**Summary.** We present the results of combined investigation of the tensile fracture of metal melts, which uses both the molecular dynamic simulations and the continuum modeling.

## 1 INTRODUCTION

Dynamic tension of a melt takes place at fast expansion of an initially solid metal, which was heated and melted by an ultra-short pulse of powerful laser [1,2] or high-current electron irradiation [3]. An initial expansion of melt is due to the pressure gradients, while the subsequent expansion is due to the inertia, which leads to a tensile state with negative value of pressure. Another situation is a reflection of a compression pulse (a shock wave followed by an unloading wave) from an interface [4], when the compression pulse transforms into a tension wave. Thermodynamic state of a melt at a negative pressure is unstable and decays by means of cavitations. It is the tensile fracture of melt and the highest absolute value of negative pressure is the tensile strength, which depends on the strain rate and temperature.

We present the results of MD simulations of the high-rate tension and fracture of pure metal melts [5] and melts with both refractory [6] and fusible inclusions. Also we investigate late stages of aluminum melt tension up to the deformation degree of about 10 including a stage of bubble liquid, a foamed melt, and a fragmentation with formation of droplets; main regularities are reviled [7] and used on the continuum level of description. Our continuum model based on the MD simulation results is described and applied to the large-scale problems unattainable for MD. In presentation with the help of the continuum model we analyze a possibility of a foamed aluminum formation under the action of a high-current electron beam.

## 2 MOLECULAR DYNAMIC SIMULATIONS

MD simulations are performed with the help of LAMMPS [8] and with using of various interatomic potentials based on the embedded atom model. Atom configurations are visualized and analyzed with the help of OVITO [9]. Crystalline lattice of atoms is set initially and then it is melted by applying a high temperature. After preparation stage, a

uniform tension of the sample is simulated by means of scaling of the atom coordinates; this scaling corresponds to the melt extension by inertia. The obtained stress-strain curves are analyzed for determination of the tensile strength. The obtained atom configurations are analyzed for investigation the melt evolution including the growth and interaction of voids and final fragmentation. Figure 1 shows an example of atom configurations obtained in MD simulations for the stage of formation, growth and interaction of voids [7].
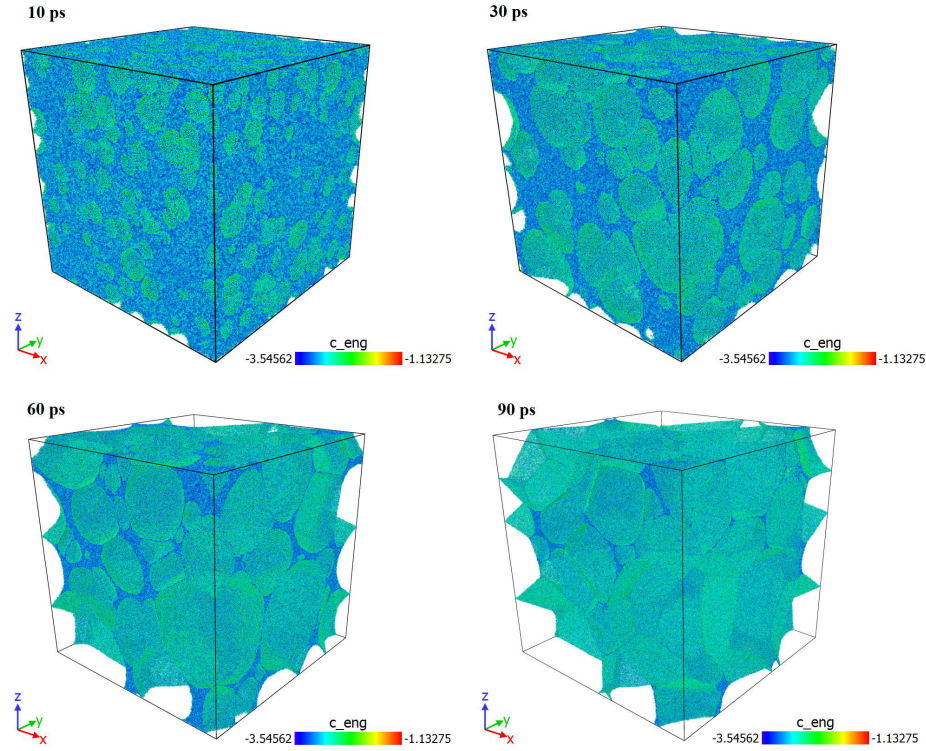


Figure 1: Nucleation, growth and coalescence of cavities: MD system at time moments of 10, 30, 60 and 90 ps, deformation degrees are 0.3, 0.9, 1.8 and 2.7, respectively. The last time moment corresponds to the volume increase in 15 times. Aluminum melt at the temperature of 1100 K, the strain rate is 30 ns$^{-1}$. Atoms are colored according to the value of their total energy ("c_eng"), which is higher for atoms on the void surfaces.

Influence of impurities is examined with using of MD simulations. By the example of Ti and Ni inclusions in Al melt, it is shown that the refractory inclusions weakly increase the tensile strength [6] due to the fact that tension is applied predominantly to the melt around inclusions, which effectively increases the strain rate. By the example of Mg inclusions in Al melt, it is shown that the fusible inclusions can temporally decrease the tensile strength several times (Table 1), but the effect weakens together with the diffusive mixing.

| System | Mg | Al+Mg | | | | Al |
|---|---|---|---|---|---|---|
| Preparation time (ps) | - | 30 | 140 | 240 | 1200 | - |
| Strength (GPa) | 0.85 | 1.75 | 2.96 | 3.38 | 3.95 | 4.28 |

Table 1 : Strength of Al melt with Mg inclusions (2.4 at.%) in comparison with pure melts. Diffusive mixing of Mg and Al atoms increases together with the preparation time.

## 3 CONTINUUM MODEL

The continuum model [5] included the equations of the nucleation and growth of voids in approximation that voids interact only through the mean field of pressure. A simplified model of the percolation transition was used in [5] for description of the transition from the bubbly liquid to separate droplets: it was supposed that the fragmentation occurs as the volume fraction of voids reaches 0.5. Further investigation [7] showed that the bubbly liquid stage lasts till the volume fraction of voids reaches about 0.95. This difference is not important for calculation of the tensile strength, but it is substantial for analysis of the foamed metal formation conditions and for the problem of micro- or nanoparticles generation during the expanding melt fragmentation. Therefore, a more precise accounting of the late stages of the metal melt evolution is included in the present version of the continuum model.

Figure 2 shows an example of 2D modeling of the copper sample dynamics under the action of the high-current electron beam (SINUS-7 accelerator [3]). The continuum model describes the size distribution of pores inside the energy deposition area of the beam. A layer of melt along the irradiated surface remains in the one-phase state and can be treated as a spalled layer similar to the case of rear spallation in solids.
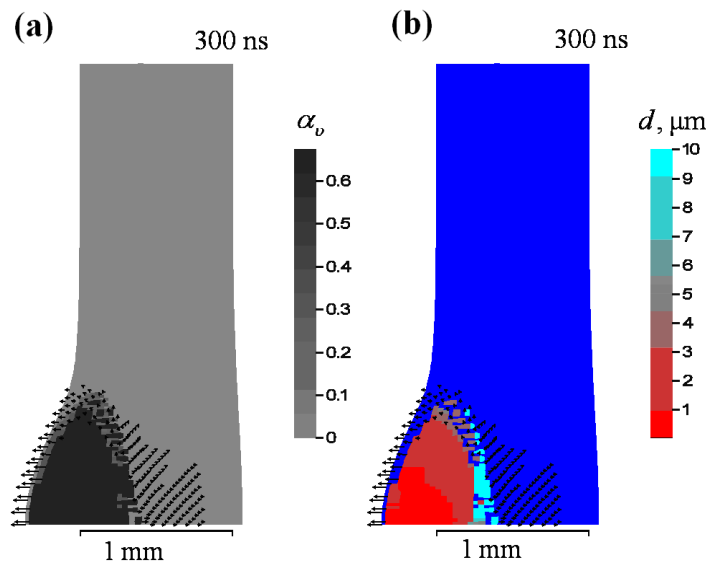


Figure 2: Calculated distributions of the volume fraction $\alpha_v$ (a) and the mean diameter (b) of voids: irradiation of copper plate with the thickness of 1 mm by the high-current electron beam (SINUS-7 accelerator [10]) with the effective beam radius of 0.5 mm. Dark blue color in (b) corresponds to the one-phase state of metal without voids. The axis of symmetry is from below. Little arrows show the substance velocity vectors.

## 4 CONCLUSIONS

- Continuum model of the metal melts evolution under the tension is developed using the data from molecular dynamic simulations. The model takes into account the late stages of the melt fracture till the complete fragmentation. It is intended for description of the molten metal dynamics in the energy absorption area of laser or electron beam, and the shock-wave processes in melts.

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