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Multi-scale modeling of phase explosion in high fluence nanosecond laser ablation and clarification of ablation depth prediction criterion

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ABSTRACT

When phase explosion occurs, accurate prediction of the ablation behavior in the high energy nanosecond laser ablation process still remains a difficult challenge. In this paper, nanosecond laser ablation of aluminum and copper with phase explosion is investigated through a multi-scale model and experimental verification. The melt ejection behavior during phase explosion is successfully predicted by combined molecular dynamics (MD) and smoothed particle hydrodynamics (SPH) simulations and validated against the experiments. The commonly adopted $0.9T_c$ (critical temperature) criterion for phase explosion boundary is also assessed with the prediction of the ablation depth for both aluminum and copper, and it is found that the $0.9T_c$ criterion does not always work. The multi-scale model developed in this work is shown to have better capability in predicting the ablation behavior when phase explosion is involved.

1. Introduction

It is generally known that the laser ablated material consists not only of evaporated atoms, but also particles or droplets formed, either directly by the laser-solid interaction, or later, through condensation (smaller particles condense onto the larger particles), collision between particles, or hydrodynamic sputtering (large particles) in the expanding plume.

In the low laser fluence regime, the particles/droplets are mainly in the nano or sub-micron scale, which are formed mainly through laser evaporation [1]. A number of models have been reported to describe particle formation and growth in the expanding vapor plume, based on condensation and nucleation theories [2–6]. In general, condensation droplets are typically formed in long-pulse (ms) and low-intensity (10^4–10^5 W/cm^2) regimes [3]; however, they can also be generated at higher laser intensity and shorter pulse (e.g. 10^8–10^{10} W/cm^2 and a few ns pulse) under the slow expansion of the vapor plume into the background gas [7].

With the increase of laser fluence, the surface temperature of a target material may rise close to 90% of the critical temperature or even higher [8,9]. Under this condition, explosive ejection of liquid melts and droplets will occur and may start dominating the ablation process, which is usually referred to as phase explosion or explosive boiling [9]. In this high fluence regime, larger particles/droplets may form with different mechanisms depending on target material and laser conditions. It was proposed based on experimental observation that the vaporized atoms and ions condense as tiny particles on the ejected larger droplets, forming an outer layer and even larger particles [10]. For metals, particles are assumed to be formed by liquid (large droplet) ejection, which can be the result of several processes. Large droplets can be ejected as a result of transient melting and motion of a liquid caused by steep pressure gradients and the vapor plume recoil pressure [11–14]. The formation of large droplets is assumed to be from the collision between small particles. According to Hergenroder [15], hydrodynamic sputtering may also play a very important role on the large particle formation in a laser ablation process.

At high laser power density, the particle size was measured to have a bimodal shape distribution [15]. Clearly, there are two mechanisms for the particle generation. One is the evaporation induced by laser ablation, which corresponds to the lower peak in the particle size distribution. The other one is due to either condensation, collision between small particles, or hydrodynamic sputtering, which corresponds to the higher peak.

It still remains a difficult challenge to capture the ejected droplets during the material removal by conventional modeling methods (for example, hydrodynamics model) using generated mesh. The mesh size needs to be several times smaller than the ejected molten materials, which requires massive computing resources. Lu [16] proposed a one-dimensional fluid model to describe the thermodynamic evolution during phase explosion. However, Lu's model could not predict the melt ejection

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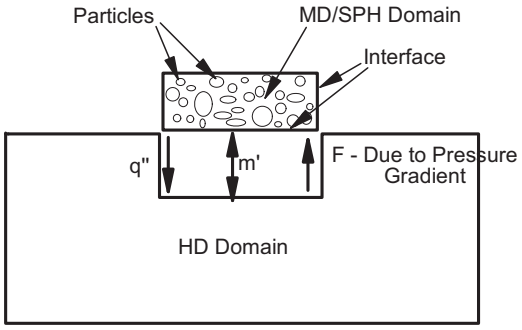

Fig. 1. Calculation domain.

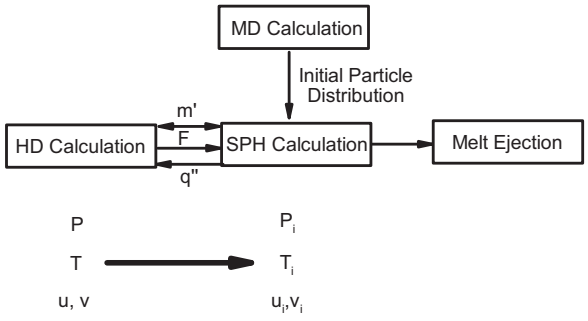

Fig. 2. Calculation flow chart for multi-scale model.

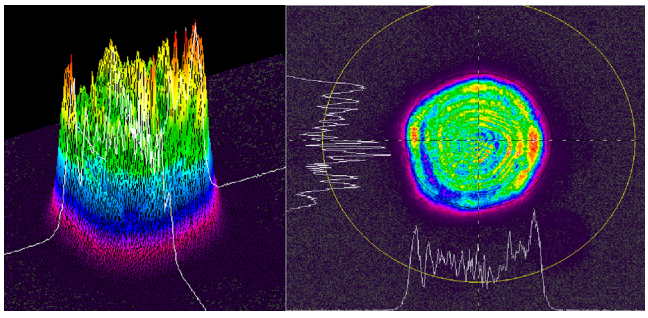

Fig. 3. Beam profile measurement, beam diameter 0.2 mm.

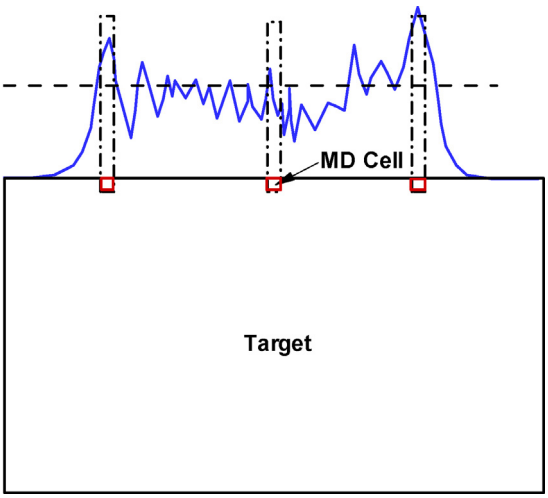

Fig. 4. Laser beam distribution and MD cells.

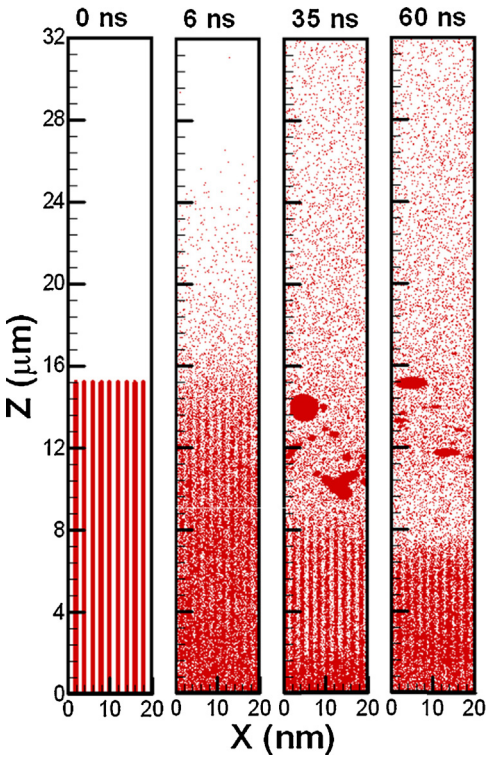

Fig. 5. Atom distribution at different time (laser fluence 12 J/cm^2, wavelength 1064 nm, pulse duration 6 ns).

behavior and the resulting ablation depth. As a walk-around, most researchers use $0.9T_c$ (critical temperature) as the ablation depth prediction criterion when handling phase explosion [17–19]. In the authors' previous work [20], $0.9T_c$ as the ablation depth prediction criterion was shown to yield good accuracy when predicting the ablation depth for aluminum with phase explosion. However, it was found that $0.9T_c$ does not work when dealing with a copper target.

There are some numerical methods proposed in literature to capture these nonlinear phenomena, such as molecular dynamics (MD) and smoothed particle hydrodynamics (SPH). Molecular dynamics (MD) simulation provides an explicit atomistic representation of material heating, vaporization, and plume expansion, and solves problems that cannot be accounted for by continuum models, such as highly non-equilibrium states and fast phase transformations induced by high fluence laser irradiation [21]. The interatomic potential V is one of the most important parameters governing MD simulation of a certain material, because this potential defines the interactions among atoms that the material consists of and dominates the properties of the material [22]. The force exerted on each atom by other atoms is also determined by the interatomic potential. Therefore, once the interatomic potential is given, MD can be used to simulate many problems with their specific external forces, initial conditions and boundary conditions.

SPH is a meshless computational method represented by a set of particles where each particle moves according to the governing dynamics [23]. In SPH, differential equations are therefore solved by a Lagrangian technique. The basic concept of SPH is that continuous media are represented by discrete particles with volume, density and mass. The particles have a kernel function to define their range of interaction, and the hydrodynamic variables are approximated by integral interpolations. Meshes are not needed in the simulation, which is a major advantage of SPH over Eulerian methods for complex geometries. However, since SPH is a mesoscale method [23] that deals with the particle size in the sub-micron to micron range, SPH alone cannot predict the initial particle formation in the