Single Pulsed Laser Ablation Simulations of Femtosecond and Nanosecond Lasers on an Aluminum lattice in a Vacuum

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Abstract

Simulations of laser ablation on an aluminum lattice in a vacuum are created using Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) and its ttm/mod fix.Single pulsed laser ablation with nanosecond and femtosecond lasers were simulated and the ablation behavior between the two were compared. The ablation threshold on the order of .1J/cm^2 was successfully reproduced in the simulations and cold ablation was observed. On the nanosecond laser, the lattice maintained its structure and no ablation was observed at its reported threshold of 5.2 J/cm^2, suggesting hot ablation to be the dominating process on the nanosecond pulse duration regime.

Background

Laser ablation is a process by which one removes material from the surface of a solid by irradiating it with a laser beam. By using a pulsed laser beam, as opposed to a continuous laser beam, we can produce the peak power needed to irradiate the material.

Cold ablation is a process where the full energy of the laser pulse is deposited to the electrons before the electrons can relax and equilibrate with the lattice, thus a large amount of energy is transferred to the lattice suddenly, causing an explosion. Hot ablation occurs when the pulse duration is less than the relaxation time and so the electrons can equilibrate with the lattice, causing heating and thus leading to vaporization. Theoretical works into laser ablation involve the two-temperature model (TTM) which describes non-equilibrated states of the electronic and lattice subsystems. The energy transport between the systems is described by a modified heat diffusion equation :

Equation 1. Generic TTM Model

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \nabla[K_e(T_e,T_l)\nabla T_e] - G(T_e)(T_e - T_l) + S(\vec{r},t),$$

C_e is the electronic heat capacity, K_e is the electronic thermal conductivity, G is the electron-phonon coupling factor, S is an added source term describing energy deposited by the laser pulse, and T_e is the electronic temperature.

Methods and Computational Setup

In order to to simulate laser ablation, the ttm/mod fix in LAMMPS was used to implement an electronic subsystem modeled as a “gas” on a grid overlaying the lattice. The energy transfer between electronic and lattice subsystems are described by the following TTM:

Equation 2. LAMMPS TTM Model

$$C_e\rho_e\frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) - g_p(T_e - T_a) + g_s T_a' + \theta(x - x_{surface})I_0\exp(-x/l_{skin})$$

The new variable introduced in this version of the TTM are g_s, which is the electron-stopping coupling factor. This was set to 0 since the effects of electron-stopping are negligible in laser ablation simulations. The last term describes the laser pulse, which travels in the +x direction. I_o is the absorbed laser intensity and l_{skin} is the skin depth which is dependent on the wavelength of the laser. For the Al lattice, C_e was taken to be linear with T_e with a Sommerfeld coefficient of 135 J/m^{3}K^2. The electronic thermal diffusivity, from which the conductivity is calculated, is taken to be 2 cm^2/s which is typical of most metals. The coupling factor g_p is taken to be 3.1*10^{17} W/m^{3}K. From the following equation:

Equation 3. Relaxation Time

$$\tau_p = 3nk_B/g_p$$

The electron-phonon relaxation time was calculated to be around 8 ps. The mean free path was taken to be 18.9 nm. The electronic pressure is $P_e = B*C_e*T_e$ and B was taken to be .274.

A 100 by 80 by 80 Angstrom(A) simulation box was constructed with a 60 by 80 by 80 A Al lattice in the middle and a 3 by 3 electron grid. The lattice was equilibrated at 300K under a NVT ensemble then placed in an NVE ensemble right before the ttm/mod was implemented. Three finalized simulations were ran, two of which were done with a femtosecond laser and one being a nanosecond laser. The femtosecond laser had parameters of 100 fs pulse duration, 630 nm wavelength, and an absorbed fluence of .1 and .01 J/cm^2. The nanosecond laser had 5 ns pulse duration, 1064 nm wavelength, and an absorbed fluence of 5.2 J/cm^2

Results

Figure 7-9. Al lattice after completion of 100 fs laser pulse (7), 900 fs after (8) and 1900 fs after (9)

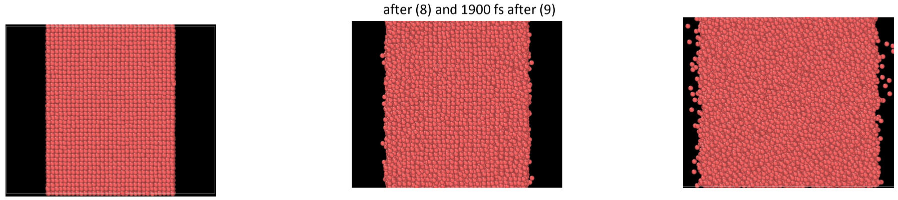
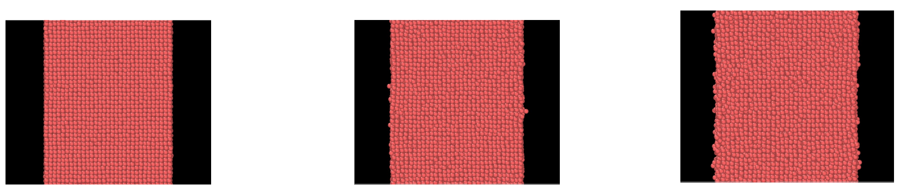


Figure 10-12. Al lattice after 2 ps (10), 7ps after (11) and 10 ps after (12)



Discussion

At a fluence of .01 J/cm^2, no ablation was observed. At .1 J/cm^2 however, ablation was observed, verifying experimental data for the ablation threshold of Al. The ablation occurred while the lattice and electrons non-equilibrated, implying cold ablation is the dominant process in laser ablation. On the nanosecond laser simulation, no ablation behavior was observed and the lattice continued to heat up and average around 1100 K 10 ps after the start of the pulse, while the electrons were at around 1900 K. Although the full pulse could not be simulated due to computational constraints, the data suggests ablation would not have occured in a single pulse and multiple pulses would be needed to engage in hot ablation. In the future with more computing power, a more in depth simulation can be executed and more features can be examined such as ablation depth.

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