Investigation of Different Heating Regimes of Laser Cleaning using Molecular Dynamics Simulations

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ABSTRACT

Different heating regimes of laser cleaning are examined using two-dimensional molecular dynamics simulations. A 12-6 Lennard-Jones potential is used to model the interactions between molecules, which comprise the contaminant particle, the substrate and the energy transfer medium (ETM). Cleaning efficiencies are determined for cases where laser energy is absorbed by the particle, the ETM, and the particle and substrate together. Particle velocities resulting from each type of laser heating are also determined. These cases are compared with the previously analyzed case where the substrate is the only medium that absorbs the laser energy.

Keywords: semiconductor manufacturing industry, particle contamination, laser cleaning, molecular simulations

1 INTRODUCTION

Particle contamination is a major source of yield loss in the semiconductor manufacturing industry [1]. In order to eliminate contamination, super-clean environments are used and surfaces are repeatedly cleaned during production. Current minimum feature sizes of integrated circuits (below 100 nanometers) require the removal of both nano- and micro-scale contaminants, whereas clean rooms and standard cleaning techniques such as wiping, scrubbing and wet-chemical cleaning are only capable of eliminating micro-scale particles [2].

Laser-assisted cleaning is a technique developed in the early 1990s that can efficiently remove micro- and sub-micro-scale particles from critical surfaces. It is a non-contact method that can be applied in two different ways. In dry laser cleaning (DLC), the particle and/or the substrate absorb the laser energy [3]. The impulse generated by the thermal expansion of the absorbing medium results in the removal of particles. In energy transfer medium (ETM) cleaning, a small amount of liquid (known as energy transfer medium) is deposited on the surface. In this case, laser energy is absorbed by any of the media or any combination of them. Particle removal is facilitated by the explosive boiling of the ETM. If the ETM is transparent to the laser energy, heat is transferred to this medium from the particle and/or the substrate via conduction [4, 5].

In this study, a two-dimensional molecular dynamics approach is used to simulate the laser cleaning process. The Lennard-Jones 12-6 potential is used to model the interactions between the molecules in the system that consist of a substrate, an ETM and a particle. In a recent study, ETM cleaning was investigated when the substrate is the medium that absorbs the laser energy. The effects of temperature and ETM thickness on the cleaning efficiencies were examined and good qualitative agreement with the literature was obtained [6]. In another study, the significance of ETM-contaminant particle interaction was analyzed. Cleaning efficiencies in the presence of a wetting and a partially-wetting ETM were determined. It was shown that a strong particle-ETM interaction was needed to facilitate cleaning when the DLC mechanism was not effective [7]. In the present study, we have investigated different laser heating regimes. Specifically, the cleaning efficiencies for different ETM thicknesses and temperatures were determined when the laser energy is absorbed only by the particle, only by the ETM, and by both the particle and the substrate.

2 COMPUTATIONAL MODEL

The system consists of a substrate, an ETM and a particle. In order to lower the computational cost, a two-dimensional molecular model of the system is employed. The Lennard-Jones 12-6 potential is used to model the interactions between the molecules in the substrate, ETM and particle.

$$\varphi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \qquad (1)$$

In Eq. (1), r_{ij} is the distance between molecules i and j, and ε is the depth of the potential well, which is a measure of the strength of interaction. σ is the distance from the origin where the potential equals zero. The results are presented in reduced units, which can be converted to specific units. Detailed information on the conversion from reduced units to dimensional units of Argon molecules is presented in the study by Smith et al. [6]. One reduced unit of temperature is equal to 121 K and one reduced unit of velocity is equal to 154.5 m/s. Potential interactions are truncated at 2.5σ (0.85 nm).

Table 1 shows the selected Lennard-Jones parameters. The parameters for the ETM are equal to unity; ETM is the reference material. For the particle-particle interaction, ε is set to 10 to ensure that the particle stays solid at high temperatures. The value of 1.5 is selected for ETM-substrate and ETM-particle interactions to obtain good wetting of the substrate and particle by the ETM.

Interaction	σ	ε
ETM-ETM	1.0	1.0
ETM-Particle	1.0	1.5
Particle-Particle	1.0	10.0
ETM-Substrate	1.0	1.5
Particle-Substrate	1.0	1.5

Table 1: Lennard-Jones Potential Parameters for Interactions between the ETM, Particle and Substrate

The initial configurations are generated using the Grand Canonical Monte Carlo (GCMC) method, where the number of molecules varies with a specified chemical potential. Figure 1 shows the initial configurations with different ETM thicknesses. In order to obtain statistical accuracy for the cleaning efficiencies, 9 additional configurations are generated for each thickness by running the GCMC simulation for an extra 100 cycles for each configuration.

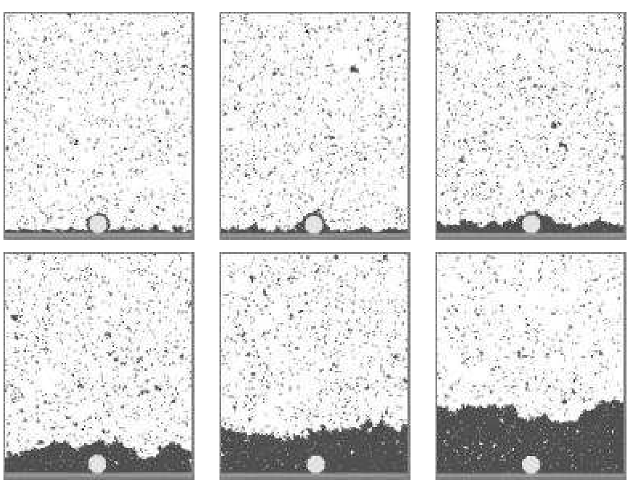

Figure 1: Initial configurations for the fluid thicknesses of 3σ (1.02 nm), 6σ (2.04 nm), 10σ (3.4 nm), 25σ (8.50 nm), 50σ (17.00 nm), and 70σ (23.80 nm).

A two-dimensional domain of size $x=202\sigma$ (68.9 nm) by $y=240\sigma$ (81.6 nm) is used in the simulations. The molecules that reach the top of the domain are reflected back into the domain. This reflection condition in the y-direction has no effect on the results since the important part of the simulation takes place in the lower part of the domain. The domain is periodic in the x-direction.

The substrate and the particle molecules have a hexagonal arrangement. The particle is circular with a diameter of 19σ (6.5 nm). The lowest layer of particle molecules is in contact with the uppermost layer of the substrate. In order to simplify the analysis, the substrate molecules are held fixed and the trampoline cleaning mechanism is not taken into account.

Each simulation was run for 30,000 time steps (0.33 ns). In the simulations, the Gaussian isokinetic thermostat is used. When the particle or the ETM absorbs laser energy, the temperature is enforced by constraining the total kinetic energy of their molecules. The temperature is raised from its base value of 0.4 (48.4 K) to a value between 1.0 (121 K) and 5.0 (605 K) after 250 time steps. A fifth order Gear predictor-corrector algorithm with a time step of 0.005 reduced units (1.1×10^{-14} s) is used to integrate the equation of motion.

3 RESULTS

Cleaning efficiencies vary with the medium that absorbs the laser energy. We determine the efficiencies at different ETM thicknesses and temperatures of the absorbing medium and compare them with the case where the substrate absorbs the laser energy.

Figure 2 shows snapshots of simulations when the laser energy is absorbed by the particle in the presence of an energy transfer medium. In this case, the temperature of the particle increases very rapidly. Heat is transferred from the particle to the neighboring ETM molecules. We observe that the ETM layer explodes radially and the particle gets ejected from the surface.

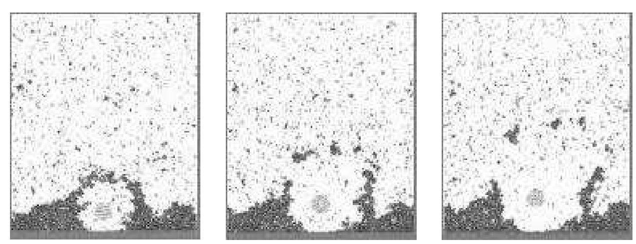

Figure 2: Snapshots of a simulation where the particle absorbs the laser light. The initial thickness of the liquid layer is 25σ and the temperature is 2.5 (302.5 K). From left to right, the elapsed time is 10000 (0.11 ns), 20000 (0.22 ns), and 30000 (0.33 ns).

Cleaning efficiencies are presented in Table 2. At an ETM thickness of 3σ, particle removal starts at a temperature of 1.3. Yet, cleaning is not 100 percent efficient until 1.9. At this temperature, no significant cleaning is achieved with high thicknesses (25, 50 and 70σ). Particle removal is retarded with thickness due to the increasing inertia of the ETM layer above. When the particle absorbs the laser light with no energy transfer medium present, it hops off the surface at very low temperatures (see Figure 3).

Thickness / Temp	3σ	6σ	10σ	25σ	50σ	70σ
1.0	0	0	0	0	0	0
1.1						
1.2	0					
1.3	10					
1.4	30					
1.5	50					
1.6	50	0	0			
1.7	50	20	10	0		
1.8	70	50	30	10	0	
1.9	100	70	50	10	10	0
2.0	90	90	50	10	20	10
2.5	100	100	100	50	70	70
3.0	100	100	100	90	100	100

Table 2: Cleaning efficiencies (percent of simulations that result in particle removal) for all fluid layers when the particle is heated. No entry means that the cleaning efficiency is 0% at that temperature.

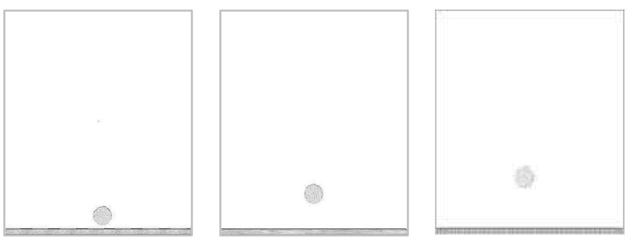

Figure 3: Snapshots of Dry Laser cleaning simulations at different particle temperatures at an elapsed time of 30000 (0.33 ns). From left to right, the temperature is 1.0 (121 K), 1.5 (181.5 K), and 2.5 (302.5 K).

Figure 4 shows snapshots of a simulation where both the particle and the substrate absorb the laser light. We observe that heating both media expels the ETM vertically away from the substrate and also, away from the particle.

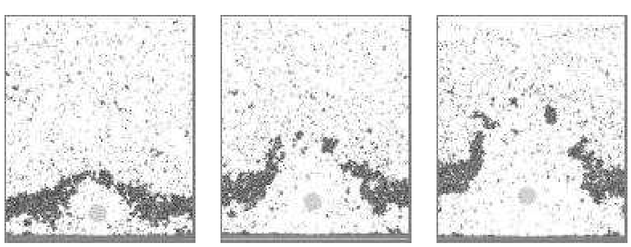

Figure 4: Snapshots of a simulation where both the particle and the substrate absorb the laser light. The initial thickness of the liquid layer is 25σ and the temperature is 1.7 (205.7K). From left to right, the elapsed time is 10000 (0.11 ns), 20000 (0.22 ns), and 30000 (0.33 ns).

Cleaning efficiencies obtained for this case are presented in Table 3. Heating the particle along with the substrate increases the efficiencies for all fluid layers. (See [6] for the cleaning efficiencies for the case where only the substrate absorbs the laser energy.) However, in this case, melting of the particle might pose a problem to the efficiency of cleaning. Note that, when only the substrate is heated, the particle remains intact even at very high temperatures.

Thickness / Temp	3σ	6σ	10σ	25σ	50σ	70σ
1.0	0	10	0	0	0	0
1.1	10	30	10	10	0	0
1.2	30	50	60	30	0	0
1.3	60	70	100	40	30	10
1.4	70	100	100	30	20	20
1.5	90	100	100	80	90	40
1.6	80	100	100	100	100	90
1.7	80	100	100	100	100	90
1.8	100	100	100	100	100	90
1.9	100	100	100	100	100	100
2.0	100	100	100	100	80	100
2.5	100	100	100	100	100	100
3.0	100	100	100	100	100	100

Table 3: Cleaning efficiencies (percent of simulations that result in particle removal) for all fluid layers when the particle and substrate are both heated.

When the ETM absorbs the laser energy, sudden vaporization takes place, as shown in Figure 5. In this case, explosive boiling of the ETM layer is the only particle removal mechanism. The ETM is expelled in every direction and the cleaning force is not concentrated at the substrate/ETM interface.

Table 4 shows the cleaning efficiencies obtained when the ETM is heated. In comparison to substrate heating, cleaning is less efficient. Cleaning efficiency increases until 10σ. However, for ETM thicknesses higher than 10σ, no significant cleaning is obtained.

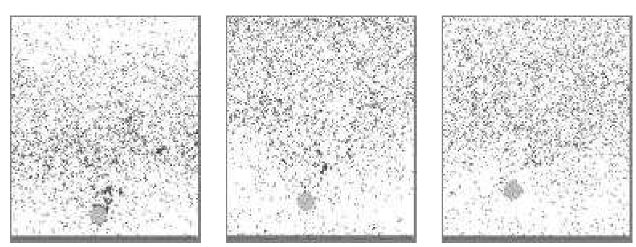

Figure 5: Snapshots of a simulation where the ETM layer absorbs the laser energy. The initial thickness of the liquid layer is 10σ and the temperature is 2.0 (242.0 K). From left to right, the elapsed time is 10000 (0.11 ns), 20000 (0.22 ns), and 30000 (0.33 ns).

Thickness / Temperature	3σ	6σ	10σ
1.0	0	0	0
1.5			
1.6			0
1.7			10
1.8		0	20
1.9		10	50
2.0		30	60
2.5	0	60	100
3.0	10	90	100
3.5	20	100	100
4.0	30	100	100
4.5	40	100	100
5.0	50	100	100

Table 4: Cleaning efficiencies (percent of simulations that result in particle removal) when the ETM is heated. No entry means that the cleaning efficiency is 0% at that temperature.

Figure 6 shows the particle velocities at different laser heating regimes. In case of DLC, the particle velocity reaches a maximum value immediately upon increasing the temperature, and then decreases at a fast rate. With an energy transfer medium, maximum velocities are sustained for longer time periods due to the viscous drag force provided by the lifting ETM molecules. When only the particle is heated in the presence of an ETM, the maximum velocities are lower than those obtained for DLC due to the retardation effect caused by the ETM layer. However, the velocities eventually become equal.

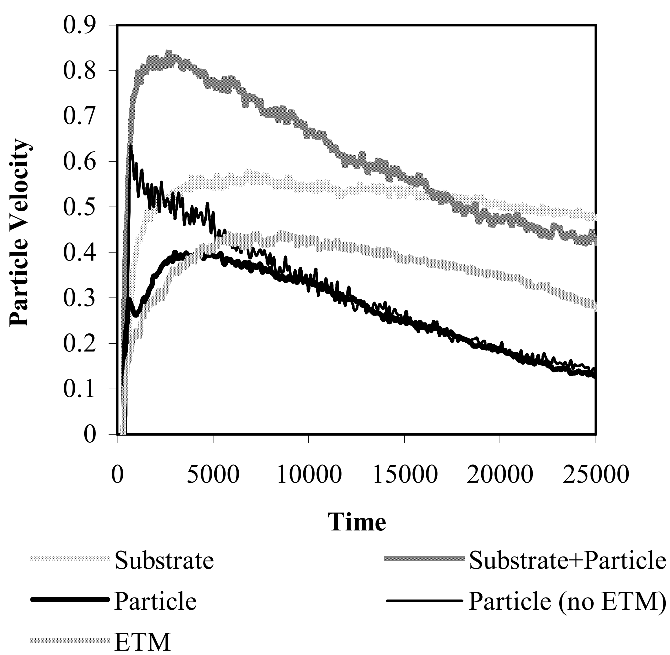

Figure 6. Change in Particle Velocities with Time (Thickness: 10 σ and Temperature=2.5 (302.5 K)).

4 CONCLUSIONS

Laser energy can be absorbed by any of the media in the cleaning system depending on its wavelength. In this study, we have analyzed the cleaning efficiencies at different laser heating regimes.

With the selected parameters, it is possible to remove the particle from the surface when the particle is heated with no ETM present. Yet, the initial acceleration provided in this case is not sustained at later simulation times. When the particle is heated in the presence of an ETM, cleaning is retarded due to the inertia of the ETM layer.

Heating the particle and the substrate is very effective for particle removal. Higher velocities are obtained in comparison to other heating regimes. However, melting of the particle may be a problem in this case.

With an energy transfer medium (substrate heating and ETM heating), maximum velocities are sustained longer. Also, it is possible to keep the particles intact at high temperatures at these heating regimes.

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