# MD Simulations on the Momentum Transfer to Nano Contaminant Particle on Wafer Surface in Collisions with Cleaning Bullets

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## ABSTRACT

In order to understand the correct mechanism of removing nano contaminant particles by momentum transfer, collision between a target contaminant particle sitting on a wafer substrate and cleaning bullet particles was analyzed through molecular dynamics simulations. Even in conditions where the contaminant particle was successfully removed from the surface, the fraction of the bullet kinetic energy transferred to the target particle was very small - 0.066 with Ar bullet, and even smaller - 0.021 with $N_2$ bullet in the nanometer size range. Those values were nearly constant regardless of the velocity and the size of the bullet particle.

***Keywords***: MD simulation, nano-cleaning, momentum transfer

## 1 INTRODUCTION

Target of nano contamination control in the state-of-the-art semiconductor fabrication is expected to decrease from 30nm to 10nm size in 5 years or less. The supersonic nano particle beam technique is one of the most promising techniques in this regards, having shown the nearly perfect cleaning of 20 or 10 nm contaminants experimentally [1]. Despite the success in experimental performance, no theory has yet been proposed on the underlying mechanism. So this study aims to clarify the basic mechanism through MD simulations on momentum transfer during collisions between target contaminant and cleaning bullet particles both in the nanometer size range.

## 2 SIMULATION METHOD

### 2.1 MD Simulation Technique

The MD simulation modeled interactions between Ar atoms using a shifted pair-wise Lennard-Jones potential, Eq. (1), where r is the distance between atoms, ε the characteristic energy, σ the length scale.

$$V_{LJ}(r) = 4\varepsilon \left[ (\sigma / r)^{12} - (\sigma / r)^{6} \right] + r\delta V \qquad (1)$$

An additional correction term $r\delta V$ is included so that the force vanishes at the cutoff distance ($r_c$), and the shifted potential, Eq. (2), was used in this study with $r_c = 2.5\ \sigma$.

$$V_{shifted}(r) = \begin{cases} V(r) - V(r_c) - \left(\dfrac{dV(r)}{dr}\right)_{r_c}(r - r_c) & \text{when } r < r_c \\ = 0 & \text{when } r \geq r_c \end{cases} \qquad (2)$$

LJ potential parameters for Ar, $N_2$ were chosen as $\sigma_{Ar}$ = 3.405 Å, $\sigma_N$ = 3.31 Å, $\varepsilon_{Ar}/k_B$ = 120 K, $\varepsilon_N/k_B$ = 37.3K. Also the atomic mass was set as $m_{Ar}$ = 40 amu, $m_{N2}$ = 28 amu, where $k_B$ is the Boltzmann constant. The natural time unit in the calculations is then $\tau = (m_{Ar}\sigma_{Ar}^2/\varepsilon_{Ar})^{1/2} = 2.16\times10^{-12}$ s. The dimensionless velocity (v*) is $v(m_{Ar}/\ \varepsilon_{Ar})^{1/2}$ with v* = 1.0 corresponding to v = 158 m/s. Dimensionless temperature T* was scaled to $\varepsilon_{Ar}/k_B$ = 120 K, and parameter values for $N_2$ was also scaled to the values for Ar. The equations of motion for each atom were integrated using Leap frog algorithm with a time step of 0.002 τ (~ $4.32\times10^{-15}$s). Atoms forming both the particles were all placed on FCC lattice points initially.

### 2.2 System Configuration

Nano-cleaning system used for MD simulation is as shown in Fig. 1 (a). The wall molecules are made practically motionless by assigning a very large mass ($10^8$). The number of molecules constituting the contaminant particle is 1056, and the number of wall molecules is 22440. Number density of the bullet, the contaminant particle and the wall is $1.0\sigma_{Ar}^{-3}$ and the temperature of contaminant particle and the wall are $2.5\varepsilon_{Ar}/k_B$ (300K). Bullet consisting of argon or nitrogen was simulated at cryogenic condition of about 36K, typical of particles formed in supersonic expansion [2]. The overall computation domain size is $140\sigma_{Ar}\times60\sigma_{Ar}\times40\sigma_{Ar}$. Periodic boundary conditions were applied in the x- and y-direction, but reflective boundary condition is used for the upper z boundary. The domain size is set larger in the x-direction at 140 $\sigma_{Ar}$ so that the effect of bullet residues to obstruct the move of contaminant can be minimized. The contaminant was allowed to adhere on the substrate during the initial 2000 time steps. After adhesion, the overall system was equilibrated for 20,000 time steps under the condition of constant temperature thermostat. Nano-sized bullet particle was shot right toward the center of the contaminant at a variety of velocities but at a constant angle of 45° to maximize the cleaning efficiency [3]. The collision process is schematically shown in Fig. 1(b). During shooting process, only the wall temperature was controlled by thermostatting.

Figure 1 (a) : Initial placement of bullet, contaminant and wall.

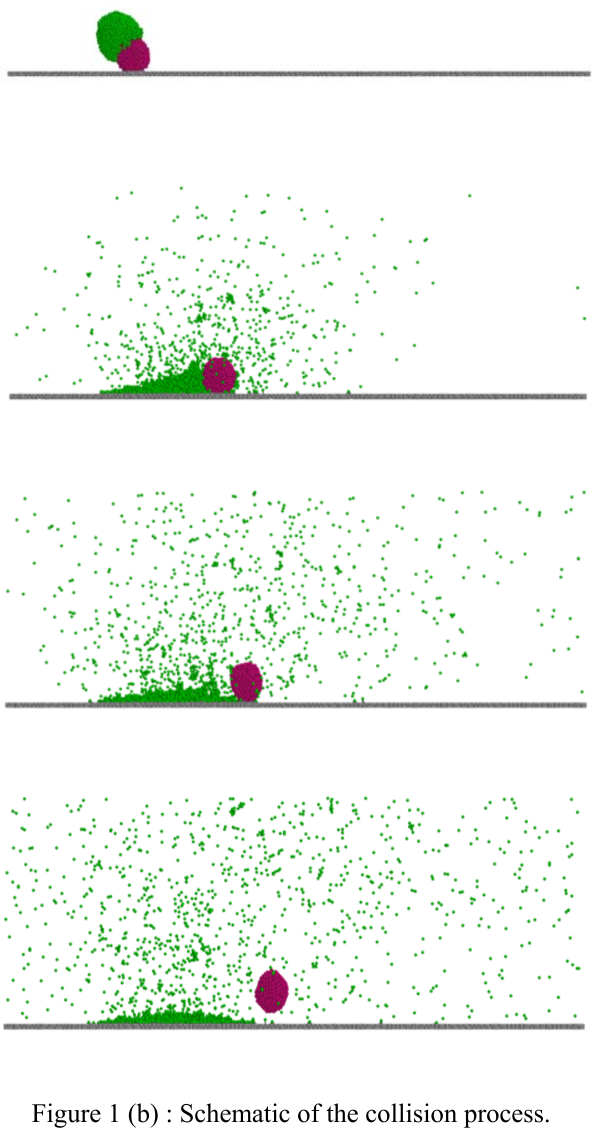

Figure 1 (b) : Schematic of the collision process.

## 3 RESULTS AND DISCUSSION

### 3.1 Conditions for removal

Removal of the contaminant is determined by two parameters - the size ($R_b$*) and the velocity ($V_b$*) of the bullet, which determines the amount of kinetic energy the contaminant gets from the bullet. Simulations were done for a target of radius 6.5 and with three different bullet velocities - 2.0, 3.0, 4.0 - and four different bullet sizes (radii) - 5.0, 6.0, 7.0, 8.0. Criterion for removal was the take-off of the contaminant from the substrate within the domain.

Final results are summarized in Table 1 for Ar bullet and in Table 2 for $N_2$ bullet with O(removed) and X(not removed). In general, removal was more sensitive to the bullet velocity than to the bullet size: larger bullet particles removed the contaminant at a lower bullet velocity, but the effect of velocity is more dominant than bullet size.

The velocity required for removal with Ar bullet was about 2.5 ~ 3 (395 ~ 484m/s), but was 4.5 ~ 5 (711 ~ 790m/s) with $N_2$ bullet, which is almost twice as high as with Ar bullet.

| $R_b$* / $V_b$* | 5.0 (1.71nm) | 6.0 (2.05nm) | 7.0 (2.39nm) | 8.0 (2.73nm) |
|---|---|---|---|---|
| 2.0 (316m/s) | X | X | X | X |
| 2.5 (395m/s) | X | X | X | O |
| 3.0 (474m/s) | O | O | O | O |

O = suceess, X = failed, $R_c$*=6.5 (2.22nm)

Table 1 : Summary of removal contaminant for Ar bullet.

| $R_b$* / $V_b$* | 5.0 (1.71nm) | 6.0 (2.05nm) | 7.0 (2.39nm) | 8.0 (2.73nm) |
|---|---|---|---|---|
| 4.0 (632m/s) | X | X | X | X |
| 4.5 (711m/s) | X | X | X | O |
| 5.0 (790m/s) | O | O | O | O |

Table 2 : Summary of removal contaminant for $N_2$ bullet.

## 3.2 Transfer of kinetic energy

Take-off of the contaminant is determined by the sliding/rolling velocity, and the centre-of-mass kinetic energy of the contaminant required for take-off should be orders of magnitude greater than the adhesion energy on the substrate. Typical time change of the centre-of-mass kinetic energy of both the Ar bullet and the target particle during the collision process was shown in Fig 2 (a), for Ar bullet with $V_b$*=2.5 and $R_b$*=8.0. In this case, the adhesion energy of the contaminant was about 200$\varepsilon_{Ar}$ and initial kinetic energy of the bullet was about 7900$\varepsilon_{Ar}$. Part of the bullet kinetic energy is transferred to the contaminant, and the other transferred to the substrate or the fragmenting bullet molecules.

The contaminant acquired about 520$\varepsilon_{Ar}$ at the moment of collision, and the contaminant velocity reduced a little bit while moving on the substrate. Finally, the contaminant took off the substrate, and the kinetic energy did not change thereafter. The fraction of the bullet kinetic energy transferred to the contaminant during the short collision was about 0.066, which is quite small.

Similar simulations were repeated for a $N_2$ bullet as shown in Fig 2 (a), for $V_b$*=5.0 and $R_b$*=8.0. Initial kinetic energy of the $N_2$ bullet was about 18700$\varepsilon_{Ar}$, and the kinetic energy acquired by the contaminant was about 400$\varepsilon_{Ar}$. From this result, the fraction of the bullet kinetic energy transferred to the target particle was obtained as 0.021, even smaller than for Ar.

The fraction of bullet kinetic energy transferred to the contaminant during collisions that resulted in successful removal for a variety of bullet conditions was summarized in Fig. 3. The fraction of transferred kinetic energy was nearly unchanged under a wide variation of velocity and size of the bullet particle, but was sensitively dependent on the species of the bullet molecule: 0.06 to 0.07 with Ar bullet and 0.02 to 0.03 with $N_2$ bullet, respectively.

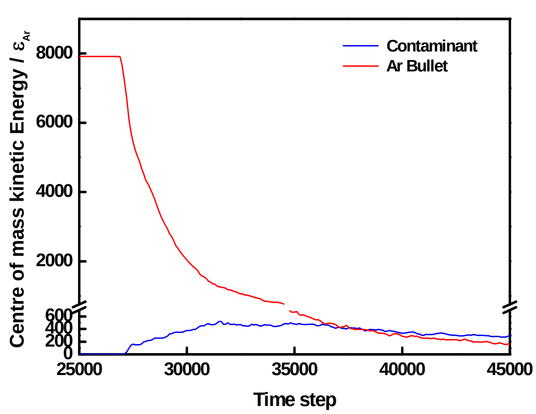


Figure 2 (a) : Change of the centre-of-mass kinetic energy with Ar bullet at $V_b$* =2.5 and $R_b$*=8.0

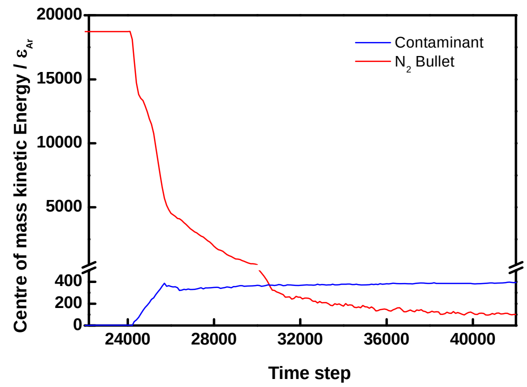


Figure 2 (b) : Change of the centre-of-mass kinetic energy with $N_2$ bullet at $V_b$* =5.0 and $R_b$* =8.0.

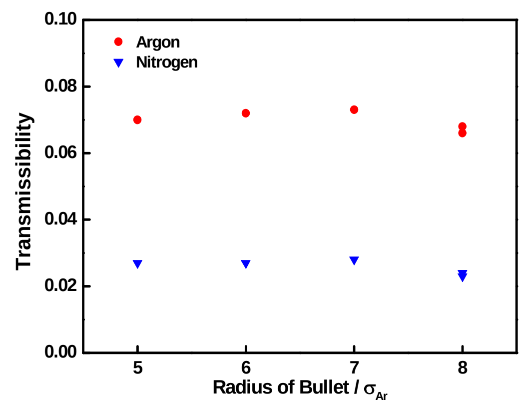


Figure 3: Fraction of the bullet kinetic energy transferred to the contaminant for two different bullets at various sizes, all for conditions of successful removal.

# 4 CONCLUSION

Momentum transfer during collisions between target contaminant and cleaning bullet particles was analyzed using MD simulation with the findings summarized as follows :

1. The cleaning effect for the changes of velocity was greater than for the change of size (mass).
2. The fraction of transferred kinetic energy showed 0.06 ~ 0.07 with Ar bullet and 0.02 ~ 0.03 $N_2$ bullet, which is nearly constant regardless of the velocity and the size of the bullet particle.

# 5 ACKNOWLEDGMENT

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