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# Characteristics of kinetic energy transfer in collisions between a fragile nano-particle and a rigid particle on a surface



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## ABSTRACT

The characteristics of kinetic energy transfer during a collision between a rigid target particle on a surface and a fragile bullet particle (BP) moving at a high velocity were analyzed by Molecular Dynamics (MD) simulation. Ar, N<sub>2</sub>, and CO<sub>2</sub> BPs were considered; their size, temperature and velocity were varied over a wide range. The fraction ( $F_K$ ) of kinetic energy transferred from the BP to the target particle was almost independent of BP size or velocity, but was sensitively dependent on BP type and temperature. The rigidity or the average potential energy of the BP was a dominant factor determining the post-collision behavior of the target particle and  $F_K$ .  $F_K$  was almost linearly proportional to the average potential energy per molecule of the BP.

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## 1. Introduction

Contaminant particles (CPs) on submicron-scale devices can significantly reduce their manufacturing yield. Sizes of semiconductor device features are expected to be decreased continuously, reaching 25 nm by 2015 for DRAM/Flash memory devices; together with this decrease, the size of CP that can cause circuit failure should be reduced to 12.5 nm (Sematech, 2011). The adhesion force per contact area between a nano-sized particle and surface increases linearly as particle size decreases (Bakhtari, Guldiken, Makaram, Busnaina, & Park, 2006), but the drag force exerting on the CP by a flow of gas (cleaning flow) is proportional to the cross-sectional area of the CP, so the efficiency with which CPs can be removed by cleaning flow decreases as CP size decreases; therefore the applicability of flow cleaning is limited to contaminants  $\geq 50$  nm (Lim, Jang, Kim, Lee, & Lee, 2005; Lin, Chioujones, Lauerhaas, Freebern, & Yu, 2007; Rimai & Quesnel, 2001; Sherman, 1999).

One promising particle-removal alternative that is applicable in the nanometer range is the particle beam technique, in which the contaminated surface is bombarded by fine BPs of volatile material at high velocity. High-velocity collisions can impart sufficient energy to remove the adhered CPs from the surface; upon collision the volatile BPs fragment into vapor molecules, which are removed easily from the surface. BPs are usually generated by homogeneous nucleation and growth during supersonic expansion of a gas. Commonly-used gases include Ar, N<sub>2</sub> and CO<sub>2</sub>, which form volatile particles easily because they cool quickly due to their high specific heat ratio (Bae, Kim, Kim, & Lee, 2010; Choi, Yi, Lee, & Lee, 2012; Yang, Lee, Choi, Yi, & Lee, 2009).

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Particle beams shot at supersonic velocities can remove CPs of 10-nm diameter when the BPs are of sizes similar to those of the CPs (Hwang, Lee, Kim, & Lee, 2011; Kim, Hwang, & Lee, 2012). The mechanism of the CP removal for Ar BPs has been analyzed by MD simulation (Choi, Yi, & Lee, 2013; Yi, Kim, Lee, & Koplík, 2005), but the general characteristics of kinetic energy transfer during collisions between BPs and CPs have not been studied yet.

The purposes of this study were to use molecular dynamics (MD) simulation to reveal the characteristics of kinetic energy transfer for BPs made of Ar, N<sub>2</sub> or CO<sub>2</sub> at various sizes, temperatures and velocities, and to derive an empirical formula for the fraction ( $F_K$ ) of kinetic energy transferred from the BP to the CP.

## 2. Simulation methods

The behaviors of the molecules comprising the BP and the CP were analyzed using MD simulation, in which Newton's equations of motion for each molecule were solved simultaneously using the Lennard–Jones (LJ) inter-molecular interaction potential function (Eq. (1)), which is applicable for Ar, N<sub>2</sub>, and CO<sub>2</sub> molecules:

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

where  $r$  (m) is the distance between interacting molecules,  $\varepsilon$  (J) is the characteristic energy and  $\sigma$  (m) is the characteristic length.  $r\delta V$  is a correction term to reduce the truncation error, so that the force vanishes at a finite cutoff distance ( $r_c$ ); the corrected potential is called the shifted potential,  $V_{shifted}(r)$  (Eq. (2)).  $r_c = 2.5\sigma$  was used in this study, following previous studies (Choi et al., 2011, 2013; Yang et al., 2009; Yi et al., 2005).

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

LJ potential parameters for Ar, N<sub>2</sub>, CO<sub>2</sub> and Si (Table 1) (Allen & Tildesley, 1989; Chen, Shibuta, Kambara, & Yoshida, 2012; Wilhelm & Battino, 1971) were sometimes used as dimensionless values (Table 2) normalized to the values of Ar; these values are asterisked in the following presentation. The equations of motion were integrated using the leap-frog algorithm (Hockney, 1970) with an integration time step of  $0.002\tau_{Ar}$  ( $\sim 4.32 \times 10^{-15}$  s).

The system for MD simulation consisted of a substrate with a CP adhered to it, and a nano-sized BP shot at a specified velocity ( $V$ , m/s) (Fig. 1). The dimensionless diameter ( $D_b^*$ ) of the BP was varied in the range of 10–16, and the number of molecules in a BP was adjusted to the BP diameter required. The substrate consisted of 22,440 Si molecules with the same number density as the BP, but was made practically motionless by assigning it a very large mass,  $4 \times 10^9$  amu =  $6.6 \times 10^{-15}$  g. The CP had diameter ( $D_c^*$ ) of 13 (4.42 nm), and consisted of 2056 LJ molecules of 20-amu mass, which is the mid-range of BP size.  $F_K$  is quite insensitive to variation of the molecular weight of the CP molecule (Choi et al., 2013). The number density of the CP molecules was twice as high as that of the BP and the potential well-depth was  $\varepsilon^* = 10$ ; this means that the CP was a little softer than an Al or Cu particle.

The size of the computational domain was  $140\sigma_{Ar} \times 60\sigma_{Ar} \times 40\sigma_{Ar}$  ( $x \times y \times z$ ). Periodic boundary conditions were applied in the  $x$ -direction and  $z$ -direction, and a reflective boundary condition was used for the upper  $y$ -boundary. The domain size was set large in the  $x$ -direction to minimize the obstructing effect of BP residues on CP movement. Initially, molecules comprising the BP and the CP were placed on face-centered cubic lattice points and the substrate molecules were placed in the diamond lattice structure. The CP was then set to adhere to the substrate under the Nosé–Hoover thermostat at 300 K, and the final adhesion energy between the CP and the substrate was  $\sim 200\varepsilon_{Ar}$ , which is comparable to that of a silicon CP of the same size (Dahneke, 1972). Because the adhesion energy does not differ much among typical materials (from silicon and oxides to metal Cu) used in wafer fabrication, the simulation conditions can be considered to represent typical process conditions.

After adhesion was completed, the overall system was equilibrated for another 20,000 time steps under constant temperature maintained by a Nosé–Hoover thermostat. The temperature of the CP and the substrate was 300 K, but the temperature of the BPs was varied depending on the simulation condition. The BP was shot toward the center of the CP at 45° incidence angle, and only the substrate temperature was controlled by the thermostat thereafter.

**Table 1**  
LJ parameters for Ar, N<sub>2</sub>, CO<sub>2</sub> and Si.

Species	Molecular weight (amu)	$\sigma$ (Å)	$\varepsilon/k_B$ (K)
Ar	40	3.41	120
N <sub>2</sub>	28	3.70	95
CO <sub>2</sub>	44	3.94	195
Si	$4 \times 10^9$	3.83	202

$k_B$ : Boltzmann constant.

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