Impacts with Initial Rotation in Nanocluster Deposition

Aruna Awasthi

Industrial Research Limited, PO Box 31-310 Lower Hutt 5040, New Zealand
(Received 10 November 2008; Accepted 9 December 2008; Published 25 December 2008)

Molecular dynamics simulations are presented for the angular collisions of 561-atom icosahedral cluster on a weakly attractive substrate. We study the effect of rotational motion of the cluster at various impact velocities and incident angles. The outcome of the collision is determined by incident kinetic energy of the cluster and the cluster-surface adhesion energy. Energy losses are greater when the collisions of the cluster with initial angular velocity are considered. At larger impact angles, the cluster loses a relatively larger amount of rotational kinetic energy by the collision. The transition from reflection to adhesion is observed at high initial angular velocities due to increase in the rotational kinetic energy and plastic deformation of the cluster. [DOI: 10.1380/ejssnt.2008.307]

Keywords: Nanocluster deposition; Cluster rotation; Molecular dynamics

I. INTRODUCTION

Collisions between clusters and solid surfaces show several unique features which have been given increased attention during recent years (for a recent review see Ref. [1]). For over 30 years, a large amount of effort has been invested in understanding thin film deposition from cluster-surface collisions. During the collision of a cluster with the surface various outcomes such as adhesion [2], scattering [3, 4], fragmentation [5–10] etc. are possible, depending on the available energy of the cluster. Our aim in the present study is to investigate collisions between clusters and surfaces at intermediate regime between the soft-landing and fragmentation regime where clusters undergo reflection. Most of the thin film studies were performed to explain some of the relationships between deposition conditions (incident energy, incident angle, cluster size, cluster temperature etc) and the resulting film properties and structures [11–13]. To date, however, little direct information has been gathered on the dynamic process of rotation of the cluster during impact. A range of earlier experimental and computational studies [14–18] on different spinning sports balls have been performed in the bat-ball collision. It is found that a ball can hit faster if it is projected without spin but it can hit farther if it is projected with a backspin due to aerodynamic lift force [17]. In general there is a tradeoff between the spin and speed that can be imparted to a ball. This has motivated us to carry out the study of cluster impact behavior which can include the effect of cluster rotation in the collision process.

The purpose of this paper is to focus on the dynamics of rotating cluster which is incident at the surface at various impact angles. Previous work using the same theoretical approach has been described for the normal and oblique collisions [19, 20]. During impact of the cluster with the surface, one or more of the following occurs: elastic deformation of the cluster resulting in adhesion of the cluster to a region, and/or plastic deformation of the cluster resulting in reflecting or bouncing or sliding of one or more clusters from a region, and/or plastic deformation of the cluster resulting in adhesion of one or more clusters to a region, and/or plastic deformation of the cluster resulting in reflecting or bouncing of one or more clusters from a region. In this paper the emphasis is on describing the effects of rotational motion of the cluster to show plastic deformation of the cluster resulting in adhesion of clusters to a weakly attractive surface.

II. METHODOLOGY

Among the various simulation techniques that may be used, molecular dynamics (MD) simulation is especially well suited to study the cluster-surface collision because this process typically occurs within a few picoseconds. MD simulations allow one to trace atomic motions and alter conditions of the system that may not be easily varied experimentally. Therefore, simulations can provide valuable information about the atomic mechanisms responsible for the resulting properties and structures. In the MD simulation method, the classical equations of motion are numerically integrated to yield a time record of position and velocity of each coordinates of the atoms. The interaction between the atoms is modeled using modified form of the Lennard Jones (LJ) potential

\[ LJ(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - C \left( \frac{\sigma}{r} \right)^{6} \right] \]

for \( r < r_c \). Here \( r \) is the inter-atomic separation (with potential cut-off \( r_c \)), \( \sigma \) is the LJ radius and \( \varepsilon \) is the depth of potential well. For our system the parameters \( \varepsilon \) and \( \sigma \) are the same for all atoms, although the constant \( C \), which is used as a scaling factor to the attractive part of the potential, is varied to control the attraction between surface and cluster atoms. The cut-off distance is set at \( 6\sigma \) to enable us to probe a collision regime where the kinetic energy and adhesion energy are delicately balanced. Newton’s equations are integrated with velocity Verlet scheme. We have simulated the collisions of 561-atom Mackay icosahedra with a (111) terminated fcc surface as shown in Fig. 1. The surface slab consists of a fixed bottom layer and 15 layers of dynamic atoms with about 8000 atoms arranged in fcc crystalline structure and exposing a (111) surface facet. The surface has the dimensions of \( 11.7\sigma \) by \( 11.3\sigma \) by \( 10.5\sigma \). Newtonian dynamics is

---

*This paper was presented at International Symposium on Surface Science and Nanotechnology (ISSS-5), Waseda University, Japan, 9-13 November, 2008.
†Corresponding author: a.awasthi@irl.cri.nz
applied to the central part of atoms while outer region follows Langevin dynamics at a temperature $T$. The friction parameter is varied linearly from 0 at the Langevin Newtonian interface to 2 at the Langevin exterior in Langevin region. This block of 5846 Langevin atoms regulates the temperature of the 1344 Newtonian atoms and absorbs energy from the cluster impact. The surface computational cell is repeated periodically in the two dimensions parallel to the (111) surface plane, with no periodic boundary conditions applied in the $z$-direction. For intra-atomic collisions (atoms within the cluster and within the surface) $C$ is taken as unity i.e. standard LJ potential whereas $C$ is varied between 0 and 1 for inter-atomic collision to control the attraction between the cluster and surface. To adopt relaxed configurations, both cluster and surface were equilibrated at the temperature of 0.13 units using $\sigma$, $\varepsilon$ and $\tau$ as characteristic length, energy and time scales, respectively. The direction of motion of the cluster is specified in terms of the angle of the velocity vector with respect to the horizontal. This angle ranges from 25-90°.

III. RESULTS AND DISCUSSIONS

Collisions are simulated for a range of parameters including the incident cluster velocity $v_0$, the angle of incidence $\theta_i$, the cluster-surface interaction $C$, and the z-component of incident angular velocity $\omega_z$. We have considered here the impacts of 561-atom cluster on the surface at $C = 0.2$ i.e. at low value of $C$, which result in the reflection of the cluster. We have first discussed the time variation of the cluster which is incident at an angle of 35° to the substrate plane with and without initial angular velocities. The effects of increasing angular velocity at $\theta_i = 35°$ on Weber number and cluster energies are explained in Section B. The cluster rotation at various impact angles is examined in the last section.

A. Time evolution of the collision with and without initial spin

This section presents the simulation results of a cluster colliding with a surface at an incident angle of 35° to the substrate plane. We selected a fixed cluster orientation relative to the surface and placed the cluster so that the separation between the cluster atoms and the surface was at least 6\sigma. The cluster was then given a prescribed velocity, $v_0 = 1.0$, towards the surface. As shown in Fig. 2(a), the time of impact process was simulated for 35\tau, with the collisions timed to occur approximately 1/4 of the way into the simulation. The time evolution of the collision was studied for three different values of z-component of initial angular velocities ($\omega_z = 0$, $\omega_z = 0.08$ and $\omega_z = 0.24$). Figure 2(a) shows a plot of center of mass position $Z_{cm}$ (where $Z$ is the coordinate component in the direction normal to the surface) versus time for no spin (solid line), $\omega_z = 0.08$ (dashed line) and $\omega_z = 0.24$ (dotted line). At the beginning of the simulation, $Z_{cm}$ decreases linearly with time during the free flight period before the cluster begins to interact with the surface. The initial distance of the cluster from the surface was chosen so that impact occurred at approximately $\tau = 8$ as is evident in Fig. 2(a). Note that after the collision ($\tau > 8$), $Z_{cm}$ increases linearly with time for all the three cases indicating that the cluster has escaped from the surface. The rebound cluster height above the surface for $\omega_z = 0$ is seen to be substantially greater than that for $\omega_z \neq 0$ which indicates that the cluster has been only partially compressed at impact. And as $\omega_z$ increases, we see that $Z_{cm}$ peak decreases indicating greater energy loss on adding initial angular velocity to the cluster.

The translational kinetic energy of the cluster, $E_{k_z}$, in the direction perpendicular to the surface versus time is shown in Fig. 2(b). Initially $E_{k_z}$ of the cluster decreases due to the energy transfer to the surface and this energy is mainly stored as elastic energy of the surface. After the cluster bounce, the magnitude of the cluster final kinetic energy is less than that of initial kinetic energy, indicating that a part of the center-of-mass energy was lost. This translational kinetic energy dissipates to cluster rotation and further on to intra and inter atomic cluster potential energy.

Time variation of total potential energy of a cluster with initial angular velocities is shown in Fig. 2(c). The total cluster potential energy per atom, $E_p$, is the sum of cluster internal energy per atom and cluster-surface interaction energy per atom (the adhesion energy, $E_{ad}$). As seen in Fig. 2(c), $E_p$ at first increases when cluster gets compressed upon collision and recovers later after the bounce. The increase in cluster potential energy at the impact is due to a substantial perturbation of the initial low energy structure. $E_{ad}$ decreases (i.e. the adhesive energy increases) in Fig. 2(d) due to the attraction between the cluster and surface. The potential energy increment of a cluster during impact indicates the deformation of the cluster. The cluster potential energy increases with increasing angular impact energy under the same incidence angle.

Figure 2(e) shows the evolution of $z$-component of the radius of gyration ($R_z$) and is a measure of the distribution of mass within the cluster about $z$-axis. This is a
useful quantity for tracking the deformation of the cluster during the impact. In all the three cases $R_z$ increases sharply at the impact. At $	au = 8$ maximum deformation occurs and this deformation also increases with the increase in angular velocity of the cluster. At $\omega_z = 0$ the deformation is small and reversible suggesting that the deformation is nearly elastic. As the angular velocity becomes higher, the collision shows evidence of irreversible (plastic) deformation. The general trend is that translation and rotation of individual atoms within the cluster couples strongly to the surface resulting in a compression phase of the cluster. Correspondingly, we note that this deformation of the cluster during impact leads to an increase in cluster temperature as shown in Fig. 2(f). This is evident from the spike in thermal kinetic energy, $E_{\text{thermal}}$, at impact followed by the drop in $E_{\text{thermal}}$ after rapid cooling of the cluster when the cluster thereafter leaves the surface. In Fig. 2(g), the reflected angles of the cluster that bounce from the surface are shown when the cluster is launched at an incident angle of 35°. The incident angle ($\theta_i$) and the reflected angle ($\theta_r$) are calculated using the initial and final velocities (represented by 0 and $f$ subscripts, respectively) with the normal and tangential components of the approach, given by the following relationship:

$$
\theta_i = \tan^{-1} \left( \frac{v_{0z}}{v_{0y}} \right) \quad \text{and} \quad \theta_r = \tan^{-1} \left( \frac{v_fz}{v_{fy}} \right),
$$

where the subscripts $z$ and $y$ refer to the normal and tangential components, respectively of the respective velocities. At $C = 0.2$ it can be seen that the rebound motion of the cluster depends on the initial angular velocity of the cluster. As the initial angular velocity increases, larger deformation of the cluster at a given velocity produces larger adhesion energy during impact. This leads to smaller rebound angle which is observed in Fig. 2(g).

### B. Effects of increasing initial angular velocity

Here, we will study the effect of increasing $z$-component of initial angular velocity, $\omega_z$, for various normal components of incident velocity ($v_{0z}$) at an impact angle of 35°. The transition from reflection to adhesion is observed when $\omega_z = 0.64$, 0.52, 0.48, 0.36, 0.28 and 0.24 for $v_{0z} = 0.16$, 0.25, 0.37, 0.47, 0.59 and 0.8, respectively. It can be concluded that when the cluster’s kinetic energy at impact falls below a threshold, it makes a transition from the reflection to the adhesion. It is convenient to characterize the collision process in terms of Weber number which is the ratio of kinetic energy and adhesion energy. Figure 3(a) shows the Weber number of the clusters at the pull off, $W_{ez} = E_{kz}/E_{cs}$ as a function of $\omega_z$ when $v_{0z} = 0.47$. This ratio is a good predictor of the outcome of the collision i.e. if $W_{ez} < 1$ the cluster would adhere to the surface and if $W_{ez} > 1$, the cluster is reflected. For low angular velocities ($\omega_z < 0.36$), the cluster undergoes less deformation which results in smaller adhesion energy during impact. This leads to larger Weber number and as $W_{ez}$ approaches and exceeds 1, the reflected kinetic energy of the cluster dominates. But for $\omega_z > 0.36$, due to greater rotational energy, the cluster undergoes plastic deformation which results in greater adhesion energy during impact. Hence $W_{ez}$ becomes smaller than unity. It is observed for all other $v_{0z}$ that the average translational energy tends to decrease with increasing rotational energy and therefore, transition from reflection to adhesion is seen. It is observed here that energy conservation between rotational and translational motion is in agreement with classical mechanics, which predicts that clusters with
higher rotational energy have less translational energy.

Figure 3(b) shows the variation of cluster potential energy, $E_c$, and the radius of gyration, $R_g$, with $\omega_z$ for $v_{0z} = 0.47$. In the low deformation regime ($\omega_z < 0.36$) there is very small increment in cluster potential energy and the radius of gyration. Whereas in the strong deformation regime, $\omega_z > 0.36$, cluster potential energy increases due to increase in the plastic deformation of the cluster as the initial angular velocity increases. The cluster temperature and rotational energy strongly influence the qualitative features of the cluster-surface collision for $\omega_z > 0.36$ as shown in Fig. 3(c). In this regime, the translational kinetic energy is greatly dominated by rotational kinetic energy of the cluster. Similar type of behaviour is also observed for other normal component of incident velocities. At low values of $\omega_z$, atomic translational properties dominate whereas atomic rotation is much influenced by the cluster impact when the initial angular velocity is increased.

C. Cluster rotation at various impact angles

In this section, the collisions of the 561-atom icosahedral cluster at various incident angles, $\theta_i$, with $C = 0.2$ are investigated at fixed prescribed impact velocity ($v_0 = 1.0$), which would allow us to see the reflection behavior at different off-normal component of initial velocities. In Fig. 4(a) we have plotted the normal coefficient of restitution ($e_z$) as a function of impact angle, since the probability of adhesion is largely determined by the normal component of the incident velocity. For oblique collisions, the normal coefficient of restitution is defined as the ratio of normal velocity components after and before impact (at peak velocity prior to and after impact): $e_z = -v_{zf}/v_{0z}$. Figure 4(a) also shows the variation of tangential coefficient of restitution with impact angle and it can be defined as the ratio of tangential velocity components near the pull off: $e_y = -v_{yf}/v_{0y}$. Here 0 and f subscripts represent the velocities before and after impact, respectively. It can be seen from Fig. 4(a) that the tangential coefficient of restitution is roughly constant and is equal to unity for no initial angular velocity whereas it decreases slightly at larger angles when $\omega_z$ is included. As $\theta_i$ increases the normal component of the incident velocity increases ($v_{0z} = v_0 \sin \theta_i$). It is observed that at low incident angles, $e_z = e_y = 1$ which is expected at low $v_{0z}$, since we expect elastic bouncing in this regime. The plot is consistent with significant deformation of the clusters at higher incident angles as $v_{0z}$ increases and there is significant energy loss i.e. $e_z < 1$. Therefore, $e_z$ shows velocity dependence as the normal component of velocity decreases $e_z$ decreases. The normal coefficient of restitution is lowered when the initial angular velocity is taken into consideration since $e_z$ is associated with the momentum loss during the impact and hence with the deformation of the cluster.

Figure 4(b) shows the variation of rotational kinetic energy $E_{rot}$ of the cluster as a function of incident angle, $\theta_i$. When the initial angular velocity is applied to the cluster ($\omega_z = 0.2$) $E_{rot}$ increases dramatically. As $\theta_i$ increases from 35° to 90° the normal component of the velocity ($v_{0z}$) also increases, the amount of rotational kinetic energy decreases due to strong deformation of the cluster which leads to an increase in contact area and adhesive energy. The cluster experiences more plastic deformation at large normal component of the velocity, $v_{0z}$, and the final cluster temperature increases. This suggests that high impact momentum normal to the surface could facilitate adhesion.
IV. CONCLUSIONS

We have studied the reflection phenomenon of the 561-atom cluster at various values of initial angular velocity at a constant impact velocity, $v_0 = 1.0$. The cluster collision with the surface includes energy transfer from cluster center-of-mass kinetic energy, to translational and rotational energy, as well as cluster potential energy and adhesion energy. The normal coefficient of restitution, $e_z$, and rotational kinetic energy decreases by changing the incident angle, $\theta_i$, from 35° to 90° which suggests that the energy dissipation is much stronger at large angles. The effects of initial angular velocities are significant on all the calculations, including $e_z$ and energy losses. Rebound occurs for low adhesion and low initial angular velocity, however, the particle is captured by the surface when the adhesion energy and rotational kinetic energy of the cluster increases. It is observed that the rotational kinetic energy of the cluster increases quite a lot for the angular impacts as compared to the normal collisions.

Acknowledgments

This study is supported by FRST funded multi-scale modeling M5 program of New Zealand through Research Project No. 33603000.

[1] W. Harbich, in Metal Clusters at Surfaces, Ed. H. H. Meiwes-Broer (Springer, Berlin, 2000), pp. 108-150.
[2] A. Tomsic, P. U. Andersson, N. Markovic, W. Piskorz, M. Svanberg, and J. Pettersson, Phys. Rev. B 115, 115422 (2001).
[3] J. D. Kress, D. E. Hanson, A. F. Voter, C. L. Liu, X. Y. Liu, and D. G. Coronell, J. Vac. Sci. Technol. A 17, 2819 (1999).
[4] E. V. Pugina, G. V. Kornich, and G. Betz, Phys. Solid State 49, 1090 (2007).
[5] I. Yamada, J. Matsuura, Z. Insepov, T. Aoki, T. Seki, and N. Toyoda, Nucl. Instrum. Methods B 164, 944 (2000).
[6] C. L. Cleveland, and U. Landman, Science 257, 355 (1992).
[7] I. Yamada, Nucl. Instrum. Methods B 112, 242 (1996).
[8] H. P. Cheng and J. D. Gillaspy, Phys. Rev. B 55, 2630 (2000).
[9] R. W. Lee, Z. Y. Pan, and M. Hou, Nucl. Instrum. Methods B 115, 536 (1996).
[10] H. Mizuseki, Y. Jin, Y. Kawazoe, and L. T. Wille, Nucl. Instrum. Methods B 87, 6561 (2000).
[11] M. Ghaly, K. Nordlund, and R. S. Averback, Philos. Mag. A 79, 795 (1999).
[12] T. Aoki, J. Matsuura, Z. Insepov, and I. Yamada, J. Vac. Sci. Technol. B 19, 634 (2001).
[13] Y. Hu and S. B Sinnott, Nucl. Instrum. Methods B 195, 329 (2002).
[14] R. Cross, Sports Engg. 6, 235 (2003).
[15] R. Cross, Am. J. Phys. 73, 914 (2005).
[16] H. Dong and M. H. Moys, Powder Technol. 161, 22 (2006).
[17] R. Cross and A. M. Nathan, Am. J. Phys. 75, 658 (2007).
[18] A. M. Nathan, Am. J. Phys. 76, 119 (2007).
[19] A. Awasthi, S. C. Hendy, P. Zoontjens, and S. A. Brown, Phys. Rev. Lett. 97, 186103 (2006).
[20] A. Awasthi, S. C. Hendy, P. Zoontjens S. A. Brown, and F. Natali, Phys. Rev. B 76, 115437 (2007).