Applied Surface Science 255 (2008) 893–896

Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Friction model to describe cluster bombardment

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ARTICLE INFO

Article history:
Available online 13 May 2008

Keywords:
Molecular dynamics
Clusters
C_{60}
Au_3
SIMS
Friction model

ABSTRACT

Short time molecular dynamics simulations were performed to model C_{60} and Au_3 bombardment of an amorphous water sample in the projectile energy range of 5–120 keV. A previously proposed friction model has been applied to describe the fundamental motion of a projectile during cluster bombardment of a solid. This simple analytical model uses a definition of friction on a single particle to describe the cluster movement through a medium. Although the mathematics of the friction model vary among systems, the projectile motion and energy deposition of a single particle into the sample as well as the reactive environment created is close to that of C_{60} bombardment.

1. Introduction

Cluster bombardment of solids has been shown both experimentally and computationally to possess many different characteristics from atomic bombardment. In particular, energetic cluster bombardment has become a useful tool for biological and organic secondary ion mass spectrometry (SIMS) experiments because cluster bombardment creates less damage accumulation in the sample and enhances the ejection yield compared to atomic projectiles [1]. However, in the computational realm, cluster bombardment creates many challenges due to the increase in system size needed to contain all the events associated with cluster projectile impact as well as the use of lower mass/bond strength solids which may contain chemistry not present in previously used atomic metal samples. The challenge arises, then, as to how to understand the motion induced by the cluster bombardment event without running full simulations that require large samples and complicated potentials which may take several months to calculate. If a simple conceptual model exists, then a fundamental level of understanding can be obtained without extensive simulations.

We propose a simple analytical model based on friction applied to a single particle moving through a material. The development of this model has been discussed previously [2]. In short, the frictional force can be expressed as a power series in the velocity with a linear term and quadratic term as,

$$m\frac{dv}{dt} = -6\pi a\eta v - \frac{1}{2}\rho A C_D v^2 \quad (1)$$

where m is the mass of the projectile, v is the velocity, t is the time, a is the initial radius of the projectile plus some interaction distance between the projectile and the sample atoms, η is a friction parameter, ρ is the density of the sample, A is a reference area of the cluster equal to πa^2, and C_D is a drag coefficient [3]. In previous simulations of fullerene bombardment of a molecular solid, benzene, at short times, it was found that the quadratic term alone is a sufficient approximation and for short times Eq. (1) reduces to,

$$\ln\left(\frac{v}{v_0}\right) = -\frac{1}{2}\frac{\rho v_0 A C_D t}{m} \quad (2)$$

where v_0 is the velocity at $t = 0$. That is, the fraction of velocity that the projectile has relative to its initial velocity follows an exponential decay where the exponent depends on the initial velocity of the projectile. The linear term in Eq. (1) shows no such dependence, and instead decays linearly with a dependence on size, time, and inverse mass of the projectile.

Here, we explore this model further by comparing results from simulations of C_{60} and Au_3 bombardment of amorphous water with previously reported simulations of fullerene bombardment of benzene. We also discuss the dynamics of cluster motion with

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doi:10.1016/j.apsusc.2008.05.113

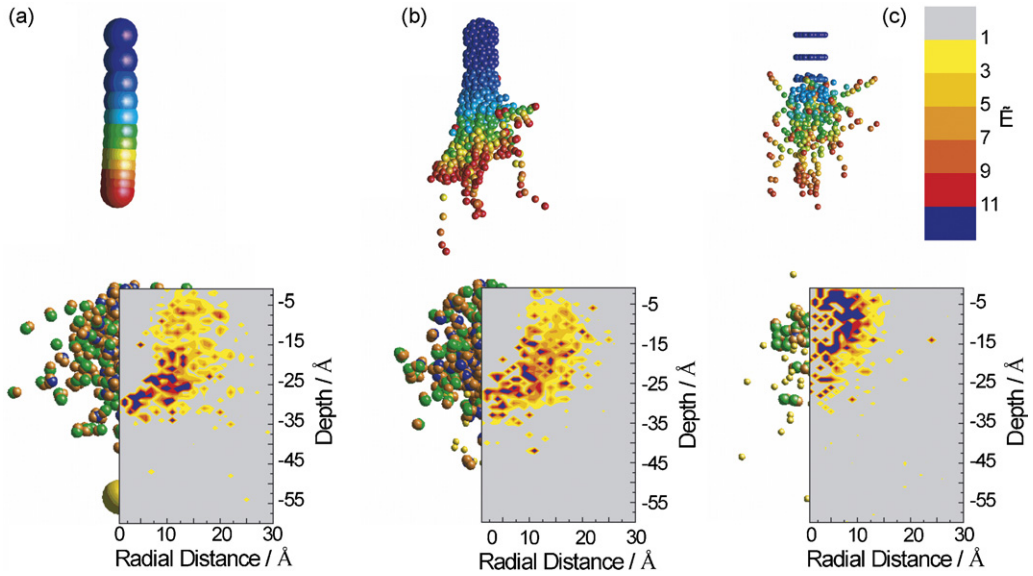

Fig. 1. (a) Results from 10-keV bead bombardment. (b) Results from 10-keV C_{60} bombardment. (c) Results from 60 separate C bombardments with 166.67 eV/projectile atom. (Top) Time-lapsed views (blue to red) of the projectile motion until 90% of the projectile energy has been deposited to the sample. (Bottom) The energy deposition profile overlaid on a snapshot of the reaction environment of the sample. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

respect to a single bead projectile and a collective of 60 separate single carbon atomic projectiles.

2. Simulation method

The friction model is tested for a water ice system for which previous molecular dynamics simulations have been performed for C_{60} and Au_3 projectiles given incident energies of 5, 10, 15, 20, 40, 80, and 120 keV and were aimed normal to the surface [4]. The simulations were run only for short times until 90% of the projectile kinetic energy was deposited in the sample. This interval has been shown to be a critical time for cluster bombardment when examining the energy deposition and its connection to the ejection yield as estimated using the mesoscale energy deposition footprint (MEDF) model [4,5]. In order to test the reaction dynamics of the sample during bombardment, simulations were also performed to model 10-keV C_{60} bombardment of water using an interaction potential that allows for dissociation of water into ions [6]. This process has a large activation energy for occurrence and therefore acts as an indicator for a wide range of reactions and electronic events that are energetically accessible during cluster bombardment.

For comparison, a simulation of a 10-keV single bead projectile with the mass and size of an intact C_{60} molecule was implemented. The bead was assigned a potential that allows interaction between the edge of the bead and the sample atoms. The potentials used are identical to the C–O and C–H potentials used for the atomistic C_{60} bombardment simulation.

Lastly, 60 separate individual carbon trajectories each with an initial kinetic energy of 166.67 eV, the same energy per atom as the C_{60} projectile at 10 keV, were calculated on the same water sample. The initial positions of the C atoms corresponded to the 2D projection of the C atom positions in the C_{60} cluster. The motivation for this calculation arises from the concept that the energy deposition rate of a cluster of n atoms can be described by n times the energy deposition rate by one atom at the same velocity [7,8].

3. Results and discussion

In order to test the assumption that cluster bombardment may be described by friction acting on a single particle moving through a solid, we have compared a simulation of 10-keV C_{60} bombardment of a reactive water sample with that of a single bead projectile. Fig. 1 b shows the results from C_{60} bombardment of amorphous water. The top snapshot is a time-lapsed view of the projectile motion where dark blue represents $t = 0$ and red represents the time at which 90% of the projectile energy has been deposited to the substrate. The C_{60} projectile is able to penetrate into the substrate in a nearly straight trajectory and begins to break up as it approaches the 90% time. The projectile deposits its energy within a depth of ~35 Å and a width of ~20 Å from the impact point as shown by the bottom of Fig. 1b. The energy deposition profile is represented by changes in $\tilde{E} = E_{exc}/U_0$, where E_{exc} is the excitation energy and U_0 is the binding energy of the substrate. Therefore, according to the legend, grey represents molecules in their initial state respectively, and yellow to blue represent energized molecules from slightly energized to highly energized. This contour plot is overlaid on the original positions of the water molecules (colored beads) that have reacted. The reaction zone created following C_{60} bombardment is very dense and located near the point of impact indicating that multiple or adjacent molecules react simultaneously [6].

The results from the bead simulation (Fig. 1a) closely mirror those of C_{60} bombardment. The bead projectile is also able to penetrate into the sample in a nearly straight line and deposits its energy in approximately the same region as the C_{60} projectile resulting in similar yields according to the MEDF model [4,5]. Likewise, the reaction profile also shows a dense near surface region where multiple molecules may react concurrently.

The sum of results from 60 separate single carbon trajectories paints a very different picture (Fig. 1c). All the figures for the 60 C atoms correspond to a sum of 60 individual calculations. The individual C atoms begin to randomize immediately upon impact with the surface as shown by the time-lapsed snapshot and do not penetrate as deeply as either the bead or C_{60} projectiles. The energy