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A COMPARISON OF THE ENERGY DENSITY DISTRIBUTION WITH ATOMIC AND POLYATOMIC PROJECTILES IN ORGANIC SIMS

David W. Ward[a], T. C. Nguyen[a], Kristin D. Krantzman[a]
and Barbara J. Garrison[b]

[a]Department of Chemistry and Biochemistry, College of Charleston
Charleston, SC 29424, USA

[b]Department of Chemistry, The Pennsylvania State University
University Park, Pennsylvania 16802

1. Introduction

Numerous organic SIMS experiments have demonstrated that polyatomic projectiles enhance the yield of secondary ions compared to monoatomic projectiles [1-4]. Recently, experiments have compared the secondary ion yield with Xe and SF_5 projectiles [5-6]. Although Xe and SF_5 have approximately the same mass, there is a significant enhancement in the yield with the polyatomic projectile. We have performed molecular dynamics simulations of the bombardment of a monolayer of biphenyl molecules on Cu(100) and Si(100)-(2x1) substrates with 0.6 keV SF_5 and Xe projectiles [7], which have shown that SF_5 produces more yield than Xe. It is hypothesized that the secondary ion yield is greater with polyatomic projectiles because the energy deposited is spread out over a larger surface area, leading to more ejected molecules from the surface. In this paper, we examine the energy density distribution with Xe and SF_5 projectiles.

2. Method

The classical method of molecular dynamics simulations is used to study the systems of interest and the details of this method are described extensively elsewhere [8]. Details of the calculations have been described previously [9] and will be described in more detail elsewhere [10]. The model systems consist of a monolayer of biphenyl molecules adsorbed on copper and silicon substrates, where the positions of the biphenyl molecules are determined by allowing the adsorbates to equilibrate at 0 K on the substrate using an algorithm based on the generalized Langevin equation (GLE). The forces among the atoms are described by the best currently available potential energy functions, the majority of which are multi-body in nature. The Xe and SF_5 projectiles are brought in at normal incidence with 0.6 keV of energy, and the orientation of the SF_5 projectile with respect to the surface is selected randomly. The results are calculated with each projectile for 150 trajectories, where each trajectory has a different aiming point on the surface.

3. Results

a. Yield and Mechanisms

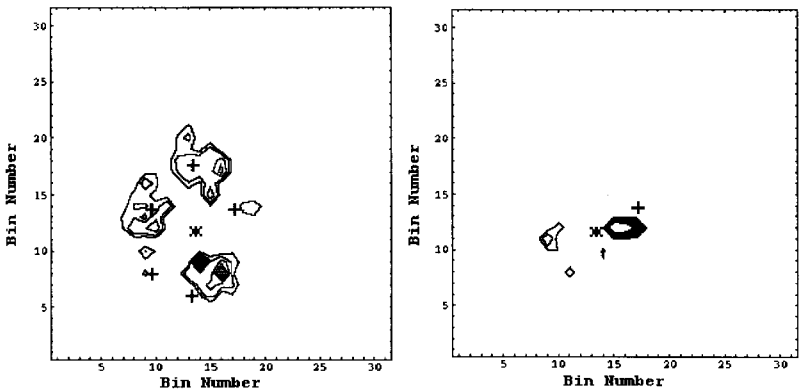
Our simulations have demonstrated that SF_5 enhances the yield compared to Xe, and that the degree of enhancement depends on the nature of the substrate [7]. On the silicon substrate, the yield with SF_5 is 2.1 times greater than with Xe. On the copper substrate, the yield with SF_5 is only 1.2 times greater than with Xe. The differences in the enhancement between the two substrates can be explained by the differences in their lattice structure. With the more open lattice structure of silicon, the SF_5 is able to penetrate the lattice and break up within the substrate underneath the monolayer of biphenyl molecules. With the more closely packed copper substrate, on the other hand, the SF_5 cluster breaks up on the surface rather than within it. The break up of SF_5 within the lattice leads to upward motion of the silicon substrate atoms, causing a greater number of ejected biphenyl molecules from the surface.

b. Energy Density

Only the energy density from the upward moving substrate atoms are considered because these are the atoms that cause ejection of whole biphenyl molecules. Contributions to the energy density from the primary particle are not included because collisions with the primary particle lead to fragmentation of the biphenyl molecules. In order to calculate the energy density distribution, the surface area is divided up into thirty by thirty bins, each with an area of four $Å^2$. For each time step, the energy within each bin is calculated by summing over the kinetic energy of the substrate atoms in the volume of the bin that have an upward momentum and are within two Å above the substrate surface. The energy density is calculated by dividing the total energy by the volume of the bin and the maximum kinetic energy density over time in each bin is recorded for the trajectory.

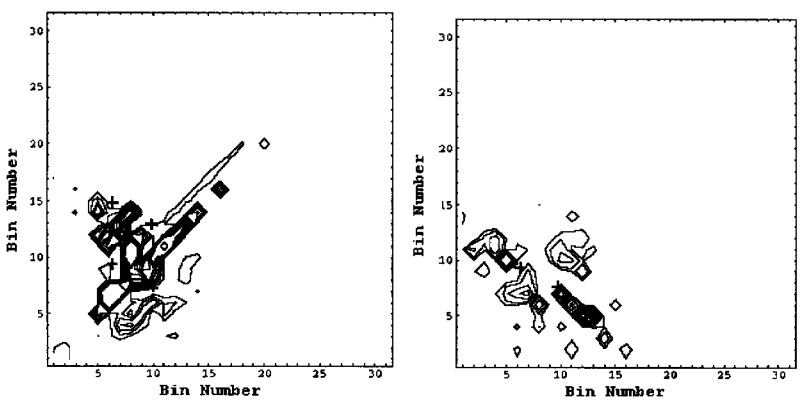
Figures 1a and 1b show plots of the maximum energy density within each bin for a typical trajectory on the Si(100)-(2x1) substrate with the SF_5 and Xe projectiles. Both projectiles have the same impact point on the surface. SF_5 produces a yield of five ejected biphenyl molecules and one fragmented molecule and Xe produces a yield of two ejected biphenyl molecules. The plus signs on the plots represent the positions of the center of mass of the ejected biphenyl molecules and the asterisk in Figure 1a represents the position of the biphenyl molecule fragmented by the impact of the SF_5 projectile. In general, positions of high energy density correlate with the positions of biphenyl molecules that are ejected. The SF_5 projectile produces a larger area of energy density on the silicon surface compared to Xe, which distributes its energy in a smaller region, and consequently, more biphenyl molecules are ejected with the SF_5 projectile.

Figures 2a and 2b show plots of the energy density with the SF_5 and Xe projectiles on the Cu(001) substrate. With this impact point, SF_5 has a yield of three biphenyl molecules and Xe has a yield of two biphenyl molecules. The magnitude of the energy density is greater on the copper substrate than the silicon substrate because of the greater mass of its substrate atoms. As in the case with the silicon substrate, SF_5 distributes the energy over a larger area than Xe. However, the increase in area is not as great as on the silicon substrate because SF_5 breaks up on the copper surface rather than within it.



a) SF_5 projectile b) Xe projectile

Figure 1: Energy density distribution on the Si(100)-(2x1) substrate. Contour lines are drawn to represent positions of energy density at values of 0.5 eV/8 Å^3, 1.0 eV/ 8 Å^3, 2.0 eV/8 Å^3, 3.0 eV/8 Å^3, and ... 10.0 eV/8 Å^3.



a) SF_5 projectile b) Xe projectile

Figure 2: Energy density distribution on the Cu(001) substrate. Contour lines are drawn to represent positions of energy density at values of 0.5 eV/8 Å^3, 1.0 eV/ 8 Å^3, 2.0 eV/8 Å^3, 3.0 eV/8 Å^3, and ... 10.0 eV/8 Å^3.

4. Summary

Plots of the distribution of the maximum energy density with the Xe and SF_5 projectiles on the Si(100)-(2x1) and Cu(001) substrates are presented for typical trajectories. Our simulations show that only substrate atoms with upward momentum cause ejection of whole biphenyl molecules, and therefore, only these atoms are included in the calculation of the energy density. In general, positions of high energy density correlate with the positions of ejected biphenyl molecules. SF_5 produces a larger area of energy density than Xe, and this is especially true on the silicon substrate. The larger area of energy density leads to a greater yield of biphenyl molecules ejected from the surface.

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