Theoretical Study of the Role of Chemistry and Substrate Characteristics in C_{60} keV Bombardment of Si, SiC, and Diamond by Molecular Dynamics Simulations

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This article presents a theoretical study aimed at understanding the reactive nature of carbon in secondary ion mass spectrometry experiments of Si with keV C_{60}^+ . Molecular dynamics simulations are performed to model the bombardment of three different substrates, Si, SiC, and diamond, with normal incident C_{60} at kinetic energies ranging from 5 to 20 keV. Projectile atoms form strong covalent bonds with both Si and C and, therefore, are incorporated into the target material. Although these substrates have the same diamond lattice structure, they differ greatly in their cohesive energy and number density. The yield is found to be a factor of two times greater on SiC than on Si or diamond. The mesoscale energy deposition footprint model is used to understand the reasons for the differing behaviors of the substrates as a result of C_{60} bombardment.

1. Introduction

In the past few years, the introduction of cluster ion beams, particularly C_{60}^+ , has put secondary ion mass spectrometry (SIMS) in the spotlight because of the possibility of its application to molecular sputter depth profiling.¹ Experiments show that C_{60}^+ bombardment produces a significant enhancement in sputter yield, i.e., the average amount of material removed from the surface in a single impact. Moreover, chemical damage induced by the ion impact is confined to a shallower region below the surface. The combination of both effects makes C_{60}^+ an outstanding candidate for the three-dimensional chemical characterization of a solid on a molecular level,¹ thus opening up a large range of applications in molecular biology^{2,3} and nanotechnology.⁴

However, depth profiling experiments of C_{60}^+ on silicon by Gillen et al.⁵ indicate unusual behavior that appears to be specific to the pairing of the projectile and the target material. At low incident kinetic energies, the sputtering signal disappears and a buildup of material is produced. When the incident kinetic energy of C_{60}^+ is increased, the sputtering signal increases and a transition from net buildup to net removal of solid material is observed. Moreover, problematic effects have been observed where initial surface erosion stops in the course of a sputter depth profile. Accumulation of material deposited on the surface results in the production of interesting topographical features, such as mounds of solid carbon deposits in the shape of “Hershey kisses”. Kozole and Winograd⁶ have also observed the formation of C containing, moundlike structures on the solid surface in depth profiling experiments of Si bombardment with 10 keV C_{60}^+ at a 40° angle of incidence.

Numerous molecular dynamics (MD) simulations of the bombardment of C and Si materials with carbon atoms and fullerene projectiles at lower incident energies and a range of incident angles have been performed by Smith, Webb, and co-workers.^{7–12} Simulations of the dimer reconstructed Si ($2 \times$

1) surface bombarded with C_{60} projectiles at 1 keV and normal incidence show that the C_{60} projectile disintegrates and sputtering of atoms and larger Si_xC_y molecules occurs.⁸ Aoki et al.¹³ have compared the collision dynamics of C_{60} and single C atom bombardment on a diamond surface and found that the cluster shows a nonlinear effect at energies ranging from 100 to 2 keV per atom. Studies by Webb et al.¹¹ have compared craters and defects caused by fullerene and single C atom impacts on graphite. Recently, Anders et al. have studied the ranges and fragmentation of fullerene molecules on a number of targets including graphite.¹⁴ However, the majority of these simulations were performed with incident kinetic energies too low to be relevant to SIMS experiments. Furthermore, many of these studies have focused on the behavior of the projectile and its motion within the substrate rather than on the sputtered yield.

In order to interpret some of the unusual observations in SIMS experiments on Si, we have performed MD simulations of the bombardment of a silicon crystal with normal incident C_{60} projectiles at incident kinetic energies ranging from 5 to 20 keV.¹⁵ The simulations demonstrate that chemical reactions occur between carbon atoms from the projectile and silicon atoms in the solid, which result in the formation of strong covalent bonds. Consequently, the simulations confirm the experimental observation of a transition from net erosion to net deposition of material. The transition occurs at ~ 12 keV in the simulations, which is comparable to the estimated value of ~ 14.5 keV in the depth profiling SIMS experiments.⁵ Additional simulations at 45° incidence¹⁶ demonstrate that more energy is transferred to the uppermost layers of the crystal than at normal incidence, which leads to an increase in sputtered yield compared to that at normal incidence. The dependence of the sputtered yield on the angle of incidence agrees with experimental results by Hill and Blenkinsopp.¹⁷

Our previous simulations of Si with C_{60} suggest that the formation of chemical bonds between projectile and surface atoms leads to a chemical modification of the bombarded solid, which in turn may change the sputtered yield. In order to study the effect of changes in surface composition, simulations of the bombardment of silicon carbide and even pure carbon surfaces, diamond and graphite, with normal incident 20 keV C_{60} have

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TABLE 1: Average Yield and Standard Deviation of Sputtered and Deposited Atoms from C₆₀ Bombardment of the Si, Diamond, and SiC Targets

incident kinetic energy (keV)	diamond		SiC		Si	
	sputtered atoms	deposited atoms	sputtered atoms	deposited atoms	sputtered atoms	deposited atoms
5	17 ± 7	50 ± 2	37 ± 6	51 ± 3	9 ± 3	58 ± 2
8	30 ± 13	53 ± 2	88 ± 2	46 ± 6	23 ± 8	55 ± 2
10	61 ± 10	47 ± 3	138 ± 29	44 ± 4	44 ± 18	56 ± 1
12	91 ± 8	47 ± 3	189 ± 35	44 ± 4	69 ± 9	55 ± 2
15	122 ± 14	47 ± 5	276 ± 35	41 ± 2	89 ± 28	55 ± 2
20	231 ± 28	43 ± 3	465 ± 50	38 ± 3	154 ± 40	55 ± 2

been performed.¹⁸ On graphite, the yield of sputtered atoms is negligible, because the open lattice allows the cluster to deposit its energy deep within the solid. The simulations suggest that the formation of a carbon deposit with a less dense, more graphitelike structure may actually quench the sputtering yield.

This paper focuses on understanding the role of the reactive nature of carbon and the effect of changing surface composition in experiments of Si with keV C₆₀⁺. Of particular interest is how the formation of covalent bonds between the projectile and substrate atoms affects both the sputtered yield and the chemical composition of the surface. MD simulations are performed to model the bombardment of three different substrates, Si{100}, SiC{100}, and diamond{100}, with normal incident C₆₀ at kinetic energies ranging from 5 to 20 keV. The unique feature of these substrates is that the projectile atoms form strong covalent bonds with the target atoms, which results in the incorporation of projectile atoms into the target. The study is restricted to a family of substrates made of group IV atoms, diamond, SiC, and Si, which represent possible compositions of the Si surface after depth profiling SIMS experiments with C₆₀⁺.

This family of compounds has the same diamond lattice structure but varies widely in two material properties, cohesive energy and number density. These quantities, as well as the energy density deposited in the near surface region, have been proposed to influence the sputtering yield^{19–26} and will be used to interpret the results of the simulations. Specifically, the model that is most universally applicable is the microscale energy deposition footprint (MEDF) model of Russo et al.,^{23–25} which uses information obtained from short time MD simulations as input to an analytic formula. The other models require quantities that are challenging to determine a priori. Results from the simulations and the MEDF model show that SiC has the highest sputtering yield by a factor of two, which represents a balance of intermediate number density and intermediate binding energy.

2. Description of the Simulations

The classical method of MD simulations is used to model the systems of interest, and the application of this method to keV bombardment of solids is explained comprehensively elsewhere.^{27,28} The Si surface is modeled by a Si{100} microcrystallite with dimensions of 200 Å × 200 Å × 120 Å containing 248 768 atoms arranged in 23 layers of 10 186 atoms with the top layer of Si atoms placed in the (2 × 1) reconstruction. The diamond surface is modeled by a similar microcrystallite, although the dimensions of 155 Å × 155 Å × 81 Å are smaller because of the smaller lattice constant. The microcrystallite for SiC contains 207 360 atoms arranged in 20 layers of 10 368 atoms with the top layer of Si atoms placed in the (2 × 1) reconstruction and has similar dimensions to the diamond microcrystallite, 155 Å × 155 Å × 86 Å. Simulations were also performed on an alternative model system for SiC with the top layer of C atoms placed in the (2 × 1) reconstruc-

tion. The size of each microcrystallite was chosen to be sufficiently large to minimize the effects of the edges of the crystal on the processes essential to the bombardment event.

The randomly oriented C₆₀ projectile was placed at a sufficient distance above the surface that the interaction potential with the substrate is negligible. The results at each incident kinetic energy were calculated as an average over four trajectories at impact points located in the center of the crystal. Each microcrystallite was surrounded by a heat bath composed of one layer of rigid atoms and two layers of atoms kept at 0 K by a frictional force, which is used to prevent energy induced by pressure waves being reflected from the boundary walls back into the surface.²⁹ This method is explained extensively in previous simulations of the keV bombardment of Ag{111} with C₆₀.²⁹ The simulations were run for 5 ps. It was found that the majority of particles were sputtered by this time and the general trends in sputtering yields are not affected by running the simulations for longer times. The time of 5 ps is shorter than that needed for Ag crystals (4–13 ps),^{29,30} water ice (20 ps),²³ or benzene (27 ps)³¹ because of the larger cohesive energy and lattice structure of the group IV materials.

An empirical many-body potential developed by Tersoff is used to model the Si–Si, C–C, and Si–C interactions.³² The empirical parameters in the potential are fit to the energetics and structure of Si, diamond, and SiC, and, therefore, the construction of the potential models the chemistry appropriate for C₆₀ bombardment of these group IV materials. The Tersoff potential is not sufficiently repulsive at short distances, and thus an exponential spline function is used to smoothly connect the Ziegler, Biersack, and Littmark (ZBL)³³ potential with the two-body Tersoff Si–Si, C–C, and Si–C potentials.³⁴

3. Results and Discussion

The beginning of the discussion focuses on how the sputtered yields depend on both the substrate and the incident kinetic energy of the C₆₀ projectile. Then, the MEDF model is used to analyze the energy deposition into the substrates and how the region where the energy deposited along with the cohesive energy and number density are able to explain the trends in sputtering yield. The motion of the projectile atoms during the initial stages of the bombardment process and the final positions of the incorporated C atoms are discussed relative to the region of energy deposition.

The number of sputtered and deposited atoms at different incident kinetic energies of the C₆₀ projectile at normal incidence is shown for the three substrates in Table 1. The numbers reported at each kinetic energy are the average over four trajectories with different impact points and the ± values are the standard deviations from the average. For the SiC substrate, the total sputtered yield is calculated as the sum of the number of sputtered Si and C atoms. The numbers shown are averages over the values obtained from simulations on the two SiC surfaces, one with Si dimers on the topmost layer and the other

Figure 1. Average sputtered yields from the simulations (solid line, solid symbol) plotted as a function of incident kinetic energy for the three substrates: SiC (square), diamond (circle), and Si (triangle). The error bars shown for the average simulations yields are the standard deviation from the average over a set of four trajectories. The patterned bar represents the range in the number of C atoms deposited from the projectile, which marks the transition from net deposition to net erosion of material. Predicted yields from the MEDF model (dashed line, open square) are also plotted for SiC as a function of incident kinetic energy. The error bars shown for the MEDF yields are estimated from the yields calculated for $R_{\text{cyl}} \pm 2 \text{ \AA}$.

with C dimers on the topmost layer. On average, the Si and C atoms make equal contributions to the total number of atoms sputtered. In the case of all three substrates, nearly all of the C atoms from the projectile are deposited into the substrate.

3.a. Sputtered Yields. The average sputtered yields from the simulations for each substrate are plotted as a function of incident kinetic energy in Figure 1. For each substrate, the sputtered yield has a linear dependence on incident kinetic energy above a certain threshold energy. This behavior has been observed in previous MD simulations of Cu cluster bombardment of Cu,³⁵ Ar₁₀₀ bombardment of Ar,^{21,22} and Ar cluster bombardment of Si.³⁶ No threshold energy has been observed in cluster bombardment of molecular solids, and there is a near-linear dependence of sputtered yield on incident kinetic energy, as seen in experimental results and previous MD simulations for C₆₀ and Au₃ bombardment of water ice,²⁴ and for simulations of the bombardment of benzene with fullerene molecules.³⁷ The substrate with an intermediate binding energy and number density, SiC, has a significantly greater yield than either diamond or Si. Even though Si has the lowest binding energy of the three substrates, it produces the lowest number of sputtered atoms and shows the smallest increase in sputtered yield with kinetic energy. The sputtered yields from diamond are about 30% greater than those from Si. However, these values are comparable in magnitude relative to the sputtered yields from SiC, which are a factor of about two times greater.

An analysis of the simulations by the MEDF model gives physical insight into the differing behaviors of the substrates as a result of C₆₀ bombardment. The basic ideas and application of the model to simulations of keV bombardment are described in detailed elsewhere.^{23–25} The MEDF model was originally developed to predict sputtered yields from short time MD simulations. The model, based on the work of Jakas et al.,³⁸ treats the bombardment induced particle ejection by two-dimensional fluid dynamics. Briefly, the model predicts that the energy deposited very early on in the bombardment process is what determines the sputtered yield at much later times. Initially, an energized cylindrical track with a characteristic radius, R_{cyl} , is created. Only particles near the surface at a depth of R_{cyl} or

less will be ejected. As atoms are ejected into the vacuum, a wider surface area is exposed, and further ejection occurs from a surface area with radius $R_s = (\tilde{E})^{1/2} R_{\text{cyl}}$, where $\tilde{E}$ is the average excitation energy of the substrate atoms relative to the cohesive energy, U_0 . The footprint from the projectile is equal to the volume of a cone with radius R_s and depth R_{cyl} . The volume of the footprint, along with the number density of the substrate, n_0 , can be used to estimate the sputtering yield, $Y = n_0(\pi/3)R_s^2 R_{\text{cyl}}$, which simplifies to $Y = n_0(\pi/3)R_{\text{cyl}}^3 \tilde{E}$.

The trends in yields from the simulations can be understood by examining three critical factors incorporated into the MEDF model, i.e., the number density and binding energy of the substrate and the region where the projectile deposits its energy in the solid. Figure 2 illustrates the application of the MEDF model to the analysis of a single trajectory of 20 keV C₆₀ bombardment of each substrate. Snapshots of the original positions of specific atoms are shown juxtaposed with contour plots of the excitation energy above the cohesive energy, U_0 , of the substrate. Each contour plot is centered in a 2 nm slice around the impact area and is drawn at the time when the projectile has lost 90% of its initial energy. The boundary between the gray and colored regions outlines the region in which there is a sufficient amount of energy to overcome the cohesive energy. Values of the radius of the energized cylindrical track, R_{cyl} , are estimated from the position of this boundary.

The figures are arranged from top to bottom in order of decreasing number density and decreasing cohesive energy. C₆₀ loses 90% of its energy at 40 fs in diamond, at 50 fs in SiC, and at 90 fs in Si. Diamond has the smallest estimated value of R_{cyl} , 11 Å, SiC has a larger value, 15 Å, and Si has the largest value, 16 Å. The average excitation energy per atom, $\tilde{E}$, of the substrate atoms within a cylinder of radius and depth equal to R_{cyl} is used to calculate the base radius, R_s , of the final ejection cone. The volumes of the ejection cones for Si and SiC are similar even though Si has a larger value of R_{cyl} , because SiC has a greater fraction of energy deposited above a depth of R_{cyl} . Diamond has the smallest value of $\tilde{E}$ because it has the highest cohesive energy and the energy is distributed over a larger number of atoms due to its higher number density. Consequently, due to its small value of R_{cyl} and $\tilde{E}$, the volume of the ejection cone for diamond is only $\sim 1/3$ of the volume of the cones for Si and SiC.

The MEDF model predicts that the sputtered yield is equal to the number of atoms within the ejection cone, a simple product of the number density and the volume of the ejection cone. The contributing factors to the MEDF predicted yield along with the MEDF yields and yields from the simulations are shown in Table 2. The values at 20 keV correspond to those shown in Figure 2. Note that the volume of the ejection cone depends on R_{cyl}^3 and is therefore highly sensitive to the estimated value. The MEDF predicted yield of SiC is a factor of roughly two times greater than Si simply because the number density is two times greater. Even though diamond has twice the number density of SiC, the volume of the ejection cone is one-third that of SiC, and, therefore, the MEDF predicted yield of SiC is also a factor of roughly two times larger than that of diamond. The large errors in the MEDF predicted yields are due to the large variance in the volume of the ejection cone with the estimated value of R_{cyl} .

The physics underlying the MEDF model assumes that energy is quickly deposited into the footprint region, and the substrate atoms undergo fluidlike motion. There are limitations to the model, as shown by an examination of Figure 2. The value of R_{cyl} is estimated from the contour plot of excitation energy even

Figure 2. Analysis of the excitation track and ejection cone for diamond, SiC, and Si. Each figure is composed of a snapshot of the original positions of selected atoms adjacent to a contour plot of the excitation energy. All the figures correspond to one trajectory at 20 keV. Each snapshot and contour plot have the same dimensions, a width equal to 40 Å from the C₆₀ impact point and a depth of 40 Å. Vertical lines are drawn on each plot at the estimated value of R_{cyl} , the radius of the energized cylindrical track. Horizontal lines are drawn at a depth equal to R_{cyl} . The diagonal lines outline an ejection cone with estimated radius R_s and depth R_{cyl} . Sputtered atoms that are originally within the ejection zone are colored as red (Si) and dark blue (C) spheres. Atoms within the cone that are not sputtered are colored as yellow spheres. Sputtered atoms that are originally outside of the cone are shown as green spheres. The final positions of substrate atoms that are not sputtered or within the cone are drawn as points.

though the plot is not cylindrical. Some atoms within the conical region are not ejected, and some atoms outside of the conical region are ejected. Russo et al. also found that the shape of the energy deposition is more spherical than cylindrical in the case of C₆₀ bombardment of water ice,²⁴ and the atoms that eject do not correspond exactly to those in the conical region.²³ More importantly in the case of the simulations presented here, the deposition of projectile atoms is not taken into account in the MEDF model. This model is not appropriate if the sputtering yield is low, i.e., less than a factor of two times greater than the number of deposited atoms. A comparison of the number

of sputtered and deposited atoms in Table 1 shows that the incident kinetic energy at which this criterion is valid depends on the particular substrate. This condition is met at incident kinetic energies greater than or equal to 8 keV for SiC, 12 keV for diamond, and 15 keV for silicon.

Using the same methodology as described previously, the MEDF predicted sputtered yields were calculated for a single trajectory for each substrate at incident kinetic energies for which the model is appropriate. In Table 2, the MEDF and simulation yields for the same single trajectory are compared. Qualitatively, the MEDF model reproduces the relative differ-

TABLE 2: Comparison of Sputter Yields Predicted by the MEDF Model and Those Obtained from the Full MD Simulations for C₆₀ Bombardment^a

Diamond				
incident kinetic energy (keV)	R_{cyl} (Å)	$\tilde{E}$	MEDF yield	actual yield
12	9	1.09 ± 0.15	98 ± 95	80
15	10	1.08 ± 0.05	200 ± 110	114
20	11	1.19 ± 0.08	295 ± 146	254
number density (atoms · Å ⁻³)	0.18			
cohesive energy (eV)	7.37			
SiC				
incident kinetic energy (keV)	R_{cyl} (Å)	$\tilde{E}$	MEDF yield	actual yield
8	10	1.22 ± 0.06	127 ± 67	79
10	11	1.45 ± 0.20	200 ± 91	124
12	12	1.34 ± 0.08	241 ± 99	169
15	13	1.48 ± 0.11	339 ± 121	258
20	15	1.43 ± 0.13	502 ± 144	506
number density (atoms · Å ⁻³)	0.099			
cohesive energy (eV)	6.165			
Si				
incident kinetic energy (keV)	R_{cyl} (Å)	$\tilde{E}$	MEDF yield	actual yield
15	15	1.16 ± 0.07	205 ± 93	72
20	16	1.24 ± 0.06	265 ± 112	185
number density (atoms · Å ⁻³)	0.05			
cohesive energy (eV)	4.63			

^a The error bars shown for $\tilde{E}$ and the MEDF yield correspond to the spread in values calculated for $R_{\text{cyl}} \pm 2$ Å.

ence in yields for the three different substrates and the dependence of yield on incident kinetic energy. Quantitatively, on the other hand, the MEDF yields are consistently higher than those determined from the MD simulations. Although the MEDF model is an approximate one, it is useful in this study because it explains the physical concepts underlying the trend in relative yields for the three substrates. The yield for SiC, the substrate with the intermediate cohesive energy and number density, is a factor of approximately two times greater than the yield from Si or diamond. In Si, the energy is deposited too deep in the surface to be effective in sputtering. In diamond, the average energy per atom is small due to its high number density and large cohesive energy, which results in a small volume of the ejection cone. In SiC, C₆₀ deposits its energy in an effective region for sputtering, which is also a key factor for the increased yield.

The MEDF model has been applied to understand the factors that lead to an increase in yield with kinetic energy. In the case of previous simulations of C₆₀ bombardment on ice²⁴ and coarse-grained benzene,³¹ the region in which the energy is deposited is fairly constant with increasing incident kinetic energy. Consequently, as the kinetic energy of the projectile increases, more energy is deposited in the same region and $\tilde{E}$ increases. Therefore, the increase in yield is mainly due to an increase in $\tilde{E}$ rather than changes in R_{cyl} or the depth in which the energy is deposited. When compared to C₆₀ bombardment of water ice, Au₃ shows a slower increase in yield with increasing kinetic energy, which is due to an increasing value of R_{cyl} .²⁴ Most importantly, as the incident kinetic energy of Au₃ increases, the energy is deposited deeper into the crystal, which is not effective in ejecting material. In the simulations of C₆₀ bombardment of Si, SiC, and diamond, the atomic solids have a much higher cohesive energy than the molecular solids. As a result, the value of R_{cyl} is smaller compared to that of ice or benzene. In Figure 1, the MEDF predicted yields for a single trajectory of SiC are

plotted as a function of incident kinetic energy along with the averages calculated from the simulations. The MEDF yields are consistently 10% higher than those from the simulations, and the relative increase with incident energy is similar. In the case of SiC, R_{cyl} and the region in which the energy is deposited increase as the incident kinetic energy increases, while $\tilde{E}$ is fairly constant. Therefore, the increase in yield with kinetic energy is due to an increase in the value of R_{cyl} .

3.b. Chemistry. In the case of all three substrates, atoms from the C₆₀ projectile form bonds with atoms in the target material, which leads to carbon atoms deposited into the target. In Figure 1, the shaded band represents the average number of projectile atoms deposited into the substrate. The yield of sputtered atoms increases with kinetic energy, while the number of deposited atoms from C₆₀ stays relatively constant. The transition from net deposition to net erosion of material is marked by the regions below and above the band. Therefore, the transition from net deposition to net erosion occurs at the smallest kinetic energy for SiC because it has the overall largest sputtered yield.

The depth of the energy deposited in the contour plots shown in Figure 2 can be understood by an analysis of the motion of the C₆₀ projectile as it impacts the surface. Figure 3 shows the movement and final placement of the projectile C atoms in the trajectories corresponding to those in Figure 2. In the left-hand panels of Figure 3, the motions of the projectile atoms from 0 to 100 fs at 10 fs intervals are overlaid on a single time snapshot of the position of the substrate atoms at 100 fs. C₆₀ is unable to penetrate intact into the dense diamond substrate, and the carbon atoms are confined to a small region, which corresponds to the region where the energy is deposited in the substrate. The effect of the substrate density on fragmentation of cluster projectiles was also observed in previous MD simulations of SF₅ on an overlayer of biphenyl molecules on Cu and Si substrates.⁴⁰ C₆₀ is able to penetrate deeper into the less dense SiC substrate and

Figure 3. Time snapshots of the C_{60} collision events at 100 fs for each of the three substrates. In the left panel, the projectile atomic motion during the first 100 fs is illustrated in a single frame overlaying a snapshot of the positions of the Si and C atoms in the substrate at 100 fs, which are shown as gray and blue points. The C_{60} atoms are shown as solid spheres, and the positions of the atoms are plotted at 10 fs intervals from 0 to 100 fs. The colors of the atoms progress through the rainbow from violet at 0 fs to red at 100 fs. In the right panel, the final positions of the implanted C atoms are shown as blue spheres, and the final positions of the substrate atoms are shown as points. Vertical and horizontal lines are drawn at the values of R_{cyl} for each substrate.

fragments more completely, which results in the transfer of energy to lateral motion of substrate atoms deeper within the substrate. On the least dense substrate Si, C_{60} is able to penetrate intact deeper into the surface and fragments at a later time, and some C atoms continue moving through channels in the Si substrate and deposit deep within the solid. Therefore, much of the energy in the vertical direction is deposited too deeply to be effective for sputtering.

Recently, simulations of Si bombardment with artificial Ne_{60} and $^{12}Ne_{60}$ clusters have been performed in order to understand how the formation of chemical bonds affects the net sputtered yields.³⁹ When compared to the results with C_{60} , both the Ne_{60}

and $^{12}Ne_{60}$ projectiles produce a large increase in the number of sputtered Si atoms at all incident kinetic energies. Nearly all of the C atoms from the C_{60} projectile are deposited in the target at all incident kinetic energies, while only a third of the projectile atoms are left remaining in the solid with the Ne_{60} and $^{12}Ne_{60}$ clusters. An important difference, however, is that the implanted C atoms are chemically bonded to substrate atoms in the surface. Although ^{12}Ne and C have the same mass, 70% of the ^{12}Ne atoms are reflected back into the vacuum. Therefore, it is clear that the primary reason for the large deposition of C atoms into Si is due to the formation of strong covalent bonds, which results in a decrease in the sputtered yield.

The final positions of the implanted C atoms are shown in the right-hand panels of Figure 3. The vertical and horizontal lines are drawn at the R_{cyl} values for each substrate in order to gain a better perspective relative to the energy distribution contours in Figure 2. In the case of all three substrates, C atoms are implanted outside of the region where most of the sputtered atoms are removed. The C atoms can make strong covalent bonds with Si and C atoms in the substrate and become permanently incorporated into the lattice. As a consequence, some of the projectile atoms hold on to atoms in the substrate and prevent them from being sputtered. The lateral distribution of implanted C atoms relative to R_{cyl} is similar for the three substrates and center around the area where substrate atoms are sputtered. However, the depth distribution relative to R_{cyl} varies significantly as the number density of the substrate decreases. In diamond, most of the C atoms are deposited at a depth above or equal to R_{cyl} , and, therefore, the volume of removed material is comparable to the volume of the altered substrate. In Si, more than half of the atoms are implanted at a depth below R_{cyl} , which leads to an altered region almost two times deeper than the sampled region. Some of the C atoms are able to channel through the open lattice of Si deep into the crystal without ejecting atoms during its path through the solid.

4. Conclusions

Simulations of C₆₀ bombardment of Si and C containing substrates show that strong covalent bonds can form between the projectile atoms and atoms in the target material, which results in the majority of C atoms being incorporated into the substrate lattice. The yield from SiC is a factor of roughly two times greater than that from either diamond or Si. The greater yield on SiC can be understood by the factors included in the MEDF model. SiC has intermediate values of two substrate characteristics, the cohesive energy and the number density. Furthermore, in SiC, the projectile deposits its energy into the region of the substrate that is most effective for sputtering.

The implication of these studies is that the use of chemically reactive projectile species like C₆₀⁺ may lead to chemical reactions at the bombarded surface, thus influencing the erosion dynamics. The formation of chemical bonds between projectile and surface atoms leads to a chemical alteration of the bombarded solid, which can result in a change in composition of material during depth profiling experiments. The structure and chemical composition of the Si surface may be severely damaged in the course of the sputtering process, and the simulations show that the sputtered yield changes greatly depending on the composition and density of the substrate.

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