

A molecular dynamics simulation investigation into the structure of fullerene C₆₀ grown on a diamond substrate

J.G. Chang ^a, C.C. Hwang ^{b,*}, S.P. Ju ^c, S.H. Huang ^b

^a National Center for High-Performance Computing, No. 21, Nan-Ke 3rd Road, Hsin-Shi, Tainan, Taiwan, ROC

^b Department of Engineering Science, National Cheng Kung University, Tainan 701, Taiwan, ROC

^c Department of Mechanical Engineering and Electro-Mechanical Engineering, National Sun Yat-sen University, Kaohsiung, Taiwan, ROC

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Abstract

This paper uses a Tersoff potential molecular dynamics simulation to investigate the interaction between C₆₀ molecules and a diamond substrate. The influence of the C₆₀ molecule incident energy upon the bonding preference, i.e. sp³, sp², sp or s is investigated. The current results reveal that the coating ratio actually increases rather than decreases as the incident energy of the C₆₀ molecules is increased from 80 to 100 eV. Investigation of the transient structural variation of the C₆₀ molecules shows that the additional increase in the bonding probability noted at an incident energy of 100 eV arises mainly from the changing of the structure from an s structure into an sp² structure. The steady structure statistical analysis results show that the original sp² structure of the C₆₀ molecules gradually transforms to an sp structure as the incident energy is increased from 1 to 40 eV. Furthermore, the existence of an s structure is identified at incident energies greater than 30 eV. Finally, it is observed that the impact of C₆₀ molecules on the diamond substrate seldom results in the formation of an sp³ structure.

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1. Introduction

Advances in manufacturing technologies now permit the use of fullerene C₆₀ in the fabrication of C₆₀ thin films or single crystals using sublimation or physical vapor deposition processes [1–5]. This facilitates the exciting development of fullerene-based applications that exploit the particular characteristics of fullerene C₆₀, namely superior mechanical, optical and electronic properties [6–9]. Significant research has been conducted into the growth of C₆₀ and other members of the fullerene family, e.g. C₂₀, C₂₈ and C₃₆, on carbon substrates [10–15] or on metal substrates [16]. Since the film properties are dependent upon the crystalline structure and the interaction with the substrate, it is essential that these factors are thoroughly analyzed and understood if the properties of the deposited film are to be optimized.

Previous studies have employed both experimental and numerical techniques to investigate the growth mechanisms of a C₆₀ thin film and the interaction of the film with the substrate. Experimental studies generally carried out film structure measurements to demonstrate the superior properties of the film-substrate interaction. Gao and Zhang [17] presented X-ray diffraction studies of C₆₀ and C₇₀ fullerene films grown on an SiO₂ substrate. Their results indicated that a fullerene film exhibits strong amorphous characteristics, but tends to a crystalline structure following heat treatment. In 1997, Schmidt et al. [18] employed high-resolution electron-energy-loss spectroscopy to study C₆₀ films grown on a hydrogen-terminated Si(1 0 0) substrate. Their study reported a considerably higher degree of order of the C₆₀ film when grown on hydrogen-terminated Si(1 0 0) as compared to when the film was deposited on a clean Si(1 0 0) substrate. Both studies attempted to define the process operating conditions that would yield optimum grown film properties. However, it is difficult to establish the dynamic interactions that take place between the C₆₀ film and the substrate during deposition from

* Corresponding author. Tel.: +886-6-2757575x63301; fax: +886-6-2766549/2766594.

E-mail address: chchwang@mail.ncku.edu.tw (C.C. Hwang).

off-line measurements of the structure. Therefore, dynamic film-substrate interactions are best explored via some form of numerical analysis. Katircioğlu and Erkoç [19] employed molecular dynamics (MD) simulation to investigate the absorption and decomposition of C_{60} molecules on an Si(111) surface at elevated temperatures. They found that an abrupt decomposition of the C_{60} molecules on the substrate occurred at 910 K. Man et al. [20] also adopted MD simulation to study the collision of C_{70} clusters with a graphite (0001) surface. Their results indicated that there is no significant difference between the nature of C_{70} -graphite and C_{60} -graphite interactions. However, the anisotropic characteristics of the film that may result when different initial orientation and spatial positioning of the cluster are considered were noted only for the C_{70} clusters. Webb et al. [21] investigated the growth of a diamond-like carbon film formed by the energetic impacts of C_{60} , C_{100} and C_{200} clusters on a graphite surface. They determined that sp^3 - and sp -bonded carbon structures were most readily formed at a cluster incident energy of 100 eV/atom.

The objective of the present study is to investigate the interaction of C_{60} molecules with a diamond substrate in order to develop a better understanding of the growth mechanisms of a C_{60} diamond film. Particular attention is paid to the structural composition of the diamond film, i.e. the relative presence of sp^3 , sp^2 , sp or s structures, following deposition of the C_{60} molecules at different incident energy intensities. The present simulation adopts the Tersoff potential model to model the atomic forces acting within the C_{60} molecules and the diamond substrate. Transient and steady state structural variations following impact of the C_{60} molecules on the diamond substrate are presented and discussed.

2. Simulation model

Fig. 1 presents a schematic representation of the C_{60} molecule and the diamond substrate used in the current simulation model. The C_{60} molecule and the diamond substrate are arranged according to their original structures, i.e. sp^2 and sp^3 , respectively. Furthermore, it is assumed that the diamond substrate has a perfect sp^3 structure and that the substrate surface comprises dangling bond structures, i.e. the surface has not been subjected to the hydrogen-terminated treatment considered in previous studies [22,23]. The simulation system undergoes a thermal equilibrium process at a temperature of 300 K prior to deposition of the C_{60} molecules on the substrate. The velocities of the C_{60} molecules are calculated according to their incident energies. Periodic boundary conditions are applied in the x and y directions. In order to prevent the whole substrate from shifting, a fixed bottom layer is intro-

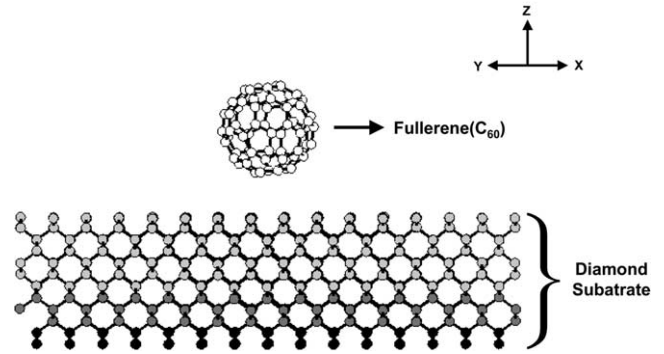


Fig. 1. Schematic representation of the C_{60} molecule and the diamond substrate used in the simulation model.

duced. The two substrate layers that lie immediately above the fixed layer are used to control the thermal state of the substrate, and are usually referred to as the thermal control layer. The Tersoff potential method is used to model the interactions within the C_{60} molecules and the diamond substrate. The Tersoff potential is a three-body potential model commonly adopted in the modeling of C–Si and Si–Ge systems [24,25] or multi-component systems. This potential is expressed by

$$E = \sum_i \sum_{j>i} f_c(r_{ij}) [V_R(r_{ij}) + b_{ij} V_A(r_{ij})] \quad (1)$$

The square bracket in Eq. (1) represents the total potential energy, which is calculated by adding the sum of the repulsive energy, $V_R(r_{ij})$, to the sum of the attractive energy, $V_A(r_{ij})$. Subscripts i and j denote atoms i and j , respectively, while the term r_{ij} represents the distance between these two atoms. The repulsive energy and attractive energy terms may be represented using the Morse-like potential form, i.e.

$$V_R(r_{ij}) = A_{ij} \exp(-\lambda_{ij} r_{ij}) \quad (2)$$

$$V_A(r_{ij}) = -B_{ij} \exp(-\mu_{ij} r_{ij}) \quad (3)$$

The cutoff function, $f_c(r_{ij})$, which limits the interaction shell located between R_{ij} and S_{ij} is given by

$$f_c(r_{ij}) = \begin{cases} 1, & r_{ij} < R_{ij} \\ \frac{1}{2} - \frac{1}{2} \cos\left(\pi \frac{r_{ij} - R_{ij}}{S_{ij} - R_{ij}}\right), & R_{ij} < r_{ij} < S_{ij} \\ 0, & r_{ij} > S_{ij} \end{cases} \quad (4)$$

In the Tersoff potential, the term b_{ij} plays an important role in determining the bond strength, i.e. the bond order. Its strength is inversely proportional to the square root of the first-neighbor coordination number (i.e. $b \propto (N)^{-1/2}$) proposed by Abell [26], and is expressed as

$$b_{ij} = \chi_{ij} (1 + \rho_i^n z_{ij}^n)^{-1/2n_i} \quad (5)$$

where ξ_{ij} is given by

$$\xi_{ij} = \sum_{k \neq i,j} f_c(r_{ik}) \omega_{ij} g(\theta_{ijk}) \quad (6)$$

Table 1
Parameters used in the Tersoff potential

Carbon											
A (eV)	B (eV)	λ ($\text{\AA}^{-1}$)	μ ($\text{\AA}^{-1}$)	β	n	c	d	h	R ($\text{\AA}$)	S ($\text{\AA}$)	
1.3936×10^3	3.467×10^2	3.4879	2.2119	1.5724×10^{-7}	7.2751×10^{-1}	3.8049×10^4	4.384	-5.7058×10^{-1}	1.8	2.1	

in which $g(\theta_{ijk})$ is

$$g(\theta_{ijk}) = 1 + \frac{c_i^2}{d_i^2} - \frac{c_i^2}{d_i^2 + (h_i - \cos \theta_{ijk})^2} \quad (7)$$

where θ_{ijk} is the bonding angle between bonds ij and ik . Note that detailed descriptions of Eqs. (1)–(7) are provided in Refs. [24,25,27–29]. The values of the parameters in Eqs. (1)–(7) adopted for the Tersoff potential in the current simulation are listed in Table 1.

3. Results and discussion

The current investigation considers the structural variations of a C_{60} molecule deposited on the (110)

surface of a diamond substrate at nine different incident energies, i.e. 1, 10, 20, 40, 70, 100, 120, 150 and 200 eV. Prior to deposition of the molecule on the surface, the substrate atoms are allowed to attain a thermal equilibrium state.

3.1. Steady C_{60} molecule morphology

Fig. 2(a)–(i) shows the C_{60} molecule steady state morphology following impact at incident energy intensities of 1, 10, 20, 40, 70, 100, 120, 150 and 200 eV, respectively. It can be seen that the final morphology of the C_{60} molecule is dependent upon the deposition incident energy. At the lower incident energies of 1 and 10 eV, the C_{60} molecule lands gently on the diamond

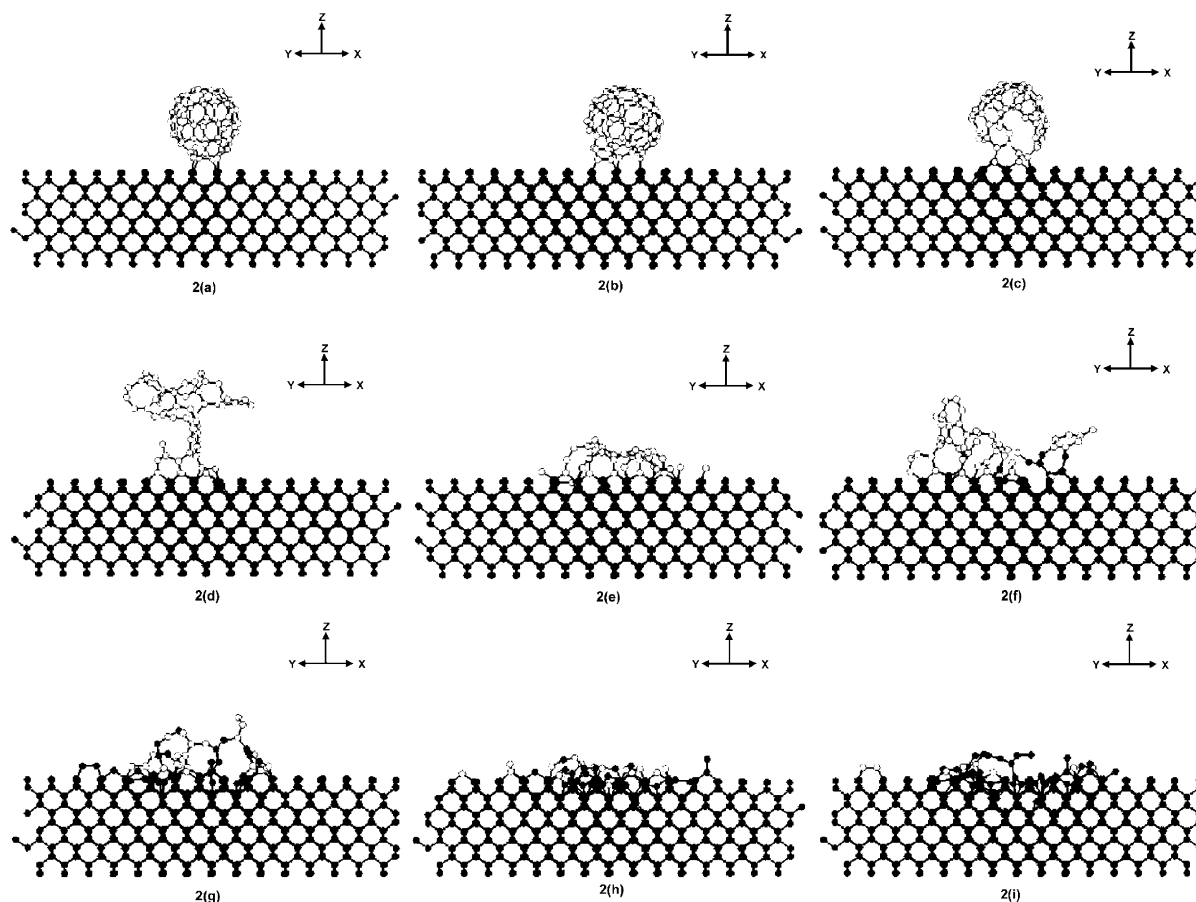


Fig. 2. Morphology of the C_{60} molecule deposited on a diamond surface at specific values of incident energy: (a) 1 eV; (b) 10 eV; (c) 20 eV; (d) 40 eV; (e) 70 eV; (f) 100 eV; (g) 120 eV; (h) 150 eV and (i) 200 eV.

substrate, and the molecule retains its original sp^2 carbon cluster structure. From Fig. 2(b), it is noted that only a very small portion of the carbon cluster is damaged at an incident energy of 10 eV. However, as the incident energy is increased to moderate levels of 20, 40 and 70 eV, the damage of the C_{60} molecule becomes more apparent. At 20 eV, the left-hand portion of the C_{60} molecule is slightly broken, but when the incident energy is increased to 40 eV, the impact of the molecule upon the substrate causes most of the molecule to become damaged. Finally, at an incident energy of 70 eV, it can be seen that the entire C_{60} molecule suffers damage upon impact.

At high incident energy intensities, i.e. those exceeding 70 eV, the C_{60} molecule structure collapses entirely and forms a “coat” on the diamond substrate. A close inspection of the collapsed C_{60} molecule morphology reveals the tendency of this coat to become flatter as the incident energy increases from 100 to 200 eV. Furthermore, analysis of the transient snapshots for incident energies exceeding 70 eV shows that some of the carbon atoms belonging to the C_{60} molecule fly away from the substrate surface. This indicates sputtering from the substrate caused by the highly energetic impact of the C_{60} molecule.

Finally, it is noted that regarding the resilience phenomenon, the results of the present study are not in full agreement with those of previous studies [22,23]. Specifically, the simulation results indicate that the incident energy of C_{60} at which a perfect C_{60} structure is preserved, i.e. the C_{60} resilience, is lower than that reported previously in studies that considered the diamond substrate surface to be a hydrogen-terminated surface [22,23]. This discrepancy can be attributed to the present assumption of dangling bonds in the diamond substrate surface. The dangling bonds surface renders the C_{60} structure more liable to damage than the hydrogen-terminated surface, and hence the resilience is lowered. C_{60} atoms tend to stick more readily to a diamond surface than to a hydrogen-terminated surface since in the latter

case, the hydrogen atoms prevent the C_{60} atoms from reacting directly with the carbon dangling bonds. The hydrogen layer also has the function of stabilizing the carbon dangling bonds and hence, reduces their reactivity. A similar conclusion has been presented in a previous study [30], which indicated that C_{60} atoms are more rarely reflected from a bare Si surface than from a Si surface with 1 or 2 hydrogen-terminated layers.

The following section considers the coating ratio of the cluster, i.e. a measure of the number of cluster atoms that become attached (or bonded) on the diamond substrate, and investigates the influence of the incident energy upon this ratio.

3.2. C_{60} molecule coating ratio

The coating ratio is a statistical measure of the percentage of C_{60} molecule atoms that remain on the surface of the substrate following impact. Fig. 3 presents the variation in this ratio at steady state conditions for incident energies in the range 1–200 eV. It can be seen that there is a significant variation in the coating ratio as the incident energy is increased, and that the curve of the variation may be broadly divided into four regions, i.e. a plateau region (I), a descending region (II), an ascending region (III) and a second descending region. The average value of the coating ratio at each incident intensity is given by the intersection of the bar and curve, while the maximum and minimum variation of the coating ratio are given respectively by the upper and lower extremities of the vertical bars. It is noted that the average value is calculated on the basis of five simulation results.

In the initial plateau region (I), the coating ratio maintains a constant value, which indicates that the C_{60} molecules do not gain sufficient energy from their impact upon the surface to escape from their bonding equilibrium positions at low incident energies. Therefore, all the carbon atoms of the C_{60} molecule remain on the surface, resulting in a coating ratio of 100%. In the second region (II), the coating ratio decreases gradually

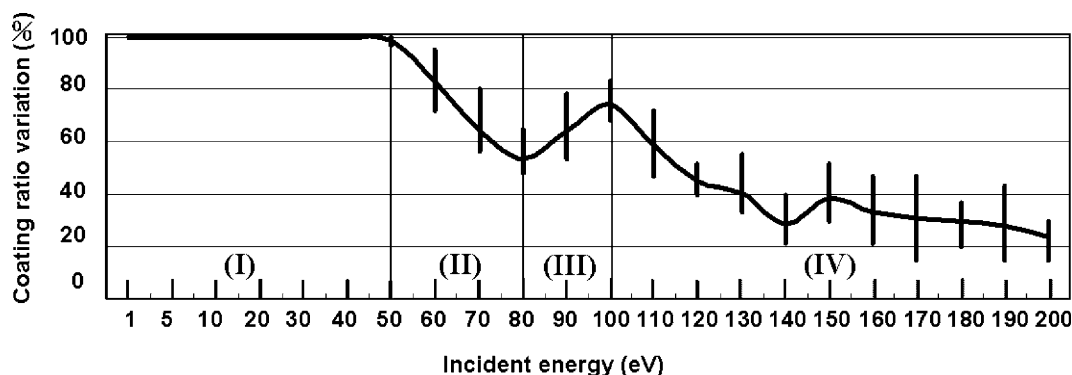


Fig. 3. Variation of coating ratio with incident energy (I) plateau region; (II) descending region; (III) ascending region and (IV) second descending region).

as the incident energy increases since the increased energy imparted to the carbon atoms by the collision on the substrate allows some of them to gain sufficient energy to escape from their bonding equilibrium positions. In the third region (III), it is noted that as the incident energy is further increased, the coating ratio does not continue to decrease, as might be expected from the results in region (II), but actually starts to increase. This result suggests that the increase in incident energy has the effect of causing a greater bonding of the C_{60} atom with the diamond substrate atom. The physical explanation for this observation is related to the internal collision cascade of the C_{60} molecule following impact on the substrate surface. In the second region (II), carbon atoms from the upper part of the C_{60} molecule escape from their bonding positions due to the kinetic energy imparted to them by successive collisions of the C_{60} atom. However, in the higher incident energy region (III), when a C_{60} molecule impacts upon the surface, the

carbon atoms located within its upper structure collide with those in the lower portion, causing them to impact directly with the substrate, where they subsequently become bonded.

3.3. Cluster structure at transient and steady states

3.3.1. Transient cluster structure variation

Fig. 4(a)–(d) shows the variation in the transient C_{60} molecule structure for the 10 ps period after impact at incident energies of 10, 70, 100 and 130 eV, respectively. In order to provide a clearer view of the transient cluster variation of C_{60} after impact, this study deliberately considers the typical behavior of one of the five simulations rather than using the statistical results obtained from the five simulations to demonstrate the transient structural variation following impact. The structural variation is evaluated by determining whether the bonding preference conforms to the s, sp, sp^2 or sp^3

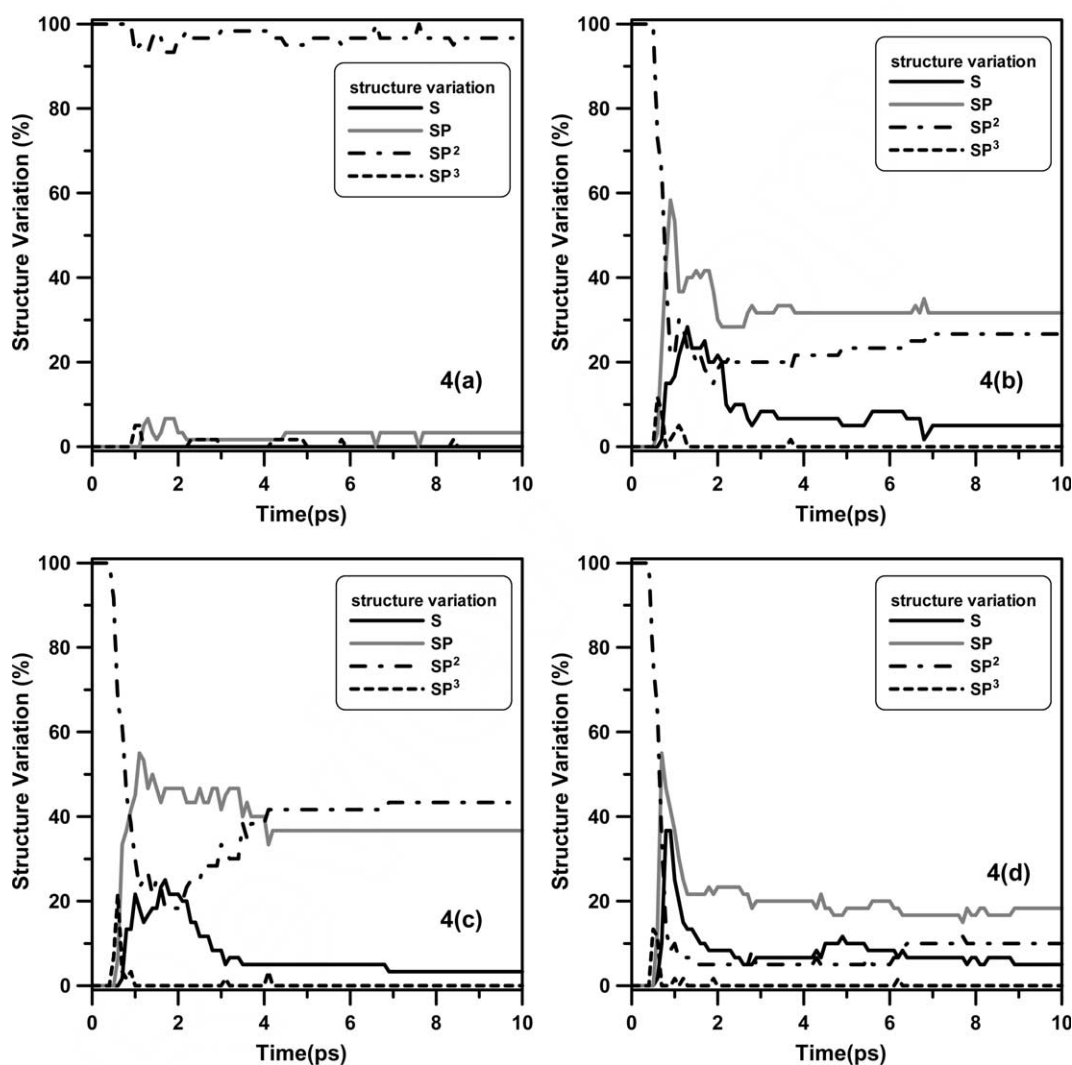


Fig. 4. Transient C_{60} structural variations at specific values of incident energy: (a) 10 eV; (b) 70 eV; (c) 100 eV and (d) 130 eV.

bonding type. This bonding preference is calculated by the atomic coordination number of a reference atom. This number indicates the number of neighboring atoms lying within the cutoff distance of the Tersoff potential from the reference atom, and provides an indication of the bonding structure, i.e. s, sp, sp^2 , or sp^3 . The additional bond angle judgment can be neglected since the three-body interaction is activated automatically by the Tersoff potential in its equilibrium bond angle structure calculation.

The data reflect both the C_{60} atoms that bond with the substrate atoms and those which re-bond with each other. Note that the atoms that fly away due to the effects of sputtering are excluded from this analysis. The data presented here can be used to verify the film structure variation after the C_{60} molecules become “coated” upon the diamond substrate. Fig. 4(a) shows the C_{60} molecule structural variation at an incident energy of 10 eV, i.e. within the plateau region (I). As would be expected, Fig. 4(a) shows a 100% sp^2 structure at the point of impact (0 ps), reflecting the original structure of the C_{60} molecule. Inspection of Fig. 4(a) indicates that the low incident energy of 10 eV is insufficient to bring about a significant change in the original sp^2 structure in the period following impact, i.e. apart from several minor “dips”, the sp^2 structure remains at 100% for the elapsed period of 10 ps considered in the current simulation. It is noted that the slight decreases in the sp^2 structure which do occur are accompanied by small increases in an sp structure. This implies that the structural arrangement within the C_{60} molecule structure changes from the original sp^2 structure to an sp structure. However, since the magnitude of the sp structural variation is small, it can be concluded that the incident energy of 10 eV is only sufficient to affect the structural arrangement of a small number of the C_{60} atoms.

Fig. 4(b) shows the C_{60} molecule structural variation at an incident energy of 70 eV, i.e. within region (II) of Fig. 3 (decreasing coating ratio with increasing incident energy). It is observed that the original sp^2 structure of the C_{60} molecule is progressively replaced by a dominant

sp structure and, to a lesser extent, an s structure. Compared to the results presented in Fig. 4(a), the structural variation of the C_{60} molecule in this case is much more dramatic, and it can be seen that the original sp^2 structure very quickly falls to a value of approximately 20% following impact. In other words, it can be concluded that an elevated incident energy of 70 eV causes significant damage to the original structure of the C_{60} molecule.

Fig. 4(c) shows the C_{60} molecule structural variation at an incident energy of 100 eV, i.e. within region (III) of Fig. 3 (i.e. increasing coating ratio with increasing incident energy). As in Fig. 4(b), the sp^2 structure falls in the period immediately following impact. However, its value does not then attain a constant value (as in the previous case). It can be seen that its value starts to rise again after approximately 2 ps, and then attains a constant value of approximately 40% after around 4 ps. The results provide evidence that the increased incident energy causes a bonding of the C_{60} atoms with the diamond substrate atoms. This conclusion is consistent with the increased coating ratio observed in region (III) of Fig. 3. Finally, it is noted that the increase in the sp^2 structure is caused by some of the atoms in an s structure reverting to their original sp^2 structure.

Finally, Fig. 4(d) shows the C_{60} molecule structural variation at an incident energy of 130 eV, i.e. within region (IV) of Fig. 3 (i.e. falling coating ratio with rising incident energy). The results confirm that the original C_{60} molecule sp^2 structure is severely damaged by the high intensity of the impact, and is replaced by an sp and (to a lesser extent) an s structure.

3.3.2. Steady C_{60} molecule structure

Fig. 5 shows the C_{60} molecule structural variation at steady state conditions for different values of the incident energy. As in Fig. 4, the data reflect both the C_{60} atoms that bond with the diamond substrate atoms and those which re-bond with each other. The C_{60} atoms that fly away from the substrate due to the sputtering effect are once again excluded. It is clearly seen that the

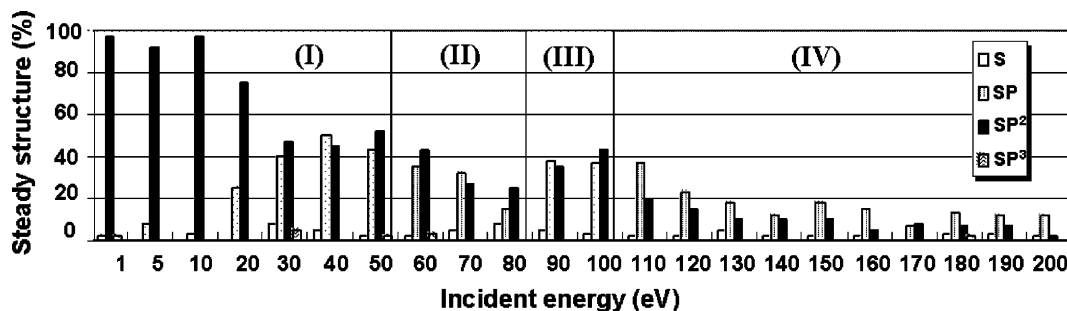


Fig. 5. Steady structure statistics at different incident energies (as in Fig. (3), (I) plateau region; (II) descending region; (III) ascending region and (IV) second descending region).

sp^2 structure of the C_{60} molecule decreases as the incident energy increases to a value of 80 eV. Furthermore, it is observed that this decrease is accompanied by a marked increase in the sp structure, and a rather smaller increase in the s structure. Therefore, it is possible to conclude that the original sp^2 C_{60} molecule structure changes primarily to an sp structure rather than an s structure for impacts at an incident energy in the range 1–80 eV.

A close observation of the value of the sp structure shows that it increases as the incident energy rises from 1 to 40 eV, at which point it attains its peak value of approximately 50%. Its value then falls gradually as the incident energy is further increased to 80 eV. The decrease in the sp structure in the latter range is accompanied by an increase in the s structure. As the incident energy increases from 80 to 90 eV, the sp structure again increases, and remains at an approximately constant value of around 40% until an incident energy of 110 eV, after which it gradually decreases as the incident energy rises to 200 eV.

The results presented in Fig. 5 suggest that the sp^3 structure is seldom generated by the impact of C_{60} molecules at the incident energies considered in the present study. A close inspection of the results shows only a minimal presence of the sp^3 structure, i.e. at 30 and 60 eV.

Finally, it can be seen that an s structure is evident for incident energies exceeding 30 eV. However, its presence is not large and, in contrast to the sp structure discussed above, no definite trends in its value are revealed as the value of the incident energy is increased. Having said that, it is clear that the relative presence of the s structure compared to that of the sp and sp^2 structures increases at incident energies exceeding 120 eV since the latter two structures become less dominant at higher incident energy intensities.

4. Conclusions

This study has presented the use of MD simulation to investigate the interactions between C_{60} molecules and a diamond substrate. The MD Tersoff potential has been employed to model the atomic forces between the C_{60} molecules and the substrate. The steady and transient structural variations of the C_{60} molecules in the period following impact have been presented and discussed. The principal conclusions that may be drawn from this study are summarized as follows:

(1) At low incident energies of less than 50 eV, the C_{60} molecules land gently on the diamond substrate, and form a perfect coat on the substrate surface. As the incident energy is increased to 80 eV, the coating ratio decreases. Interestingly, as the incident energy is further increased to 100 eV, the coating ratio increases. The transient structural analysis indicates that one of the

typical behaviors, i.e. an increase in the sp^2 structure, is prompted by atoms reverting from an s structure to their original structure. Finally, the coating ratio is seen to fall as the incident energy increases from 100 to 200 eV.

(2) Analysis of the steady state structural data reveals that the original sp^2 structure of the C_{60} molecule transforms primarily to an sp structure as the incident energy is increased. It is found that the value of the sp structure increases to its peak value at an incident energy of 40 eV and then gradually decreases as the incident energy is further increased to 80 eV. Its value subsequently increases as the incident energy rises to 100 eV and once again falls as the incident energy is increased to 200 eV. The sp^3 structure is only generated for C_{60} molecule impacts occurring at incident energies of 30 and 60 eV. However, its presence is small. Finally, the appearance of the s structure does not exhibit a definite trend as the incident energy increases.

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