Molecular dynamics study of deposition mechanism of cubic boron nitride

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Abstract

We have performed molecular dynamics simulations of bombardment of graphitic boron nitride (gBN) by energetic boron and nitrogen particles in order to examine the roles of ion bombardment in ion/plasma-assisted deposition of cubic boron nitride (cBN) thin films. We have found that the interaction of the energetic particles with gBN creates four-fold coordinated local structures (sp\textsuperscript{3}-formation) inside gBN. We have also found that clusters of sp\textsuperscript{3}-formations are created as a result of successive bombardment, some of which have cBN-like structures. On the basis of these results, we propose an atomic-scale model of cBN nucleation in which successive sp\textsuperscript{3}-formation converts gBN into cBN. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Ion- and plasma-assisted deposition of cubic boron nitride (cBN) thin films is a subject of great interest for several reasons. First, for example, cBN itself is a fascinating material with many remarkable properties. It has hardness close to diamond, excellent thermal stability, chemical inertness, transparency, high thermal conductivity, low dielectric constant, and wide band gap [1]. It is notable that cBN has several advantages over diamond: (i) it is inertert against iron and oxygen [1], and (ii) it has successfully been doped both as p- and n-type [2]. Owing to these properties, many potential applications are envisioned for cBN thin films. Due to the extreme hardness and stability, cBN thin films are a natural candidate for protective coatings. Especially, cBN thin films can be used as coatings for steel and optical elements because of its inertness against iron and transparency, respectively. Due to its electronic properties, they can be used as UV photodiodes [3], high-temperature and high-power semiconductor devices, etc. Secondly, the successful synthesis of cBN thin films by ion/plasma-assisted methods is one of the examples that best demonstrate the ability of these energetic techniques to achieve the growth of materials that conventional non-energetic methods have failed to synthesize. It is usually accepted that, in vapor-phase deposition of boron nitride, some form of ion bombardment during growth is necessary to obtain cBN-containing films [4], and that without ion bombardment, only graphitic boron nitride (gBN), an sp\textsuperscript{3}-bonded form of BN, is grown. Lastly, the subject is also interesting from a scientific viewpoint, since it is the intersection of two fields, namely the study of ion–solid interactions and the theory of crystal growth. Clarifying the elementary processes in which interactions between energetic particles and matter lead to the formation of a novel phase such as cBN is a great challenge. For these reasons, the subject has been pursued energetically for nearly two decades.

Currently, BN films with a high cBN content are grown by various ion/plasma-assisted deposition methods. However, many problems are to be solved before the cBN thin film technology is to be realized. For example, (i) it is found that non-cubic phases, such as gBN, grow before cBN nucleation and remain as an interlayer in the film [5], (ii) the epitaxial growth of single crystal films is not yet achieved, and (iii) the adhesion of the film to the substrate is poor primarily due to the large residual stresses created by ion bombardment [6]. Over the years, the deposition techniques have been greatly improved, and some solutions have been found for these problems. For example, it has been found that the intensity of ion bombardment can be reduced once the cBN phase is nucleated, and in this way films with smaller stress have been grown [7]. Despite such progress,
the road to the realization of the cBN thin film technology is still unclear. Therefore, a comprehensive growth model of cBN and the atomic-scale insights into the growth processes are desired. The atomic-scale processes have rarely been investigated, because the atomic-scale in situ observation of the growing film, which itself is extremely difficult, is made nearly impossible by the use of ion bombardment. Because of this, most of the growth models proposed so far are either kinetic models based on some assumed atomic-scale processes or phenomenological models constructed to explain experimental data. We discuss here two major growth models, namely ‘subplantation model’ [8] and ‘stress model’ [9,10]. (For extensive discussion of growth models, we refer to a review by Mirkarimi et al. [7].) Both models are based on the fact that ion bombardment creates defects in the material. In the subplantation model it is argued that the concentration of the defects increases local density, which leads to the formation of the high-density phase, namely, cBN. In the stress model, on the other hand, the stress created by the defects is considered to promote the formation of cBN, which is the high-pressure phase. In both models, therefore, the atomic-scale structure and formation mechanism of the bombardment-induced defects are important. Owing to the difficulty of atomic-scale study, these features are rarely investigated. In this context, atomic-scale computer simulations of the growth processes are quite useful in augmenting the lack of experimental facts, and in providing basis for kinetic growth models. These are the objectives of the present study.

Several computer simulations have been performed in the field of cBN deposition. Programs such as TRIM (transport of ions in matter) [11] have been used in the calculation of the distribution of ions inside films, mainly to back up kinetic growth models [12]. However, these calculations, like kinetic growth models, depend on the assumed atomic-scale processes: ions are assumed to create defects inside the target, but the structure and formation mechanism of defects in gBN are not well understood. Since we are concerned with such processes, more detailed simulation methods capable of yielding atomic-scale knowledge are necessary. The molecular dynamics (MD) method, which we have employed in this study, is one of such methods.

MD simulation of deposition of cBN on cBN substrate by energetic boron and nitrogen particles has already been performed by Albe et al. [13]. The model of the cBN substrate used in their simulation consisted of 1216 atoms with 32 atoms per layer. The impact of 300 energetic particles on dimer-reconstructed boron-terminated (100) surface was simulated for different energies from 10 to 600 eV. In their simulation, a low-density amorphous network was observed to grow on the partially destroyed cBN substrate surface. Unfortunately, no cBN formation was observed. They noted that cBN phase formation is a process occurring on much longer time scales than that of their simulation.

MD study of the nucleation of cBN on (or inside) gBN, on the other hand, has not yet been attempted, although clarifying the nucleation mechanism is the key in controlling the thickness of the gBN layer, the size and orientation of cBN crystallites, residual film stress, etc. Therefore, we have performed MD simulations of bombardment of gBN by energetic boron and nitrogen particles, to examine the interactions between energetic boron and nitrogen particles with gBN, and their roles in cBN nucleation. In Section 2, the method of simulation is presented. In Section 3, the simulation results are discussed in connection with cBN nucleation. Especially, the simulation results are discussed in connection with cBN nucleation. Especially, the structure of defects induced by bombardment and their formation mechanism are described in detail. We also propose an atomic-scale nucleation model of cBN based on the results of MD. In Section 4, concluding remarks are given.

2. Methods

In the present study, we have simulated bombardment of gBN by energetic boron and nitrogen particles using the molecular dynamic method. MD is a method of predicting the behavior of a system of atoms by solving the equation of motion for each particle. The reliability of the method is mainly determined by the way the atomic forces are evaluated. The forces can be evaluated quantum-mechanically or by taking derivatives of analytical interatomic potential functions constructed to reproduce experimental or quantum-mechanically calculated results. In this paper, an interatomic potential developed by Albe et al. [13,14] is used. This potential has a functional form similar to a Tersoff potential [15,16], and is fitted to a wide range of ab initio data of various boron–nitrogen clusters and BN polymorphs. The functional form of Albe’s potential is presented in Appendix A.

The algorithm of MD is basically as follows: (i) First, forces on the constituent particles at the moment are calculated as a function of their positions, (ii) then the accelerations are obtained by solving the equations of motion, and then (iii) the particle positions and velocities at the next instant are calculated using the accelerations. In the present study, the velocity Verlet algorithm [17] is employed. The time step is chosen to be 0.1 fs. In practical simulations, exchange of energy between the system and the surrounding needs to be incorporated in the algorithm. In the present case the temperature of the system is regulated using the Berendsen’s method [18]. In this method, the system is coupled with an external heat source, and the heat is exchanged at the rate proportional to the difference in the temperature. The proportionality constant, which controls the rate of heating and cooling, is determined by a parameter called coupling time constant.

The gBN target used in the simulation is a model of gBN interlayer that grows before cBN nucleation. To construct
the target suitable for the simulation of the nucleation processes, we now discuss some features of the gBN interlayer. First, it is generally found that the basal planes of the gBN interlayer is parallel to the film normal [9]. Secondly, the interlayer has compressive stress due to ion bombardment. Lastly, the interlayer of gBN seems to be the mixture of hexagonal BN (hBN) and rhombohedral BN (rBN) [19], and there is a question as to which of the two serves as cBN nucleation sites. The two graphic phases, hBN and rBN, differ in the way the basal planes are stacked. The structure of hBN and rBN is shown in Fig. 1 along with the structure of cBN and wurtzite BN (wBN). The stacking sequence of hBN basal planes may be described as AA', with successive layers placed directly above each other. On the other hand, rBN has ABC stacking sequence, with successive layers displaced to each other along the direction of the BN bond by exactly one bond length. It is notable that rBN is structurally similar to cBN: geometrically, rBN can be transformed into cBN by puckering rBN basal planes into (111) layers of zinc blende structure, and shortening the layer separation. To incorporate the first feature into the simulation, the basal planes of the model gBN target are oriented parallel with the film normal. The second feature may be incorporated by shrinking the separation between basal planes. But in the present study, the experimentally found equilibrium value, 3.33 Å, is used throughout the bombardment simulations. As to the third point, rBN seems more important, as rBN is found at the nucleation sites [20], and as rBN is structurally similar to cBN. We have, however, performed simulations of bombardment of hBN as well as that of rBN, for comparison. The models of the rBN and hBN targets are shown in Fig. 2. Both targets contain 1008 atoms, consist of six basal planes, and have a thickness of about 30 Å. Periodic boundary conditions are imposed for directions parallel to the target surface. The 144 atoms at the bottom of the target are fixed to prevent the target from being pushed downward by the impact. The bond length of gBN is initially set to be 1.462 Å, which is the equilibrium length under Albe’s potential.

After the target is equilibrated at the specified temperature for 1 ps, neutral B and N projectiles are alternately shot against (1100) face of the target. We have performed several simulations of the impact of 50 projectiles at the rate of one in 200 fs, varying the energy of the incoming particles, \( E_p \), and the temperature of the heat source, \( T_s \): (i) \( E_p = 10, 25, 50, 100, 200, 300, 400, \) and \( 500 \) eV with \( T_s = 700 \) K, and (ii) \( T_s = 300, 700, \) and \( 1000 \) K with \( E_p = 50 \) eV. In these simulations, the direction of incidence is parallel with the film normal. The positions of impact are selected by using random number series. To verify that the result is not random-number dependent, three simulations using different random number series are performed for each condition.

In bombardment simulations, the interval between impact is generally chosen to ensure the equilibration of the target before the successive impact. This means that (i) the particle either finds its stationary position in/on the target, or leaves

| sp\(^3\)-bonded | sp\(^3\)-bonded |
|------------------|------------------|
| ![Image](https://via.placeholder.com/150) | ![Image](https://via.placeholder.com/150) |

![Image](https://via.placeholder.com/150)

**Fig. 1.** Crystal structure of hBN, rBN, wBN and cBN.
the target, that (ii) the shock waves caused by the impact are dissipated, and that (iii) the target temperature returns to its equilibrium value. Through test runs, we have confirmed that the interval of 200 fs is enough for the first and the second conditions. To ensure the third condition, the coupling time constant of the Berendsen’s method is chosen to be 10 fs. We note that only the target atoms are coupled to an external heat source. This may not be suitable if the number of impacting particles is large, but sufficient for the present simulations. We also note that the interval of 200 fs is not long enough to allow diffusion processes.

The coordination number of atoms is monitored throughout the bombardment simulation. The coordination number of an atom is defined as the number of neighboring atoms lying within the distance of 1.7 Å. We note that the equilibrium bond lengths under the present potential is 1.462 and 1.555 Å for gBN and cBN, respectively. The number of four-fold coordinated atoms is considered to be the measure of the sp³ content of the system in the following analysis.

3. Results and discussion

3.1. Creation of four-fold coordinated local structures due to bombardment

Fig. 3 shows a snapshot of a part of the rBN target after bombardment, which shows the formation of several point defects induced by bombardment. As can be seen in the enlarged images (Fig. 4), they have four-fold coordinated tetrahedral structure typical of sp³-bonded structure, and hence their formation contributes directly to the increase in the sp³ content of the target. Moreover, more than half of the four-fold coordinated defects have the BN4 and NB4 configurations, which are the constituents of cBN. In the case of \( E_p = 50 \) eV and \( T_s = 700 \) K, for example, 66–74% of the four-fold coordinated defects have the BN4 and NB4 configurations. These facts imply that the bombardment-induced defects play important roles in cBN nucleation. To emphasize this, we call these defects and their formation process sp³-formation. There are two types of sp³-formation observed in the simulations, namely sp³-bridge (Fig. 4(a)) and sp³-protrusion (Fig. 4(b)). We note that both of them are found in the hBN bombardment simulations as well.

The creation process of sp³-formations shown in Figs. 3 and 4 is illustrated in Fig. 5. These illustrations are based on the snapshots obtained in the rBN bombardment simulation. The formation mechanism is as follows. First, an energetic particle (nitrogen in this case) penetrates the target surface and channels through the gap between basal planes (stage 1). Then, the particle collides with a basal plane, displacing an atom onto the adjacent basal plane (stage 2). The bonding

![Fig. 2. Models of the (a) rBN and (b) hBN targets and the coordinate system used in the simulation.](image1)

![Fig. 3. Snapshot of a part of the system after bombardment. Four-fold coordinated local structures are enclosed in rectangles.](image2)
of the collided atom (boron in this case) with another atom (nitrogen) of the adjacent basal plane creates a bridge-like four-fold coordinated local structure with \( \text{NB}_3\text{-BN}_3 \) configuration, which we call \( \text{sp}^3 \)-bridge (stage 3). Finally, the particle is adsorbed on top of a basal plane atom. This results in the formation of an \( \text{sp}^3 \)-protrusion (stage 4). We note that this is only an example, and that \( \text{sp}^3 \)-bridges and \( \text{sp}^3 \)-protrusions are not necessarily created in pairs.

A further evidence indicating the role of \( \text{sp}^3 \)-formation in cBN nucleation is that clusters of \( \text{sp}^3 \)-formations are created inside gBN as a result of successive bombardment (Fig. 4(c)). In the case of rBN bombardment simulations, some of them, such as shown in Fig. 4(c), have a cBN-like structure. This suggests that successive \( \text{sp}^3 \)-formation has the potential to achieve cBN nucleation. Following the creation process of \( \text{sp}^3 \)-formations and cBN-like clusters recorded in the snapshots, we have constructed an atomic-scale model of cBN nucleation. The nucleation model is presented in Section 3.2. In Section 3.3, we discuss quantitative aspects of \( \text{sp}^3 \)-formation.

3.2. cBN nucleation model

In the present study it is found that the interaction of energetic particles with gBN creates clusters of \( \text{sp}^3 \)-formations such as shown in Fig. 4(c). On the basis of this result, we propose a model of cBN nucleation in which gBN is transformed into cBN by successive \( \text{sp}^3 \)-formation. In the case of rBN, geometrical consideration suggests that there are two conceivable pathways of cBN nucleation, as illustrated in Fig. 6. The first is transformation of rBN into cBN by successive creation of \( \text{sp}^3 \)-protrusions (Fig. 6(a)). The second is transformation of rBN into cBN by successive

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**Fig. 4.** Bombardment-induced four-fold coordinated local structures, observed in the simulations. Examples of (a) \( \text{sp}^3 \)-protrusion, (b) \( \text{sp}^3 \)-bridge, and (c) cluster of four-fold coordinated local structures. In (c), only those atoms belonging to BN\(_4\) and NB\(_4\) configurations are shown.

**Fig. 5.** Mechanism of \( \text{sp}^3 \)-formation.

**Fig. 6.** Model of cBN nucleation based on the present results. Transformation of rBN into cBN by successive creation of (a) \( \text{sp}^3 \)-protrusions, and (b) \( \text{sp}^3 \)-bridges.
creation of sp³-bridges (Fig. 6(b)). In the case of hBN, on the other hand, there appears to be no pathways as simple as those of rBN. This is because rBN is structurally close to cBN, while hBN is not.

The rBN-to-cBN transformation by sp³-protrusions, illustrated in Fig. 6(a), proceeds as follows. First, a projectile coming near as sp³-protrusion (stage 1) is trapped between the protrusion and the adjacent basal plane, creating a BN$_3$–NB–NB$_3$ configuration (stage 2). Then another projectile is trapped between a two-fold coordinated atom of the configuration and the basal plane, creating a BN$_3$–NB$_3$–N$_2$B$_5$ configuration (stage 3). As these processes continue, the two rBN basal planes are converted into cBN(111)-like planes, while an extra cBN(111)-like plane consisting of deposited projectiles grows between them. As can be seen in Fig. 6(a), the orientational relationships between these cBN(111)-like planes are indeed that of cBN. We note that the BN$_3$–NB–NB$_3$ configuration of stage 2 have actually been observed in the simulations, while the subsequent processes have not yet been observed.

The rBN-to-cBN transformation by sp³-bridges, as illustrated in Fig. 6(b), is the process responsible for the creation of cBN-like cluster shown in Fig. 4(c). The mechanism is simple: A projectile colliding with a target atom adjacent to an sp³-bridge (stage 1) creates another sp³-bridge next to the previous one (stage 2), and the repetition of this process converts the two rBN basal planes into two (111) layers of cBN.

It is interesting to discuss the relation between the conventional growth models and our nucleation model. We note that our model is atomistic, and cannot be compared directly to kinetic or phenomenological models. Rather, it forms the basis of kinetic models. In this sense, our nucleation model is consistent with the subplantation model; in both models cBN nucleation results from cluster formation of bombardment-induced defects. The difference is that the individual defect has not usually been considered to be sp³-bonded, while the present results suggest the defect itself has an sp³-like configuration.

3.3. Quantitative aspects of sp³-formation

In this section we discuss the conditions that yield the large number of sp³-formation. It is true that the present simulations are not entirely kinetically accurate because the short duration of the simulation does not allow thermal processes, and because the bombardment rate is significantly faster than that of experiments. But thermal processes are slow, especially in strongly bonded materials such as BN, and hence do not affect the results appreciably.

The number of four-fold coordinated atoms in the system is plotted for the rBN bombardment simulations (i) against time in Fig. 7(a), (ii) against the temperature of the heat source in Fig. 7(b), and (iii) against the energy of energetic particles in Fig. 7(c). The following features are apparent in these plots. First, one can see from Fig. 7(d) that the sp³ content increases almost steadily. This suggests that the rate of creation of sp³-formations is faster than that of the annihilation. In fact, sp³-protrusions seem to be quite stable, and are not destroyed unless they are collided by energetic particles. The sp³-bridges are less stable but last long enough to contribute to the cluster formation. These facts support our model that sp³-formation plays important roles in cBN nucleation. Next, the temperature of the heat source

![Fig. 7. Number of four-fold coordinated atoms in the rBN target plotted against (a) time, (b) the temperature of the heat source T_0, and (c) the impact particle energy E_p. In (d), the number of four-fold coordinated atoms in the hBN target is plotted against E_p. The numbers '1', '2', and '3' refer to three simulations with different random number series determining the positions of impact. The label 'avg' refers to the average over the three simulations. In (a), E_p = 50 eV and T_0 = 700 K. In (b), E_p = 50 eV. In (c) and (d), T_0 = 700 K.](image-url)
does not appear to affect the results considerably, as can be seen in Fig. 7(b). This is because the thermal processes are slow in this range of temperatures (300–1000 K). Lastly, two threshold values, 25 and 100 eV, are visible in Fig. 7(c): the number of four-fold coordinated atoms increases rapidly around 25 eV, reaches a plateau at 50 eV, and increases again above 100 eV. It is notable that the number of four-fold coordinated atoms exceeds the number of projectiles for $E_p \geq 300$ eV. The value decreases above 300 eV, apparently due to increasing bombardment damages. These results suggest that the energy of the order of several hundred electron volts is ideal for maximizing the number of sp$^3$-formation. This is in fact consistent with most of the threshold values for cBN formation found in deposition experiments. For example, Hofssass et al. found the threshold value of 125 eV for cBN formation in mass selected ion beam deposition of BN films [21].

We have identified the atomic processes determining the two threshold values, 25 and 100 eV, by examining snapshots. The first one, 25 eV, corresponds to the penetration barrier. It is notable that this penetration barrier is not related to the displacement energy of the surface atoms. The barrier exists because the one- and two-fold coordinated surface atoms tend to adsorb incoming particles in order to achieve higher coordination. The second threshold, 100 eV, corresponds to the threshold for knock-on processes. A knock-on means the process in which a target atom collided by an energetic particle becomes energetic itself. These knock-on atoms create sp$^3$-formations just as incoming particles do, thus contributing to the increase in the sp$^3$ content.

The number of four-fold coordinated atoms in the system is plotted for the hBN bombardment simulations against incoming particle energies in Fig. 7(d) for comparison. The tendency is similar to the case of rBN, except second threshold is not entirely visible. Such a minor difference can be attributed to the fact that the surface atoms of the present hBN target are all two-fold coordinated, whereas those of the rBN target include one-fold coordinated atoms.

4. Concluding remarks

Using MD method with the interatomic potential developed by Albe et al., we have performed simulations of bombardment of gBN by energetic particles of boron and nitrogen. Our aim is to clarify the mechanism of bombardment-induced nucleation of cBN. We have found that the interactions of projectile with the target create four-fold coordinated local structures, which we call sp$^3$-formations. Clusters of sp$^3$-formations are created as a result of continued bombardment. On the basis of these results, we have proposed a model of cBN nucleation in which gBN is transformed into cBN by successive creation of sp$^3$-formations. Especially for the case of rBN, two atomic pathways of cBN nucleation have also been presented.

The novelty of the present results is that defects created in gBN by bombardment are themselves four-fold coordinated local structures, contributing directly to the increase in the sp$^3$ content. This possibility has not been considered in the former studies on ion/plasma-assisted deposition of cBN. We again emphasize the need of detailed experimental and theoretical study of bombardment-induced defects in order to establish the basis on which growth models are to be constructed. We are currently investigating the bombardment-induced defects using first-principles calculations.

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Appendix A. Potential for a system of boron and nitrogen atoms

In the present study, a Tersoff-like potential developed by Albe et al. (Albe’s potential) [13,14] is employed in the calculation of the interatomic forces. This potential, fitted to a wide range of ab initio data, is capable of describing various BN polymorphs and clusters.

Albe’s potential is a sum of the pairwise term, $\phi_{ij}$ over all pairs of atoms lying within the range of interaction $r_{co} = R + D$:

$$\Phi = \frac{1}{2} \sum_i \sum_{j \in N(i)} \phi_{ij}$$

$$\phi_{ij} = f_c(r_{ij})[f_k(r_{ij}) - b_i f_A(r_{ij})].$$

Here $N(i)$ denotes the set of neighbors of the $i$th atom, i.e. the set of atoms that lie within $r_{co}$. The repulsive term $f_k(r)$ and the attractive term $f_A(r)$ have forms similar to a Morse potential, as proposed by Brenner [22]:

$$f_k(r) = \frac{D_0}{S - 1} \exp(-\beta \sqrt{2S}(r - r_0))$$

$$f_A(r) = \frac{SD_0}{S - 1} \exp(-\beta \sqrt{2S}(r - r_0)),$$

where $D_0$ and $r_0$ are the dimer energy and bond length; $S$ and $\beta$ are fitting constants. The cutoff function $f_c(r)$ is

$$f_c(r) = \begin{cases} 
1 & r \leq R - D \\
\frac{1}{2} - \frac{1}{2} \sin[\pi(r - D)/(2D)] & |r - R| \leq D \\
0 & r \geq R + D
\end{cases}$$

The bond-strength factor $b_i$ is a function of positions of all the neighbors of the $i$th atom, and includes terms depending
on bond angles:

\[ b_{ij} = \left( 1 + \gamma \chi_{ij} \right)^{-1/2n} \]

\[ \chi_{ij} = \sum_{k \neq j} f_c(r_{ik}) g_{ik} w_{ijk} \]

\[ g(\cos \theta_{ijk}) = 1 + \frac{\mathbf{c}^2}{d^2} - \frac{\mathbf{c}^2}{d^2 + (h - \cos \theta_{ik})^2}, \]

\[ w_{ijk} = \exp\left(\lambda_1 (r_{ij} - r_{ik})^3\right), \]

where

\[ \cos \theta_{ijk} = \frac{r_{ij} r_{ik}}{r_{ijk}} \]

The parameter set for Albe’s potential is listed in Table 1.

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