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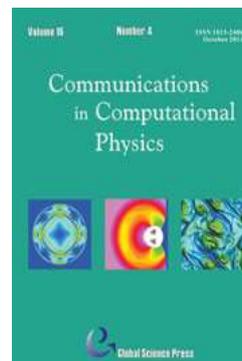
Dynamics of the Formation of the Nitrogen-Vacancy Center in Diamond

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Abstract. We present results of simulations of the energetics and dynamics involved in the realization of the NV (nitrogen-vacancy) center in diamond. We use the self-consistent charge-density functional tight-binding approximation and show that when the nitrogen resides on a single substitutional site, it fails to attract a vacancy, hence no NV center can be formed. However, if it occupies a split interstitial site and two vacancies reside on the second or third neighbor sites, an NV center will form following annealing at temperatures as low as 300°C and 650°C, respectively. These results provide guidelines to experimentalists on how to increase the efficiency of NV formation in diamond.

1 Introduction

The nitrogen vacancy (NV) complex in diamond, in particular the negatively charged NV$^-$ center, offers promising applications as a qubit. These may be the basis for future quantum computers. Amongst the advantages of this center are the luminescence wavelength, its long coherence time, operation at room temperature and the fact that it is located in diamond, offering a unique environment exhibiting unprecedented mechanical, electrical and optical properties. Since diamond is bio-compatible, NV centers, when located in nano diamond, may serve in many biological/medical applications [1,2].

However, it is still unclear how to optimize the formation of NV centers in diamond in a form in which they may be efficiently used. The requirements of this center, to be

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applicable, include being able to accurately place it at the desired location in the diamond, in an environment that is free of disturbing spins. In other words in as perfect a diamond environment as possible. Hence it is important to find ways of optimizing the formation of this center so as to fulfill the above requirements.

Substantial experimental efforts have been devoted to find ways to efficiently form NV centers and to study their properties [3–10]. Most experimental approaches rely on ion-implantation, both for the introduction of nitrogen atoms at pre-determined locations and to provide ample vacancies in the vicinity of the nitrogen to allow the formation of the NV complex. Therefore co-implantation of nitrogen and vacancy producing inert ions (carbon and noble gases) has been extensively studied. Routes that enhance the diffusion of the vacancies or the nitrogen impurities, as a result of heating have also been investigated.

In order for the NV complex to have the energy levels required for use as a qubit and for other spin related manipulations, an extra electron needs to be attached to the NV^0 center, thereby rendering it negatively charged. In other words, it is the NV^- that is the complex which must be formed in the diamond [5, 7, 17]. Experimental attempts to preferentially form an NV^- center seem to indicate that ample electrons need to be present i.e. the NV should reside in an n-type environment. It is, however, unclear if the attachment of the extra electron occurs during the formation of the NV complex or only at a later stage. In this study we address the dynamics and energetics for NV formation disregarding its charge state. We believe that no major changes to our results would be due to the attachment of an extra electron. However, a computation of dynamics for an NV^- center is currently beyond our scope.

Several computations (at different levels of accuracy) have been made regarding the energetics of different nitrogen/vacancy complexes, their formation energetics [11–15] and the properties of the nitrogen interstitials in diamond [16]. The most precise method [11, 17–19] deals with different structural combinations of defects in diamond, which includes nitrogen atoms and vacancies. The information obtained from these, specifically the diffusion barrier calculation of the vacancy and the substitutional nitrogen, is helpful for the study of NV center formation. None of the computations known to us addressing the NV center in diamond deal with the *dynamics* of the NV formation, nor with the possible effects that charge states in the system may have on the diffusion of the species in diamond and their effect on the NV formation.

It should be mentioned that extensive first principle computational publications regarding the NV center in silicon exist in the literature. These, however, describe the results of static first principle computations for silicon [20–22] but do not consider the dynamics of the NV creation in silicon. Since silicon and diamond have vastly different properties, (despite their similar geometrical structures) the silicon results are not applicable to diamond.

In this paper we present tight binding ab-initio molecular dynamics simulations to explore the *dynamics and energetics* of the formation of the NV center in diamond. These are essential for a full understanding of the NV formation mechanism, providing guide-

lines for the experimentalists how to optimize the NV formation in the laboratory by ion implantation. In the next section we present an overview of our study, and make connections to experimental studies as appropriate. In Section 3 we describe our methodology in detail, including a description of the two scenarios we compare: process A, where a nitrogen atom initially resides on a substitutional site, and process B where it is initially placed on an interstitial site. Section 4 is devoted to our results, in Section 5 we discuss under which conditions these results are realistic and in Section 6 a summary and conclusions are presented.

2 Overview

Our simulations of the energetics and dynamics involved in NV formation concentrate on diamond samples that already contain nitrogen atoms and vacancies located at different "initial" positions in the diamond. They do not explicitly model specific experimental ways of creating these initial conditions. However once the desirable configurations for efficient formation of NV defects are found from computations, experimental ways of actually creating these in the laboratory can be designed and implemented. Some possible routes to achieve these are presented below.

To model the creation of the NV complex in diamond the sample must include a nitrogen impurity and some vacancies. The nitrogen atom can, in principle, reside on a substitutional site, as occurs when it is introduced into the diamond during growth, or it can reside in different interstitial sites, such as is likely to occur following ion implantation. The vacancies in the diamond sample can be isolated vacancies located on carbon sites or can form complexes, such as divacancies. These may be located at different distances from the nitrogen. Vacancies are commonly introduced experimentally into the vicinity of the nitrogen impurity by damaging processes such as those that result from inert ion-implantation or electron irradiation. The laboratory formation of the vacancies can be carried out at different temperatures: cold – to freeze-in the impurities and defects or hot – to assist their instantaneous diffusion leading to different vacancy locations and configurations. Annealing is applied to the samples containing the nitrogen and ample vacancies to enhance the diffusion of vacancies to meet with a nitrogen atom to form the desired NV center. Experimental results of nitrogen implanted in diamond show a significant increase in the NV center photoluminescence intensity and coherence time after further vacancy implantation and thermal annealing at temperatures in the range of $600-800°C$ [5,6,10,23,24].

3 Calculations

The simulations described in this paper cover a range of initial states and dynamic processes, meant to mimic different conditions of actual experiments carried out in the laboratory. The diffusing species (N and V) are assumed, like in papers of others [11,12,16,25]

to be uncharged. While commonly assumed in various computations, it may not hold for some cases. For example when the dynamics takes place in a charged environment (depending on the Fermi level position). Nevertheless, it is reasonable to assume that inclusion of charges in the simulations will, most likely, only enhance the formation of the NV complex, computed here for neutral species only.

3.1 Methods

Previous calculations by our group have modeled the dynamics of the formation of the split interstitial following ion bombardment of diamond [26] as could be observed by direct visualization of the sample at the different computational steps. In another study we modeled the local implantation related damage required for the creation of a flat diamond membrane surface [27] under different temperature treatment schedules, providing guidelines for experiments on the "liftoff" of diamond membranes [28]. In the present study, tight binding ab-initio molecular dynamics simulations were applied to explore the dynamics and energetics of the formation of the NV center in diamond. Different initial sample structures and annealing temperatures were employed in order to determine which would provide the most efficient route to the creation of NV complexes, and thereby guide laboratory experiments. The self-consistent charge-density functional tight-binding (SCC-DFTB) method [29], as implemented in the program DFTB-Plus [30] has been applied with the pbc-0-3 parameter set [31]. This type of modeling provides, in contrast to the full Car-Parrinello modeling, sufficient detail on the electronic structure while allowing for reasonably long run times on large enough samples to approximate real experimental conditions. The DFTB-Plus model has been used previously to study NV site's properties [18,32].

3.2 Computational details

The initial samples were $3\times3\times3$ unit cells – 216 carbon atoms in a diamond structure with full periodic boundary conditions. Nitrogen atoms were inserted at different sites (substitutional or interstitial) in the crystal and the samples were annealed using molecular dynamics simulations at room temperature ($300°$K). Then, carbon atoms were selectively removed from the crystal to form different vacancy configurations at different locations with respect to the nitrogen. Fig. 1 depicts the full sample in one initial configuration where a nitrogen atom was inserted at an interstitial site and two carbon atoms were removed (above and to the right of the nitrogen); after annealing, the nitrogen atom resides in a split interstitial site. The atomistic figures were drawn with AViz [33, 34], and the bonds are drawn to guide the eye.

Two processes which could possibly lead to the formation of an NV center were considered: Process A where a nitrogen atom initially resides in a substitutional site and a single vacancy is located in its neighborhood (on one of the 2nd, 3rd or 4th nearest neighbors), and process B where a nitrogen is inserted into an interstitial site and two adjacent
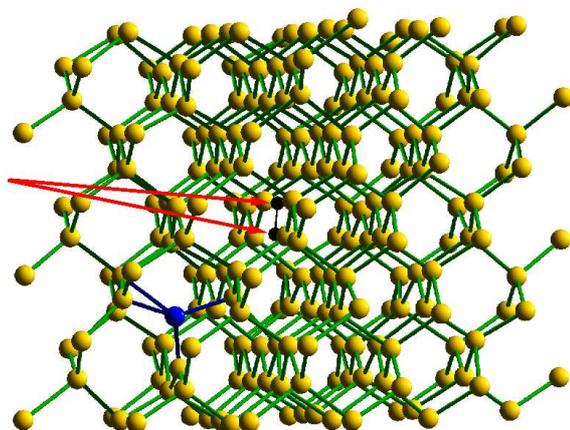
Figure 1: (Color online) An initial configuration of the full sample where a nitrogen atom (blue ball, with blue "bonds") was inserted and two carbon atoms were removed from their initial positions above and to the right of the nitrogen. The red lines guide the eye to the vacant sites and small black balls indicate their locations. After the annealing at $300°$K, the nitrogen atom resides in a split interstitial site. This is a realization of process B.
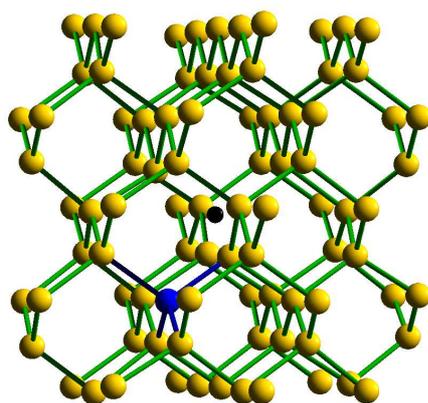

Figure 2: (Color online) An initial configuration of part of the sample for process A where the vacancy (small black ball) is located at the 2nd nearest neighbor site from the nitrogen (blue ball).

vacancies (a divacancy) are located at different sites in its neighborhood.

In process A, a nitrogen atom initially resides in a substitutional site. This mimics the case when nitrogen containing diamond is grown at high pressure/high temperature or by CVD methods [10]. To introduce a nitrogen in a substitutional site, a carbon atom was simply replaced by a nitrogen. To introduce a vacancy a carbon atom is removed from a location in the 2nd, 3rd or 4th nearest neighborhood of the nitrogen. Fig. 2 shows a closeup of an initial configuration of process A where a nitrogen atom (dark, online blue) resides in a substitutional site and a vacancy (represented by a small black circle) is located at the 2nd nearest neighbor site from the nitrogen.

In process B, a nitrogen atom was initially placed in an interstitial site, as is usually the case when nitrogen is inserted into diamond by ion implantation, then the sample was annealed using molecular dynamics simulations at room temperature (300°K). After annealing, the interstitial nitrogen atom always resided in a split interstitial site [19] (as is explained below). Then a divacancy was created at several selected locations with respect to the initial interstitial nitrogen (at a 2nd, 3rd, or 4th nearest neighbor).

The dynamics of different cases of both processes were examined following annealing at a range of temperatures (0−1200°C) for 6-20ps of molecular dynamics which correspond to 6000-20000 computational cycles. Temperature was applied to the sample, as is commonly done, by giving the appropriate kinetic energy to the sample atoms. The energetics and the paths of the motion of the atoms/vacancies into their final configurations were followed.

4   Results

There are two main differences between the two processes. One lies in the initial placement of the nitrogen. In process A it resides on a substitutional site and an additional carbon atom was removed from a nearby site. In process B the nitrogen was initially placed interstitially. Process A was direct and in process B there were two stages with a divacancy created only after initial annealing. As explained above, both are realistic from an experimental viewpoint.

4.1   Process A

This is the substitutional case, illustrated in Fig. 2, with results displayed in Figs. 3 and 4.

4.1.1   Statics and energetics of process A

The formation of an NV center from a process A initial configuration should be achieved by displacing a vacancy toward the nitrogen atom. This is equivalent to displacing a carbon atom from its site toward the vacancy site, leaving a vacancy next to the nitrogen. This is a direct process, therefore it was possible to compute the energy barrier for these displacements. The energy of the system was computed at sequential steps of the motion of the carbon atom from its initial site towards the adjacent vacancy, i.e. stages in the V-C exchange, which eventually can result in the formation of an NV complex. There are three possible cases; one with 2 next-nearest neighbour vacancies, one with a single vacancy and one with two vacancies that are nearest neighbours. In Fig. 3 the energy barrier of the displacement toward the NV configuration for the single vacancy case is shown in the middle curve. As can be seen, for the case where a single vacancy is located at a 2nd nearest neighbor site from the nitrogen (shown in Fig. 2), a potential barrier of 1.90eV has to be overcome in order to form an NV center [15], resulting in an energy gain of 2.16eV (middle curve in Fig. 3). A particularly low barrier of only 0.75eV is found for the
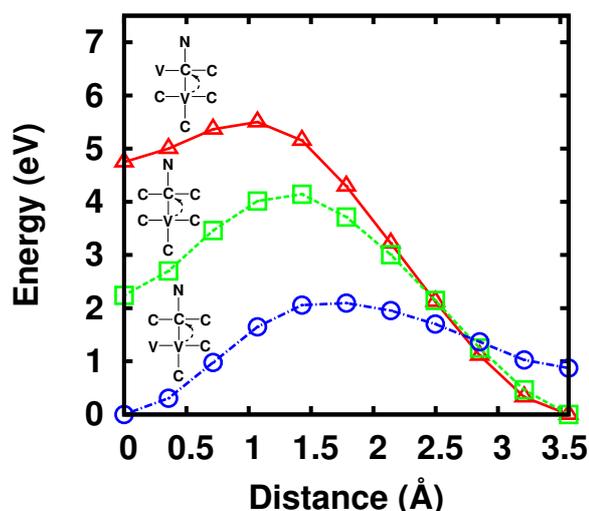
Figure 3: (Color online) The computed energy barriers (in eV) as a function of radial distance (from the center of the energy well at the origin) for selected cases of process A (substitutional site for the nitrogen atom) with three different vacancy/nitrogen initial configurations (indicated schematically). The distance is symmetric around the origin at 0Å, which is at the center of the energy well.

exchange of a carbon and a vacancy for the case in which a second vacancy is located next to the carbon atom (upper curve). However the resulting configuration is N-2V and the energy gain is some 4.75eV (in agreement with previously calculated energetics [11]). In the case where the initial configuration is a divacancy located at a second neighbour to a nitrogen located in a substitutional site, a 2.10eV barrier for the exchange of a carbon with a vacancy is found here (lowest curve). The resulting configuration is an NV center with another vacancy in the second nearest neighbour site, but since there is no energy gain in the exchange (the energy at the end of the process is higher than that at the beginning) it is unlikely to occur.

4.1.2 Dynamics of process A

Dynamic simulations of the attempts of the system to form an NV center for nitrogen initially located in a substitutional site with a vacancy located at different distances away were made at different temperatures. Tracking the sample energy and the mutual locations of the vacancy and the nitrogen for a large range of temperatures ($0-1200°$C), starting from different initial vacancy locations (2nd, 3rd and 4th neighbors of the nitrogen) failed to show any formation of a stable NV center. A typical result for the distance between the vacancy and the nitrogen during the MD simulation at 900°C is shown in Fig. 4. Random jumps of the vacancy towards and away from the nitrogen are evident, but the vacancy never remains in the nearest neighbor site of the nitrogen long enough to form a permanent NV defect.
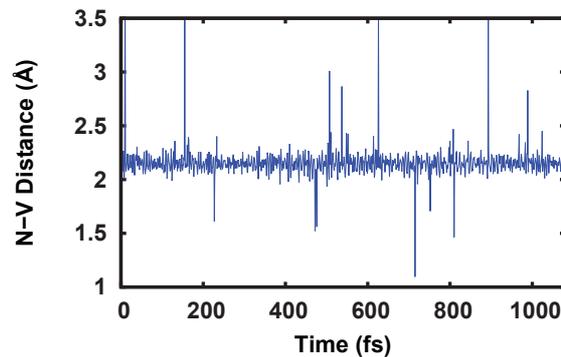
Figure 4: (Color online) The distance between the nitrogen and the vacancy as a function of time during the MD simulation for process A at 900°C.

4.2 Process B

The initial configuration in process B was a nitrogen in a split interstitial site, and a divacancy located at the 2nd, 3rd, 4th and 5th nearest neighbor site relative to the nitrogen. Figs. 7(a) and 6(a) show the initial configurations where the divacancy is located at the 2nd and 3rd nearest neighbour sites, respectively. Dynamic simulations were made for a range of temperatures ($0-1200$°C).

4.2.1 Statics and energetics of process B

The formation of an NV center in process B is a multi-stage process. The first stage includes a local change in the neighboring carbon atoms configuration, and then a diffusion of the nitrogen atom toward the near vacancy site occurs. The energy of this process was deduced by following the energy of the sample during the MD simulations (see Fig. 5).

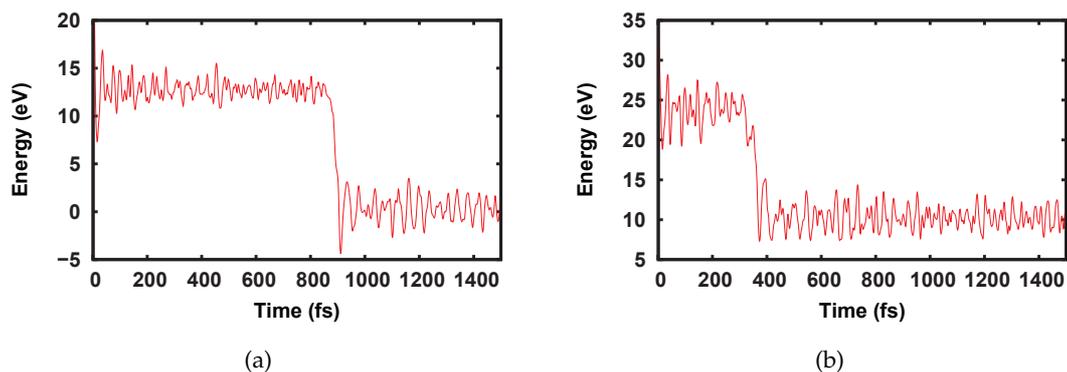(a)   (b)

Figure 5: (Color online) The total sample energy as a function of time during the NV formation in process B, where the divacancy was initially in the 2nd (a) and 3rd (b) nearest neighbor relative to the nitrogen. The sample temperatures during these MD simulations were 300°C in (a) and 650°C in (b).

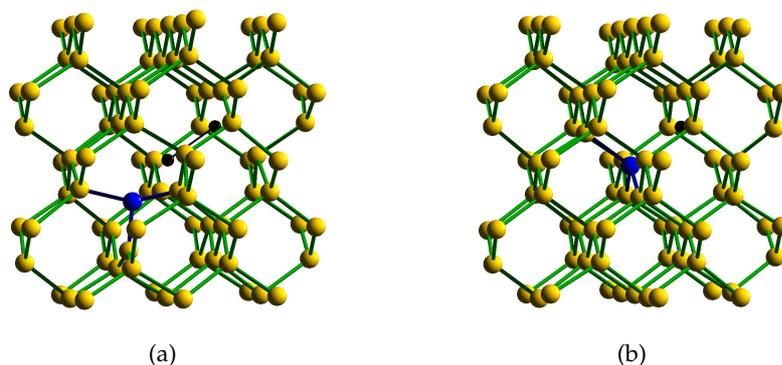(a)   (b)

Figure 6: (Color online) The initial and final configurations of process B where the divacancy is initially located at the second nearest neighbor to the nitrogen (see Table 1). In (a) a nitrogen atom (dark, blue online) is forced into the diamond and finally resides in a split-interstitial site and two adjacent vacancies (indicated by small black dots) are created. The final configurations after annealing (NV center) is shown in (b).

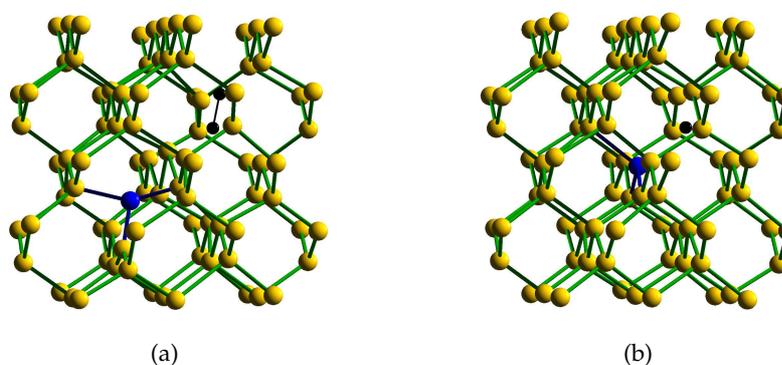(a)   (b)

Figure 7: (Color online) The initial and final configurations of process B where the divacancy is initially located at the 3rd nearest neighbor to the nitrogen (see Table 1). In (a) a nitrogen atom (dark, blue online) is forced into the diamond and finally resides in a split-interstitial site and two adjacent vacancies (indicated by small black dots) are created. The final configuration after annealing (NV center) is shown in (b).

4.2.2 Dynamics of process B

From observing the atomic motion at different temperatures, we found:

1. When the divacancy is initially located at a 2nd nearest neighbor site relative to the nitrogen, during annealing at temperatures $T \geq 300°C$ the nitrogen diffuses from its site to the divacancy and finally forms a stable NV center. Fig. 6 shows closeup views of the initial (a) and final (b) configurations of simulations for this case.

2. When the divacancy is initially located at a 3nd nearest neighbor site relative to the nitrogen, during annealing at temperatures $T \geq 650°C$ there is a complex diffusion process where a carbon atom diffuses from its site to the divacancy, and the nitrogen diffuses to the vacancy which is left, and finally a stable NV center is formed. Fig. 7 shows the initial (a) and final (b) configurations of the simulations of these cases.

3. For a divacancy more distant from the nitrogen no permanent formation of NV center was observed during longer simulations (20,000fs) even at 1200°C.

4.2.3 Additional information about process B

These results agree with experimental results where nitrogen implanted in diamond show a significant increase in the NV center photoluminescence intensity and coherence time after thermal annealing at temperatures in the range of $600-800°$C [23, 24].

We plotted the energy of the samples during the diffusion process in these two cases – a divacancy initially 2nd neighbor to the nitrogen (Fig. 5(a)) and a divacancy initially 3rd neighbor to the nitrogen (Fig. 5(b)). The energy drop in the 2nd neighbor case, occurring after 900fs at 300°C (Fig. 5(a)), indicates the formation of the stable NV center, abruptly reducing the sample's energy by 12.43 eV. A similar abrupt drop occurs in the 3rd neighbor case, in this case after 300fs at 650°C (Fig. 5(b)). In this case fluctuations are observed during the jump which indicate the complex diffusion process which finally forms a stable NV center, reducing the sample's energy by 13.42eV. The reason for the high energy values are the formation energy of the N-V bond, added to the decrease of the N-V split interstitial energy. This is quite distinct from the lack of a jump in the case of process A.

4.3 Summary

Animations of several processes can be found in the supplementary material to our recent reviews [35, 36]. In Table 1, a summary of the results of the two processes is listed. (The energies of the 4th neighbor were found to be equal to those of the 3rd neighbor, therefore they are not noted.)

Table 1: Summary of NV formation processes and results.

Process	A	B
Initial Configuration	N in substitutional site carbon vacancy	N in interstitial site carbon divacancy
Results		
NV formation energy gain - 2nd neighbor	2.160eV	12.43eV
NV formation energy gain - 3rd neighbor	2.166eV	13.42eV
Dynamics	Distance, Fig. 4	Energy, Fig. 5
Statics	Single step 3 cases, Fig. 3	
Final configuration	**No NV**	**NV** for the 2nd & 3rd nearest neighbor
Temperature range	$T < 1200°$C	$T < 650°$C

5   Discussion

An important question concerns whether the simulated initial configurations are realistic. In actual damaged diamond, there are neither specific locations for the defects nor specific clustering of vacancies, since the damage occurs randomly during the experiment. A defect distribution in damaged diamond, (i.e. sp^2 bonded carbons) similar to that occurring in actual experiments was computed by us as a part of our simulation of the conversion of a heavily damaged diamond layer into graphite versus its regrowth to diamond following annealing [27]. In these simulations, damaged layers were "created" at different depths by repetitively shooting carbon atoms from different locations at different energies. We found [27] that when the damage is created at a low temperature followed by a high temperature anneal, a sharp interface between heavily (high sp^2 fraction) and only lightly damaged diamond occurs, as is desirable for membrane formation by graphite etching. In contrast, an extended gradual damage profile, which presumably contains many vacancies and divacancies is found when the damage is created at high temperatures. This process should result in a damaged region in the diamond rich in vacancy complexes (divacancies etc.) a situation which is shown here to be favorable for efficient NV formation.

6   Conclusions

We have presented results of simulations of the energetics and dynamics involved in the formation of the nitrogen-vacancy (NV) center in diamond. Different initial locations and configurations were introduced for the nitrogen and for vacancy complexes. We have shown that only for nitrogen atoms residing in the diamond crystal as split interstitials will the nitrogen be able to diffuse at low temperatures. In order that the vacancies can be mobile and therefore find a nitrogen atom to form an NV center, the vacancies in the diamond should preferably be in the divacancy configuration. Under these conditions the NV center will already form at the rather low temperature of $300-650°C$. Experiments show that nitrogen atoms in the diamond crystal are likely to reside in interstitial positions, when introduced by nitrogen ion-implantation (prior to annealing) whereas the nitrogen will occupy substitutional sites when diamond is grown in the presence of nitrogen [10]. In previous simulations we showed that divacancy complexes are mainly formed by damaging diamond at high temperatures. These are shown here to be a prerequisite for the formation of NV centers at low temperatures. Hence the proposed route for efficient realization of NV centers in diamond is to first damage a pure diamond at high temperature ($T > 1000°C$) by implantation of inert ions, followed by nitrogen implantation into the diamond containing defects at low temperatures. Annealing the thus obtained diamond containing nitrogen and vacancies is expected to result in the formation of NV centers at rather low temperatures ($T \sim 650°C$).

Acknowledgments

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