Commun. Comput. Phys.
doi: 10.4208/cicp.261014.200515a

Vol. **19**, No. 2, pp. 380-392
February 2016

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

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Received 26 October 2014; Accepted (in revised version) 20 May 2015

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.

PACS: 07.05.Tp, 81.05.ug, 61.72.jn, 61.43.Bn, 61.80.-x, 03.67.Lx

Key words: NV center, diamond, irradiation effects in solids, computer modeling and simulations, color centers crystal defects, disordered solids.

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-