



Energetics of dopant atoms in subsurface positions of diamond semiconductor

Takehide Miyazaki^{a,*}, Hiromitsu Kato^b, Sung-Gi Ri^b, Masahiko Ogura^b,
Norio Tokuda^b, Satoshi Yamasaki^b

^a *Quantum Modeling Group, Research Institute for Computational Sciences, National Institute of Advanced Industrial Science and Technology, Umezono 1-1-1, Tsukuba 305-8568, Japan*

^b *Diamond Research Center, National Institute of Advanced Industrial Science and Technology, Umezono 1-1-1, Tsukuba 305-8568, Japan*

Received 7 May 2006; accepted 12 July 2006

Available online 26 September 2006

Abstract

We present a set of *ab initio* energetics for a substitutional boron (B) impurity atom in subsurface positions, from the topmost to the fifth atomic layer, of both C(001)-2 × 1 : H and C(111)-1 × 1 : H. We compare the calculated surface-B binding energies with those obtained for P [T. Miyazaki, H. Kato, H. Okushi, S. Yamasaki, e-J. Surf. Sci. Nanotech. 4 (2006) 124]. The surface-P binding energies become larger as the position of P is closer to the two surfaces. They are up to ~4 eV for C(001)-2 × 1 : H and ~2.6 eV for C(111)-1 × 1 : H, respectively. For B, in contrast, the binding energies are within ~0.5 eV for both surfaces. An implication of our finding in the context of a mechanism for P and B doping in diamond is discussed.

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Keywords: Diamond; Doping; Energy; Binding; Surface; Theory; Functional; Atom

1. Introduction

Diamond is a typical wide band-gap semiconductor, with the energy gap being ~5.5 eV. Due to this nature, there are some potential applications of diamond semiconductors such as electron emitters, optoelectronic devices and biochemical sensors. In order to put the usefulness

* Corresponding author. Tel.: +81 29 861 5404.

E-mail address: takehide.miyazaki@aist.go.jp (T. Miyazaki).

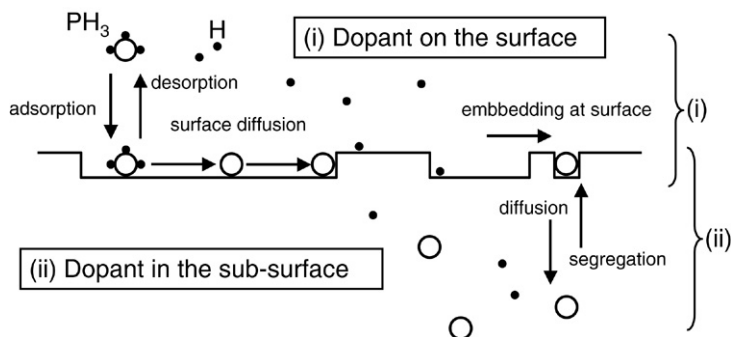


Fig. 1. Schematic illustration of doping model. The figure illustrates the P-doping process using phosphine in the CVD gas phase. One may simply replace phosphine with diborane to draw the B-doping process. Although the model has been developed for the doping of silicon, we assume at the moment that this model may also apply to the doping of diamond.

of diamond semiconductors into practical technology, it is at least necessary to make both *n*-type and *p*-type conductive materials by doping with impurity atoms *at a high efficiency*. Currently, the elements established for *n*- and *p*-type doping of diamond are phosphorus (P) and boron (B), respectively.

Doping of diamond semiconductors is mostly performed during their crystal growth with chemical vapor deposition (CVD). A long-standing problem with CVD doping of diamond is that the efficiency of *n*-type doping with P is much lower than *p*-type doping with B. For example, the efficiency of P-incorporation (for a definition of the *incorporation efficiency*, see [1]) is very low at present ($\sim 0.02\%$ and $\sim 2\%$ for the (001)- and (111)-films, respectively) [2]. For B, in contrast, the efficiency may be made much higher (35% [3] and 57% [4]). It is obvious that the P-incorporation efficiency in the (001)-oriented diamond surface is too low. Since the diamond films with the (001) orientation is very important for practical use [2], the improvement of P-incorporation in this surface is regarded as one of the urgent tasks in the diamond research community.

Keeping the above in mind, a goal of our study is to understand, from a theoretical point of view, a cause to hamper the P-incorporation in the (001)-oriented diamond films. Fig. 1 shows a schematic model of the impurity doping process. The figure illustrates the P-doping process using phosphine in the CVD gas phase. One may simply replace phosphine with diborane to draw the B-doping process. According to this model, the impurity doping process may be divided in two qualitatively different situations: (i) the dopant *on the surface* [5] and (ii) *in the subsurface* [6]. The model has been developed for the doping of silicon. We assume at moment that this model may also apply to the doping of diamond. Although both situations should affect the impurity incorporation efficiency, here we would like to focus our attention on situation (ii), where the efficiency of impurity incorporation is suppressed by the segregation of the impurity to the surface. The surface segregation may occur strongly when the binding of the impurity to the surface is strong.

We have already performed a set of *ab initio* energetics of substitutional P impurity atoms in the subsurface regions of hydrogenated (001) and (111) surfaces of diamond [7]. In order to assess the efficiency of impurity incorporation in the situation (ii) of the doping process (Fig. 1), we have estimated the impurity-surface binding energies as a function of the depth of the respective impurity atoms in the subsurface regions (Fig. 2; for a definition of the binding energy, see the result section). We have found that the binding energy becomes larger as the depth

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