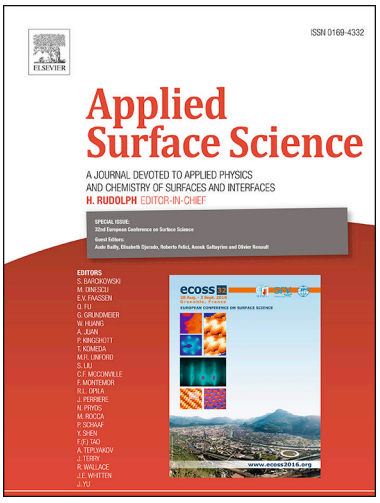
Accepted Manuscript



Full Length Article

First Principles Calculations of the Adsorption and Migration Behaviors of N Atoms on the H-terminated Diamond (001) Surface

Xuejie Liu, Hongchao Wang, Pengfei Lu, Yuan Ren, Xin Tan, Shiyang Sun, Huiling Jia

PII: S0169-4332(18)32394-8
DOI: https://doi.org/10.1016/j.apsusc.2018.08.251
Reference: APSUSC 40288

To appear in: *Applied Surface Science*

Received Date: 29 June 2018
Revised Date: 23 August 2018
Accepted Date: 28 August 2018

Please cite this article as: X. Liu, H. Wang, P. Lu, Y. Ren, X. Tan, S. Sun, H. Jia, First Principles Calculations of the Adsorption and Migration Behaviors of N Atoms on the H-terminated Diamond (001) Surface, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.08.251

First Principles Calculations of the Adsorption and Migration Behaviors of N Atoms on the H-terminated Diamond (001) Surface

Xuejie Liu*, Hongchao Wang, Pengfei Lu, Yuan Ren, Xin Tan, Shiyang Sun, Huiling Jia.
School of Mechanical Engineering, Inner Mongolia University of Science and Technology, Baotou, Inner Mongolia 014010, People's Republic of China
*Corresponding Author: Xuejie Liu. Address: Arding Str. No. 7, Baotou, Inner Mongolia, 014010, People's Republic of China. Tel. and Fax: +86 472 595 2268; E-mail: xuejieliu2000@yahoo.com

Abstract

In this paper, the adsorption and migration behaviors of nitrogen (N) atoms on the hydrogen -terminated diamond (001) surface [H-Ter-D (001) surface] were investigated. The adsorption energy, the electron charge and the magnetic moment were calculated through first principles methods. The investigation results show that on the fully H-Ter-D (001) surface, all surface C atoms have saturated bonds. However, the N atom can abstract the H atom from a surface carbon atom nearby or lead to the bond breaking of the dimer carbon atoms to form bonds with the surface carbon atoms. The maximum energy of adsorption reaches to 3.47 eV, corresponding to a stable configuration structure. The charge analysis and the density of state analysis further reveal that the N atom adsorbed has unpaired electrons, which provides the opportunity for adsorption of CH radicals. On the H-Ter-D (001) surface with one open radical site (1ORS) slab, the N atom can abstract the H atom from a surface carbon atom nearby and bond with the dimer carbon atoms. The adsorption energy rises to 4.85 eV. On the H-Ter-D (001) surface with the 2ORS slab, the activation energy for a N atom to migrate along the dimer chain to the next dimer is 1.31 eV. Moreover, the adsorption of the N atom on the 1ORS surface promotes the adsorption of a C atom nearby and improves the ability of C atom migration, which is beneficial for the growth of the diamond grains. According to the charge transform analysis, the electronegativity of N atoms plays an important role in their adsorption behaviors. In addition, when the N atom has been adsorbed on the H-Ter-D (001) surface, it could still be abstracted by the other deposited N atoms; this phenomenon may be the reason for a low deposition efficiency of N atoms in the N-doped diamond films.

Keywords:

N-doped diamond films; Adsorption and migration behavior; First principles methods; Activation energy; N atom abstraction.

1. Introduction

Nitrogen doped diamond film, because of its excellent characteristics, is considered an ideal material for many applications, such as in N-V color centers for a single photo [1], semiconductor devices [2], electrochemical biosensing [3], thermionic electron emission [4], sterilization [5], photoelectron emission, [6], and field emission [7]. Many studies focused on the influence of N incorporation into the diamond film during deposition on the film growth and film structure [8-17]. Their findings indicate that the N atom addition to the C/H gas mixtures can enhance the growth rates of diamond films [8-10] and promote the growth of the (100) facet grains [9, 11-17].

Seeking to explain these observations, several theoretical studies have been conducted [18-20]. Larsson and co-workers investigated the hydrogen abstraction and the adsorption of CH radicals on the