

# Mechanical properties of the interface structure of nanodiamond composite films: First-principles studies



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## ARTICLE INFO

### Article history:

Received 2 September 2015

Received in revised form

23 November 2015

Accepted 28 November 2015

Available online 2 December 2015

### Keywords:

Nanodiamond

Composite film

Interface structure

Mechanical properties

First principles

## ABSTRACT

The elastic properties of the interface structure of nanodiamond composite films are investigated using first-principles calculations. The nanodiamond grains in the films are surrounded by a monolayer heterogeneous interface. The interface phase comprises B, Si, P, and Ge. The elastic constants, bulk, shear and Young's modulus of the interface structures are all obtained with first principle calculations. Calculated elastic constants of the diamond (001) interface are larger than those of the (111) interface. For the B, Si, P, and Ge interface structures, as the average atomic distance increases, the average Young's modulus decrease, which follows the sequence  $\bar{E}_B > \bar{E}_{Si} > \bar{E}_P > \bar{E}_{Ge}$ , with corresponding values of 927.05, 843.841, 840.152, and 819.805 GPa. The ductility and plasticity, as well as the anisotropy values ( $A$  and  $A^U$ ) of the interface structures were discussed based on the obtained mechanical parameters. The results show that P interface structures demonstrate ductile property when stressed longitudinally, whereas the other interface structures are all brittle. Then the visualization of the directional dependence of the Young's modulus are also presented. These reflected an interesting results. For the B, Si, and Ge interface structures, whether they show isotropy or anisotropy depends on the crystal structure, while it depends on the direction of the applied strain for the P interface structures.

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## 1. Introduction

Nanocrystalline diamond (NCD) and ultrananocrystalline diamond (UNCD) films have recently attracted considerable interest. The presence of dopants in these films significantly influences material properties. Boron-doped and phosphorus-doped NCDs have been demonstrated as novel materials owing to their unique optical and electrical properties [1–4]. Other studies, to overcome the insufficient adhesion of nanodiamond films, diamond/ $\beta$ -SiC composite interlayers have been synthesized on several substrates, such as Si, W, Mo and WC-Co [5,6]. However, the mechanical properties of nanodiamond composite films have yet to be determined. In addition, the optimal elements to dope NCD and UNCD films need to be identified to improve the mechanical properties of these films effectively. Therefore, the mechanical properties of each type of film should be investigated and correlated with their structure and bonding environment. Results of such an investigation could provide a reference for the synthesis of NCD and UNCD films.

Nanodiamond films are usually grown in chemical vapor deposition (CVD) environments. According to previous works [7,8], CVD nanodiamond films can be roughly divided into two categories: NCD films and UNCD films. NCD films (grain size: <100 nm) grow in a columnar manner, with the grain size coarsening with film increasing thickness. By contrast, UNCD films (grain size: ca. 2–5 nm) generally grow in argon-rich and hydrogen-poor CVD environments. The growth process of UNCD films requires a high, stable renucleation rate ( $10^{11} \text{ cm}^{-2} \text{ s}^{-1}$ ). Hence, grain coarsening does not occur. Clearly, UNCD films consist of nanostructures. However, UNCD films have many defects and  $\text{sp}^2$  carbon bonding between grains. Some studies even consider UNCD films as composite films with UNCD and amorphous structure [9]. Significant changes in the chemical composition and microstructure of UNCD films remarkably influence the morphological and mechanical properties of the composite films. For example, Liu et al. [10] prepared UNCD films by microwave plasma CVD using  $\text{CH}_4/\text{H}_2/\text{Ar}$  plasmas and reported that the Young's modulus of the prepared UNCD films ranges from 542 GPa to 667 GPa. The Young's modulus of UNCD films could be enhanced from 400 GPa to 750 GPa by altering the hydrogen content from 5% to 20% in the deposition atmosphere [11]. Williams found that the Young's modulus of UNCD films could be as low as 440 GPa [12].

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In this study, a monolayer heterogeneous interface structure is built between grains. This structure is specifically designed to investigate the mechanical properties of nanodiamond composite films with a monolayer heterogeneous interface structures. The effects of different dopant elements and different crystal faces on the mechanical properties of the films are also examined. Focus is given on the theoretical analysis of the elastic properties of the interface structures. The interfacial phase comprises B, Si, P, and Ge; consequently, the covalent radii of the atoms are relatively close. Among them, Si and Ge are grouped with C found in diamond, whereas B and P belong to the group adjacent to the group of C. Therefore, lattice distortion cannot easily occur.

## 2. Calculation details and model

First-principles calculations were performed by employing scalar relativistic all-electron Blöchl's projector augmented-wave approach [13,14] based on density functional theory (DFT) and implemented in a highly-efficient Vienna ab initio simulation package [15–17]. Pseudo-potentials, a plane-wave basis set, and periodic boundary conditions were employed to determine the Kohn–Sham ground state. The interaction between electrons and ions was described with ultrasoft pseudo-potentials [18]. The exchange-correlation potential was treated within the generalized gradient approximation (GGA) of Perdew et al. [19]. A plane-wave energy cutoff of 400 eV was considered in the calculation. The  $k$ -point meshes for Brillouin zone sampling were constructed using Monkhorst–Pack scheme [20] with a  $5 \times 5 \times 3$  grid for all interface structures in the calculation of mechanical properties. The criteria for terminating the electronic and ionic iterations were an energy difference of  $10^{-3}$  and  $10^{-4}$  eV to balance calculation accuracy and cost. After structural optimization, calculated forces were converged to less than 0.01 eV/Å.

Two models of diamond were built, namely, diamonds (001) and (111), with a monolayer interface after full relaxation. Previous studies have reported on the calculation of a stable interface structure [21]. Fig. 1(a)–(c) shows diamond (001) with a substitute interface, consisting of 128 atoms in a  $4 \times 4 \times 8$  diamond supercell. In its middle position, an arrangement of C atoms has been replaced by B, Si, P, and Ge atoms. The size of the structure is approximately  $(6.24 \times 6.24 \times 13.38) \text{ Å}^3$ . Fig. 1(d)–(f) show diamond (111) with a substitute interface, containing 36 atoms in a  $3 \times 2 \times 6$  diamond supercell, with the size  $(3.64 \times 3.64 \times 4.633) \text{ Å}^3$ . An arrangement of C atoms has been replaced by B, Si, P, and Ge atoms in its middle position.

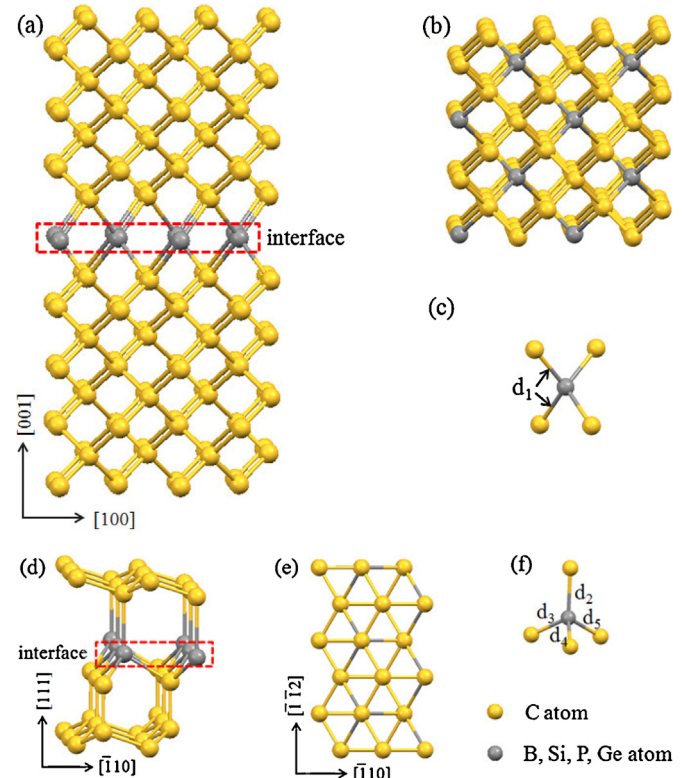
## 3. Results and discussion

### 3.1. Mechanical properties of diamond and interface structures

The athermal elastic constants  $C_{ij}$  were calculated within the total-energy method, where the unit cell was subjected to a number of finite-size strains along several strain directions. The elastic strain energy is given by

$$\Delta E_0 = \frac{V_0}{2} \sum_{i=1}^6 \sum_{j=1}^6 C_{ij} \varepsilon_i \varepsilon_j \quad (1)$$

where  $\Delta E_0 = E_{0-\text{total}}(V_0, \delta) - E_{0-\text{total}}(V_0, 0)$  is the total energy difference between the deformed and initial unit cells,  $V_0$  is the volume of equilibrium cell, and  $C_{ij}$  is the elastic constant. The monolayer interface structure, with the atoms ranged orderly, is similar to the structure of the crystalline, and the interface only affects the arrangement of the atoms nearby while it doesn't change the



**Fig. 1.** Monolayer interface in diamond crystallites. (a–c) Diamond (001) interfaces after full relaxation: (a) arrangement of the interface phase atoms located in its middle position, (b) corresponding top view, and (c) corresponding arrangement of the interface phase atoms to carbon first neighbors; (d–f) diamond (111) interfaces after full relaxation: (d) arrangement of the interface phase atoms located in the middle position, (e) corresponding top view, and (f) corresponding arrangement of the interface phase atoms to carbon first neighbors. Light/Yellow atoms are C, dark/gray atoms are B, Si, P, and Ge. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

structure of diamond, so the mechanical property of the interface structure is still calculated as the cubic system. Four independent elastic constants, namely,  $C_{11}$ ,  $C_{12}$ ,  $C_{44-x}$ , and  $C_{44-y}$ , are required to describe its elastic properties completely [22,23]. The elastic constants  $C_{11}$  and  $C_{12}$  can be deduced by straining the lattice vectors according to an isochoric tetragonal deformation and a uniform hydrostatic pressure, respectively. The elastic constants  $C_{44-x}$  and  $C_{44-y}$  are related to the elasticity in shape, which are shear constants. They cause changes in shape without a change in volume, while  $C_{44-x}$  is a transverse strain and  $C_{44-y}$  is a longitudinal strain. The tetragonal and rhombohedral distortions were obtained by compressing and expanding the  $a$  and  $c$  lattice parameters [24]. These constants were calculated to optimize crystal structures at zeroth external pressure and conform to the following relations. Four different strains  $\delta$  are shown in Eqs. (2)–(5), represent  $C_{11}$ ,  $C_{12}$ ,  $C_{44-x}$ , and  $C_{44-y}$  respectively. Here only the configuration strain of diamond (001) interface structure is given (Fig. 2).

$$\varepsilon = \begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & (1+\delta)^{-2} - 1 \end{bmatrix} \quad (2)$$

$$\varepsilon = \begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix} \quad (3)$$

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