



Letter

Interface structure of nanodiamond composite films: First-principles studies

Xuejie Liu^{a,b,*}, Suhui Zhang^a, Yongjun Jiang^a, Yuan Ren^a^a School of Mechanical Engineering, Inner Mongolia University of Science & Technology, Baotou, Inner Mongolia 014010, PR China^b Gengdan Institute of Beijing University of Technology, Beijing 101301, PR China

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ABSTRACT

This study presents novel nanodiamond composite films, in which nanodiamond grains are surrounded by a monolayer heterogeneous interface. Calculations of diamond (001) and (111) with and without the interface were conducted using the first-principles method. Results showed that silicon particles cannot become a solid solution in diamond crystallites. Thus, the silicon interface can exist among diamond grains. The interface in diamond (001) is more stable than that in diamond (111).

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1. Introduction

The hardness of thin solid films can be significantly improved by nanocomposite structures. The Ti–Si–N super hard nanocomposite film is a special example. The deposition of TiN films with less than 5% silicon addition can lead to structural transformation from the TiN columnar structure to a glass-like composite structure, in which nanocrystalline TiN is surrounded by a monolayer Si–N. This transformation can increase the hardness from approximately 20 GPa of TiN films to 50 GPa of Ti–Si–N films [1–4]. Whether or not nanodiamond composite films are harder than natural diamonds can be determined by analyzing the structure, mechanical properties, and formation mechanism of these films. The present study specifically investigated on the interface structure of nanodiamond composite films.

According to previous works [5–7], chemical vapor deposition (CVD) nanodiamond films can be roughly divided into two categories: nanocrystalline diamond (NCD) films (grain size: <100 nm) and ultrananocrystalline diamond (UNCD) films (grain size: ca. 2–5 nm). NCD films usually grow in carbon-lean and hydrogen-rich environments. The growth process of NCD films starts with high-density nucleation, which initiates nanometer-sized diamond domains that grow in a columnar manner. The grain size of NCD films

coarsens with film thickness. By contrast, UNCD films generally grow in argon-rich and hydrogen-poor CVD environments. The growth process of UNCD films requires a high, stable renucleation rate ($10^{11} \text{ cm}^{-2} \text{ s}^{-1}$) [5]. Hence, grain coarsening does not occur. UNCD films consist of equiaxed grains 2–5 nm in size, even if the film thickness is over micrometers. Clearly, UNCD films consist of nanostructures. However, UNCD films have many defects and sp^2 carbon bonding between grains. Some studies even consider UNCD films as composite films with UNCD and amorphous structure [8–13]. Ti–Si–N nanocomposite structures open the possibility of overcoming the problem of UNCD films by building a monolayer heterogeneous interface structure between grains.

Research on diamond/ β -SiC coatings has shown that the β -SiC phase can exist between diamond crystallites [14–16]. The present study investigated the monolayer heterogeneous interface structures between UNCD grains using the first-principles method.

2. Calculation method and model

In this research, first-principles calculations were carried out with the VASP code [17,18] based on density functional theory [19–21]. 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 [22,23]. Exchange–correlation potentials were treated through the generalized gradient approximation [23]. The parameter settings were optimized to provide reasonable total energy convergence. The plane wave cut-off (ENCUT) was 400 eV. The k -points, which were settled in a $5 \times 5 \times 5$ uniform grid for Brillouin zone integration, were generated by using the Monkhorst–Pack method [24]. 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.

* Corresponding author. Address: Arding Str., No. 7, 014010 Baotou, Inner Mongolia, PR China. Tel./fax: +86 472 5952268.

E-mail address: xuejeliu2000@yahoo.com (X. Liu).

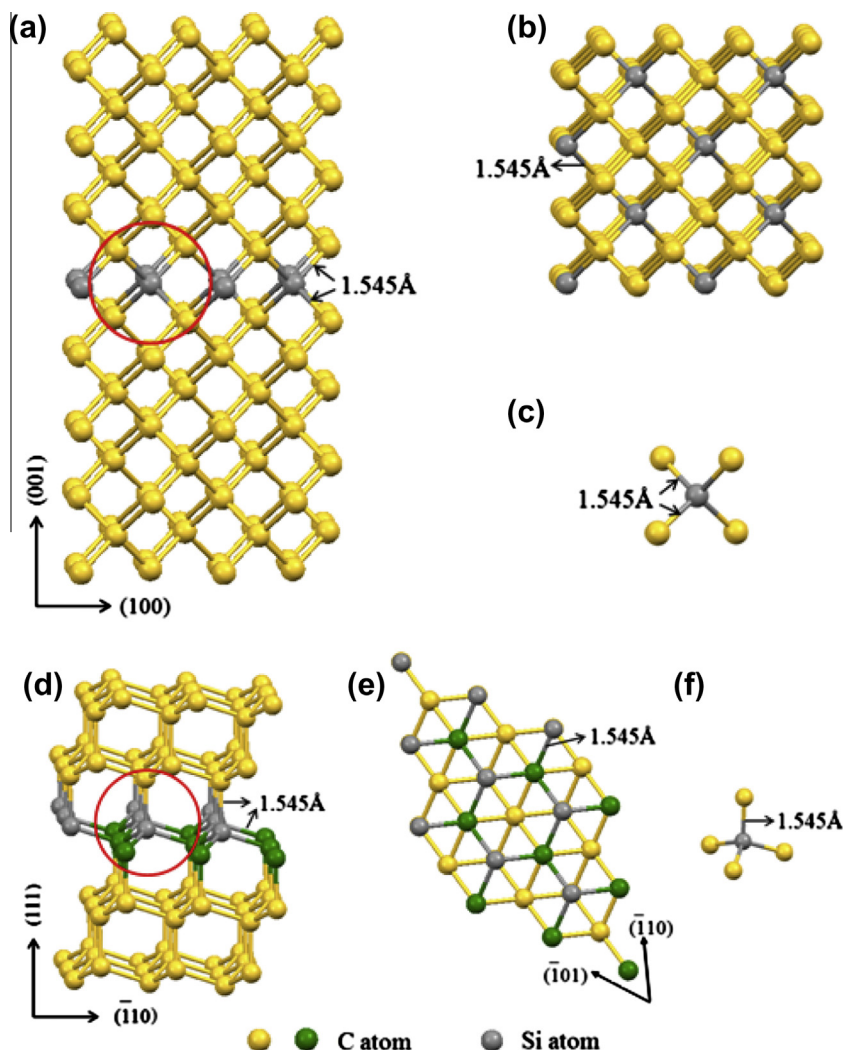


Fig. 1. Monolayer silicon interface in diamond crystallites. (a–c) diamond (001) interfaces before full relaxation: (a) arrangement of silicon atoms located in its middle position, (b) corresponding top view showing the Si–C bond distances, and (c) corresponding arrangement of silicon to carbon first neighbors. (d–f) diamond (111) interfaces before full relaxation: (d) arrangement of silicon atoms located in the middle position, (e) corresponding top view showing the Si–C bond distances, and (f) corresponding arrangement of silicon to carbon first neighbors. Yellow and green atoms are C, which are in different layers. Gray atoms are Si. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Four models of diamond were built: pure diamond (001) and (111) without an interface and diamond (001) and (111) with a monolayer silicon interface. Fig. 1(a–c) shows diamond (001) with a substitute interface, which consists of 128 atoms in a $4 \times 4 \times 8$ diamond supercell. In its middle position, an arrangement of C atoms is replaced by Si atoms. Fig. 1(d–f) shows diamond (111) with a substitute interface, which contains 90 atoms in a $3 \times 3 \times 10$ diamond supercell. An arrangement of C atoms is replaced by Si atoms in its middle position.

3. Results and discussion

The accuracy of the single atom energy must be confirmed to achieve structural optimization. Basic calculations of an atom and a crystal of carbon and silicon were conducted based on the first-principles method. The calculation results (Table 1) show that the lattice constant and cohesive energy of both agree well with the experimental values. Therefore, the energies of single atoms of carbon and silicon could be considered accurate.

The total and cohesive energies of pure diamond (001) and (111) supercells were calculated. Structural optimization was achieved by minimizing the total energy of the supercell. As a result, the lattice constant obtained is 3.567 Å, which agrees well with the experimental value. The total and cohesive energies of diamond

(001) and (111) supercells with a monolayer interface were also calculated with the same lattice constant and the same volume of pure diamond model. Table 2 lists the results of the above calculations. Furthermore, the energies of diamond (001) and (111) supercells with a monolayer interface under full relaxation were calculated. Full relaxation was carried out by completely relaxing the model along the X, Y, and Z directions. Doing so allows the atoms to find their lowest energy position automatically. Table 3 lists the

Table 1
Calculation results and relevant experimental values of lattice constant, cohesive energies, and energies of a single silicon atom and a carbon atom.

	C	Si
Energy of single atom (eV)	−1.3933	−0.8173
Lattice from calculation (Å)	$a = 3.568$	$a = 5.46$
Lattice from experiment (Å) [25]	$a = 3.567$	$a = 5.43$
Difference in the percentage of lattice (%)	0.03	0.5
Cohesive energy from calculation (eV/atom)	7.73	4.62
Cohesive energy from experiment (eV/atom) [25]	7.37	4.63
Difference in the percentage of cohesive energy (%)	4.6	0.1

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