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Structural properties and growth evolution of diamond-like carbon films with different incident energies: A molecular dynamics study

Xiaowei Li, Peiling Ke, He Zheng, Aiying Wang*

Ningbo Key Laboratory of Marine Protection Materials, Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo 315201, PR China

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ABSTRACT

Structural properties and growth evolution of diamond-like carbon (DLC) films with different incident energies were investigated systematically by the molecular dynamics simulation using a Tersoff interatomic potential for carbon-carbon interaction. The results revealed that the density, sp^3 fraction and residual compressive stress as a function of incident energy increased firstly and then decreased; when the incident energy was 70 eV/atom, the density could reach to 3.0 g/cm^3 with the maximal compressive stress of 15.5 GPa. Structure analysis indicated that the deviation of both bond angles and lengths from the equilibrium position led to the generation of a large residual stress, while the high compressive stress mainly attributed to the decrease of both bond angles and lengths among carbon atoms. The growth of DLC films underwent a formation process of "Line-Net" structure accompanied with the interaction of many atomic motion mechanisms, and the "Point" stage was only found for DLC films with low incident energy.

1. Introduction

Diamond-like carbon films (DLC) owning high hardness, low coefficient of friction, superior optical property and good chemical inertness, have been widely used as a protective coating in the industrial fields of cutting tools, molds and so on [1,2]. Especially for the good biocompatibility, DLC films are being considered as a strong candidate for the medical applications, such as heart valves [3,4], vascular stent [5] and artificial joint [6]. However, one of the most significant limitations of this coating is the high level of residual compressive stress which deteriorates the adhesive strength between the film and the substrate and leads to the failure of coated surface. Therefore, continuous efforts are being devoted to reducing residual stress and to improving physical properties of DLC films [7–12].

It is well known that the properties depend on the microscopic structure of the deposited layer. But no experimental method exists for characterizing this microstructure from the viewpoint of atomic scale. Computational simulation techniques provide a robust method for deeper insight of the microscopic structure and properties of a DLC film. Many previous works have reproduced the structure and property variations with kinetic energy of deposited carbon atoms by the molecular dynamics (MD) simulation, which led to understand the deposition process in atomic scale [13–15]. However, the relationship of the origin and distribution of stress with structure evolution is not fully understood yet. In addition, the explanation for the growth mechanism of DLC films is still controversial. For example, the subplantation mode was generally accepted as the growth mechanism of DLC films [16,17], while Marks et al. [18] deduced a new model of energetic burial from the film deposition by MD simulation.

In the present study, the deposition of DLC films with different incident energies was carried out via MD simulation to systematically investigate the structure, properties and growth mechanism. The dependence of properties on incident energy, the origin and distribution of residual stress as well as the growth mechanism combined with the atomic motion mechanism were mainly analyzed.

2. Computational method

In order to simulate the deposition and structure of DLC films by MD simulation, the three-body empirical potential Tersoff was used to describe the interaction between the deposited carbon atoms and the diamond substrate [19]. The Tersoff potential has been proved to be an effective and accurate potential for carbon system.

Energetic atoms of C impacted on a diamond (001) single crystal substrate of $25.2210 \times 25.2210 \times 24.0758$ Å^3 in the x, y and z directions, which contained 2800 carbon atoms with 100 atoms per layer and was equilibrated at 300 K for 100 ps before deposition. The

* Corresponding author.
E-mail address: aywang@nimte.ac.cn (A. Wang).

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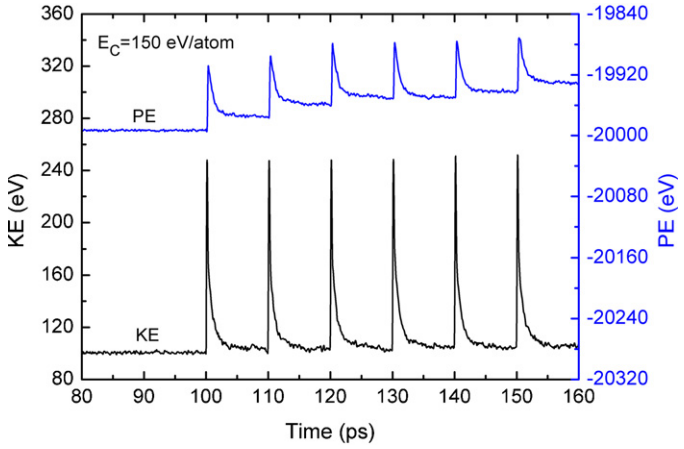

Fig. 1. Energetic variation during the deposition process when the incident energy is 150 eV/atom.

incident C atoms were deposited at the position of 10 nm above the substrate surface at a random $\{x, y\}$ position. While the positions of atoms in the bottom two layers were frozen to mimic the bulk substrate, all the other atoms were unconstrained. The incident kinetic energy of C atoms was changed from 1 eV/atom to 150 eV/atom and 2000 impacts were simulated. The periodic boundary conditions were applied in x and y directions and the time step was fixed at 1 fs.

The time interval between two sequential deposited C atoms was 10 ps, which induced an impracticable ion flux of $1.57 \times 10^{27}/\mathrm{m}^2$ s. Fig. 1 shows the changes in potential energy (PE) and kinetic energy (KE) of the system during depositing the first six incident C atoms. The energy change in the system indicates that the time interval of 10 ps is enough for relaxing the atomic structure and diminishing the unrealistic effect of high carbon flux on the deposition process. The temperature of the substrate was rescaled to 300 K by the Berendsen method [20] after the atomic rearrangement caused by the bombardment of incident atom was finished. Thus it can be said that the present simulation reasonably mimic the real deposition behavior even if the simulation was under an accelerated condition.

3. Results and discussion

Fig. 2 shows the final morphologies for DLC films with the incident energies of 1 eV/atom, 70 eV/atom and 150 eV/atom, where colors represent the different coordination numbers. When the incident energy is 1 eV/atom (Fig. 2a), a film with high roughness is generated; the incident atoms have little effect on the arrangement of substrate atoms, causing an obvious interface between the film and the substrate. With increasing incident energy to 70 eV/atom, the film has a good compact structure, smaller thickness and smooth surface (Fig. 2b); because the incident energy is much higher than the cohesive energy of diamond (7.6–7.7 eV/atom), the incident atoms can implant into the diamond lattice resulting in the intermixing layer at the interface, which may induce a high stress due to impairing the regular structure of substrate. When the incident energy is 150 eV/atom, a looser structure with many defects is produced again, implying the change of mechanical properties.

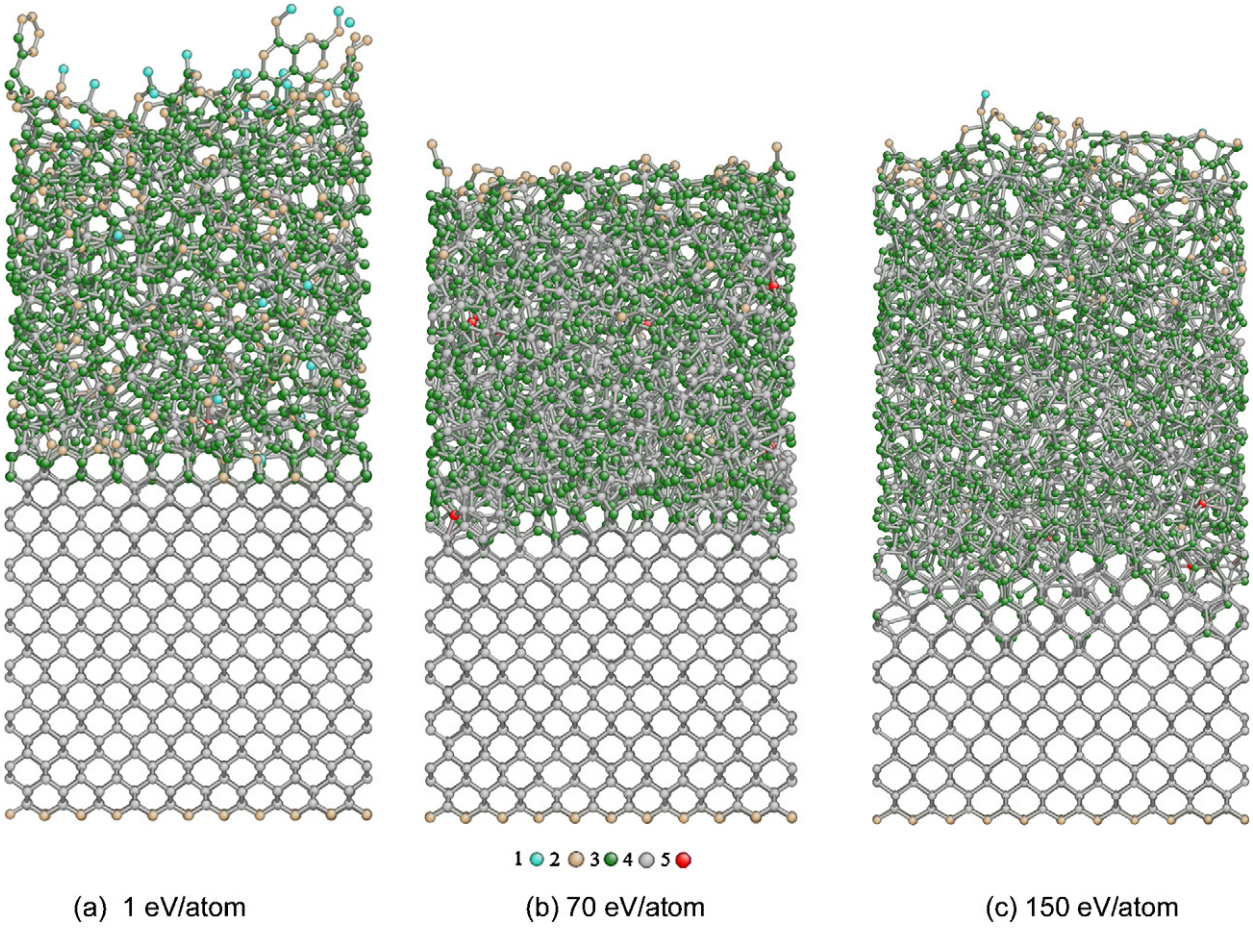

Fig. 2. Coordination configurations of films under different incident energies, where colors represent the different coordination number.