The Structure and Properties of ta-C Film with Dispersion of Incident Beam Energy

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ABSTRACT

Structures and properties of tetrahedral amorphous carbon (ta-C) films are investigated as a function of Gaussian distribution of incident carbon beam energy. The ta-C films are synthesized by controlling the standard deviation (σ) of Gaussian distribution from 0 to 10. The Brenner type interatomic potential was used for carbon-carbon interaction. Densities (3.14 ± 0.03 g/cm^3) and *sp^3* bond fractions (53.7 ±1.7 %) were not significantly changed with varying standard deviations (σ). On the contrary, the compressive residual stresses of ta-C film were changed remarkably with changing the standard deviation. The residual stress was reduced from 6.0 to 4.2 GPa with the standard deviations (σ). The decrease of residual stress corresponds to the disappearance of a satellite peak of the second nearest neighbor of the radial distribution function. The relationship between the structure of ta-C film and dispersion of incident beam energy was investigated.

Keywords: Tetrahedral amorphous carbon, Molecular dynamics simulation, Dispersed incident energy, Compressive residual stress

1 INTRODUCTIONS

Tetrahedral amorphous carbon (ta-C) films made by filtered vacuum arc of graphite have been used for the protective coatings of various tools and components owing to their superior mechanical and optical properties[1-4]. However, the residual compressive stress should be reduced for the applications since the high level of the residual stress induces spontaneous delamination of the film from a substrate. Therefore, many studies focused on the structural factor to be significant to control the residual stress.

Molecular dynamics studies are very useful methods to investigate the structural properties and stress behavior of ta-C film in the atomic scale. Growth behavior of ta-C film was successfully simulated by using energetic carbon atoms which bombard the diamond or silicon substrate[5,6]. However, most previous simulation studies have dealt with monochromatic kinetic energy of the deposited carbon atoms. Monochromatic incident energy is suitable for modeling calculation of deposition system. However, the incident energy is not monochromatic in real situation. In the case of filtered cathodic vacuum arc (FCVA) system, the incident carbon ion has the energy range of incident beam. It is the difference between the most experimental conditions and modeling calculations. It is required to investigate the effect of the energy dispersion of incident beam.

In the present work, we synthesized the ta-C films with the varying the standard deviation of the incident energy, which is assumed to follow the Gaussian distribution with standard deviation (σ). In this case, we investigated the structures and properties such as density, *sp^3* bond fraction, radial distribution function (RDF) and residual stress of ta-C film and compare with that of ta-C film using by monochromatic incident energy. The structure, density and *sp^3* bond fraction did not show significant behavior. However, the residual stress of ta-C film changed with standard deviation (σ) of Gaussian distribution. We observed the satellite peak of the second nearest peak from radial distribution function showed the same tendency with residual stress of ta-C film. We investigated the physical meaning of these satellite peaks and the relationship between these satellite peaks and the residual stress of ta-C film.

2 CALCULATIONS

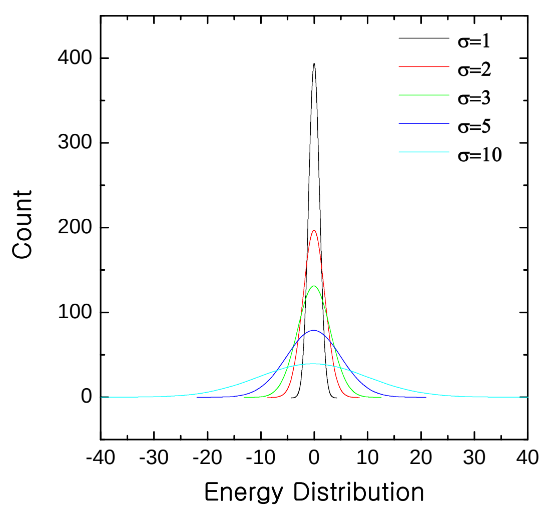

Figure 1. Gaussian distribution with standard deviation (σ)

The initial substrate is of a perfect $6a_0 \times 5\ a_0 \times 6\ a_0$ (Here, a_0 is equilibrium lattice constant of bulk diamond 3.567 Å) diamond lattice consisting of 1512 carbon atoms with 72

 NSTI-Nanotech 2005, www.nsti.org, ISBN 0-9767985-1-4 Vol. 2, 2005

atoms per layer. Before the deposition, the substrate is sufficiently relaxed to its minimum potential configuration and almost equilibrated at 300 K for 1 ps. The ta-C films were produced on a diamond (100) surface by bombardment of 3000 carbon neutrals with the average incident energy (75eV). Energetic carbon neutrals are deposited onto the substrate with normal incidence and randomly chosen location. The Brenner interatomic potential was used for the carbon atoms[7,8].

In order to investigate the structural properties of ta-C film as a function of the dispersion in the incident kinetic energy, the ta-C film was growth using by the Gaussian distribution function for incident carbon atom energy. The highly dense and residual stressed ta-C films were synthesized, when the incident energy is between 50 and 100 eV. Therefore, the average value of incident energy was chosen 75 eV. The standard deviation (σ) of the Gaussian distribution was controlled from 0 to 10 as shown in Fig. 1. The incident energy of the each atoms is dispersed with the standard deviation (σ) of the Gaussian distribution function.

3 RESULTS AND DISCUSSIONS

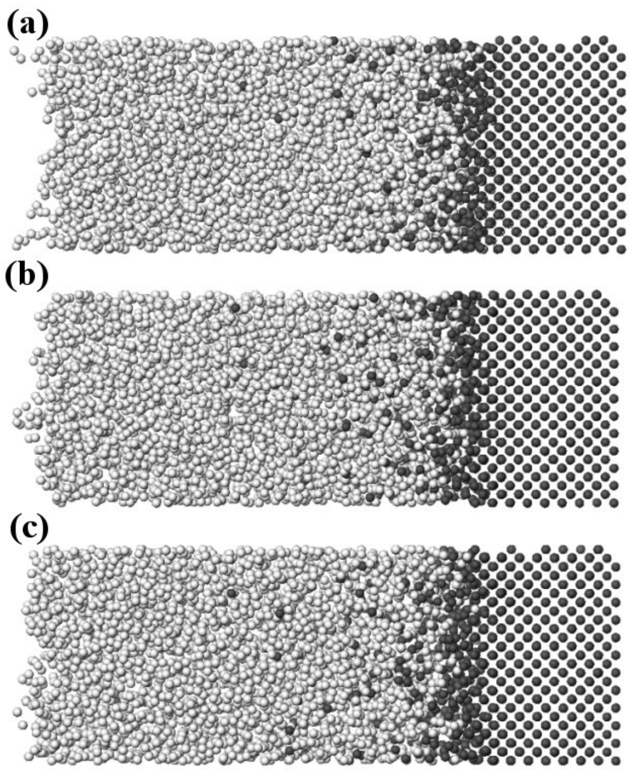

Figure 2. The atom configurations of synthesized ta-C films at each standard deviation (σ) 0 (a) 3 (b) 10 (c)

Figure 2 shows the atoms configuration of synthesized ta-C films at each standard deviation (σ) after 3000 carbon atoms deposited to substrate. White and grey balls of the configuration, which are shown in Fig. 2, represent incident carbon atoms and substrate carbon atoms, respectively. Due to the average incident energy (75 eV) is much higher than the cohesive energy of diamond (7.4-7.7 eV/atom)[9,10], intermixing occurs between film and substrate. The incident atoms bombarded to the substrate atom and the substrate surface was amorphized due to the significant agitation of the substrate atoms. Since the amorphous structure generated by the bombardment cannot return to their equilibrium phase at this temperature, a highly stressed and dense surface layer was formed on the substrate surface. However, the atom configurations with the standard deviation did changed largely that is shown in Fig. 2.

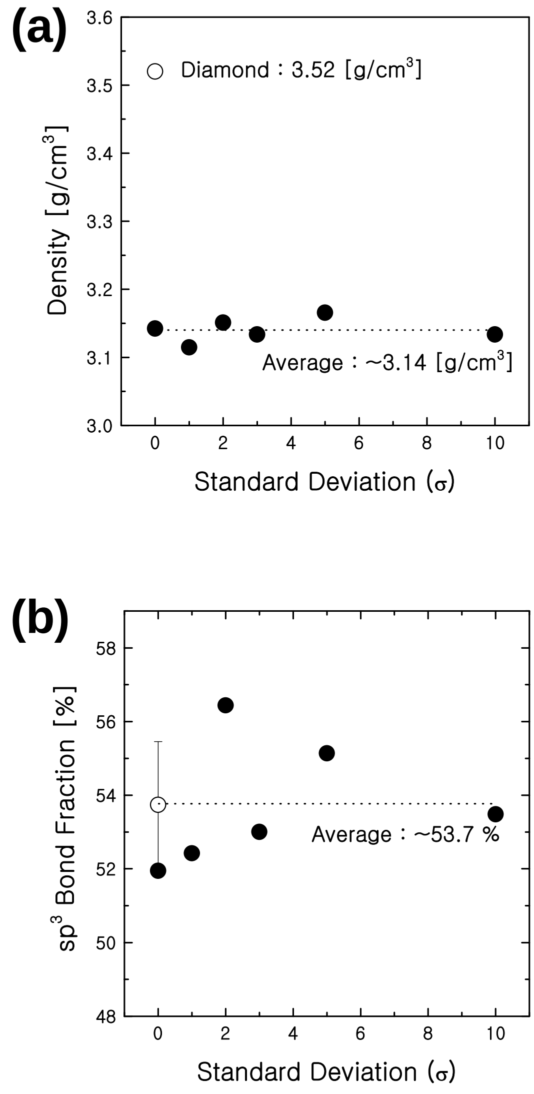

Figure 3. Density (a) and sp^3 bond fraction (b) of ta-C film with standard deviation (σ)

Figure 3 shows the behavior of density and the sp^3 bond fraction with standard deviation (σ). The average density and the sp^3 bond fraction of ta-C films deposited are 3.14 g/cm^3 and 54 %, respectively. They did not show any significant changes as the standard deviation varied.

However, the residual stress decreased with the standard deviation of incident beam energy and exhibited a minimum when the standard deviation (σ) was 3 as shown in Fig. 4.

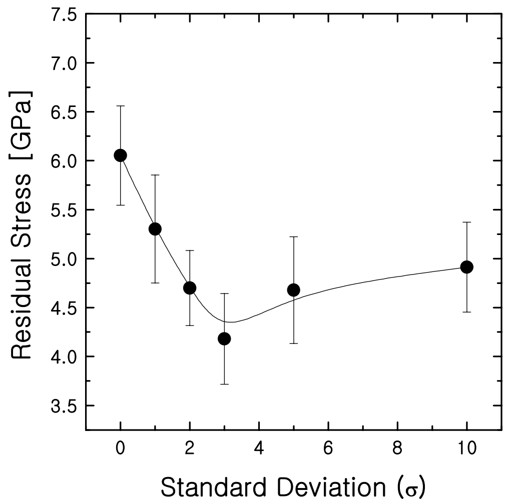

Figure 4. Residual stress behavior of ta-C film with standard deviation (σ)

It has been generally believed that the residual stress has a close relationship with the density and sp^3 bond fraction of film. It is well known that the high residual stress of ta-C film is due to high density and sp^3 bond fraction of ta-C film. However, in spite of the reduction of residual stress of ta-C from 6.0 to 4.2 GPa, the density and sp^3 bond fraction did not significantly change. Therefore, the reduction of the residual stress cannot be understood from the density and sp^3 bond fraction arguments.

In order to reveal the reason for the stress reduction, the radial distribution function (RDF) of these films were investigated. Figure 5 showed the radial distribution functions of ta-C film with standard deviation (σ) except the substrate atoms and surface atoms of ta-C film. The plots clear show the typical behavior of the amorphous structures of ta-C film. The satellite peak of second nearest peak (as indicated as arrow in Fig. 5) was observed. These peaks can be also observed from the previous molecular dynamics studies[5,9,12,13]. In our previous work suggested that the meta-stable state is generated by the localized thermal spike due to the collision of the high-energy carbon atoms, which induced the distortion of bond angle and bond distance between carbon atoms[14]. The satellite peak of second nearest neighbor represented the number of the strained bond defects by distorted the bond length and angle, when the ta-C films were synthesized. Therefore, the intensity of strained bond defects has the relationship between the residual stress of ta-C film. The intensity of the satellite peak at 2.1 Å of the second nearest neighbors showed the same tendency with stress behavior of ta-C film as shown in Fig. 6.

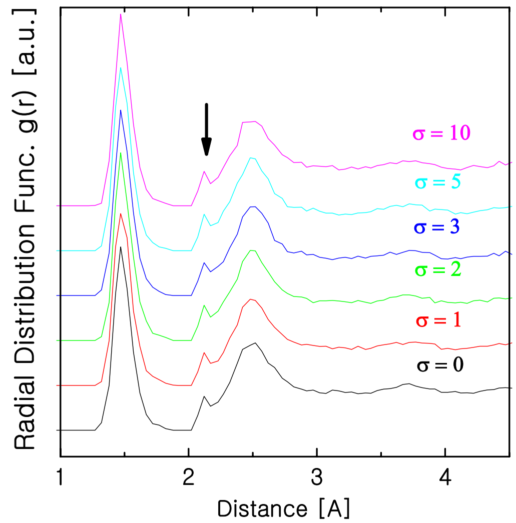

Figure 5. Radial distribution functions of ta-C film with standard deviation (σ)

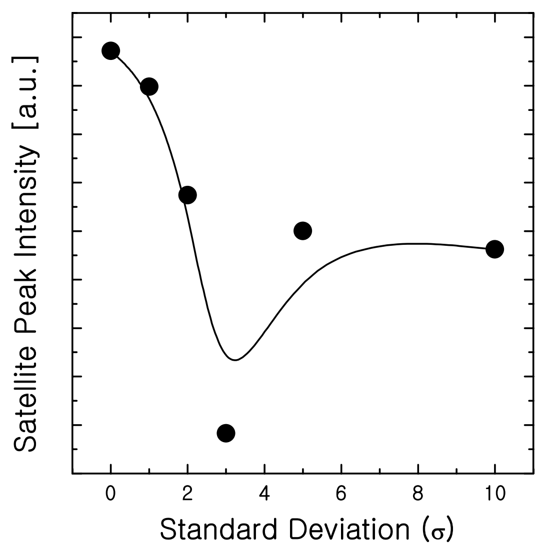

Figure 6. Satellite peak intensity behavior of ta-C film with standard deviation (σ)

4 CONCLUSIONS

We investigated the structure and properties of ta-C films using dispersed incident energy instead of monochromatic incident energy. The density and sp^3 bond fraction of synthesized ta-C film did not showed significant behaviors with standard deviation (σ). However, the residual stress of ta-C films reduced and had the minimum value when the standard deviation (σ) was 3. The intensity of satellite peak of second nearest peak, which means that of strained bond defects, shows the same tendency with residual stress. The strained bond defects are also the one of the reason of generation residual stress of ta-C film. The present simulation result shows that the residual stress can be reduced by controlling the number of strained bond defects. It is provided by the energy dispersion of the incident carbon atom

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