Effects of sputtering of a-C:H films on the chemical composition

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Abstract: We simulated effects of Ar^+ and Ne^+ irradiation to a-C:H films on their structure and chemical compositions using the SRIM code. Compared to Ar ions, Ne ions tend to sputter more H atoms out than C atoms. This tendancy brings about reduction of H concentration of a-C:H fims as well as efficient structure change from sp^2 to sp^3 configuration. Eventually, harder a-C:H films are realized by Ne^+ irradiation compared to Ar^+ one.

Keywords: a-C:H films, sputtering, ion energy, Ar ions, Ne ion.

1. Introduction

Carbon is a material that can have a wide range of structures depending on its bonding configurations. The structures include diamond, graphite, glassy carbon, graphene, fullerene, and carbon nanotubes, while amorphous carbon (a-C) can also be classified into various categories depending on its properties. This is due to the fact that carbon has three types of hybridized orbitals: sp^3, sp^2, and sp^1. Due to its material abundance and the various structures and properties, carbon is one of the most useful and the most frequently utilized material. However, the various structures of carbon related materials often lead to difficulty of the fine control of structures and properties. This is ture for amorphous hydrogenated carbon (a-C:H) films, which consist of sp^2 and sp^3-hybridized bonded carbon atoms and hydrogen atoms [1, 2].

Using H-assisted plasma CVD reactor we developed, we demonstrated conformal, sub-conformal and anisotropic deposition on trenched Si substrates by selecting dissociation degree of source gases, flux and kinetic energy of ions impinging onto surface, and atomic hydrogen flux [3-13]. This demonstration clearly shows that kinetic energy of ions impinging on a-C:H films is the key to the feature profile evolution, in other words, deposition profile. Such ion irradiation to films also modifies structures and chemical compositions of the films. This paper compares effects of Ar^+ and Ne^+ irradiation to a-C:H films on their structure and chemical compositions using the SRIM code.

2. Simulation method

We simulated effects of Ar^+ and Ne^+ irradiation to a-C:H films using the SRIM code. Simulations were performed on a-C:H films with 35% hydrogen content and 1.8 (g/cm^3) film density, bombarded by 100 eV Ar and Ne ions at an incident angle of 0 degree. The total number of incident ions was 10000 and the calculation area was 3 nm in deapth from the surface..

3. Results and discussion

Figures 1 and 2 illustrate the penetration profiles of Ar, and Ne ions into a-C:H films. Ne ions have a larger spread parallel to the film surface than Ar ions. This is caused by a significant change in the direction of travel of the massive ions when they collide with each other in the a-C:H film. The penetration length of Ne ions is smaller than that of Ar ions, namely Ne ions penetrate into a relatively shallow region. The penetration depsth profiels of Ar and Ne ions

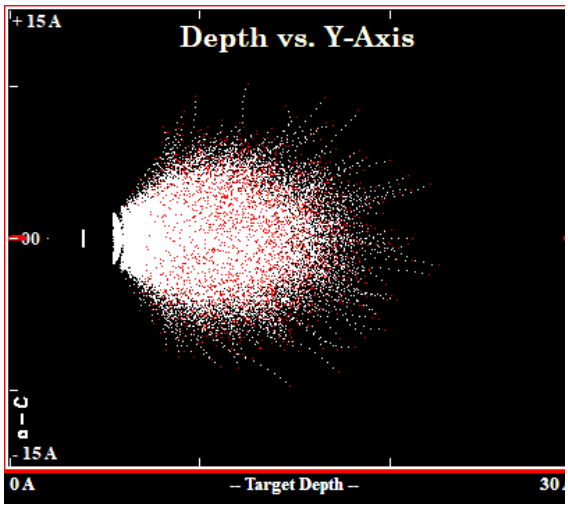

Figure 1. Penetration profile of Ar ions into a-C:H films.

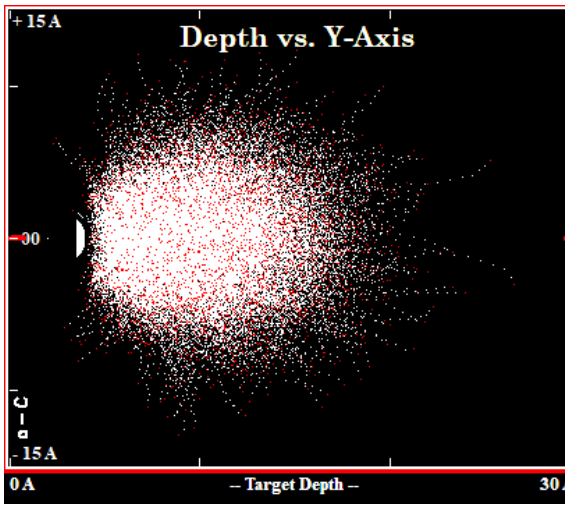

Figure 2. Penetration profile of Ne ions into a-C:H films.

show the following things. The Ar ion density is 1.4×10^7 ($atom/cm^3$) /($atom/cm^2$) at a depth of 1.3 nm. Given that 500 (atom/cm2) Ar ions are implanted, 1.4×10^7 multiplied by 500 gives a density of 7.0×10^9 ($atom/cm^3$) of Ar ions there.

Figures 3 and 4 show the original positions of sputter out C and H atoms induced by irradiation of Ar ions and Ne ions. Table I shows sputtered out H atoms and C atoms as

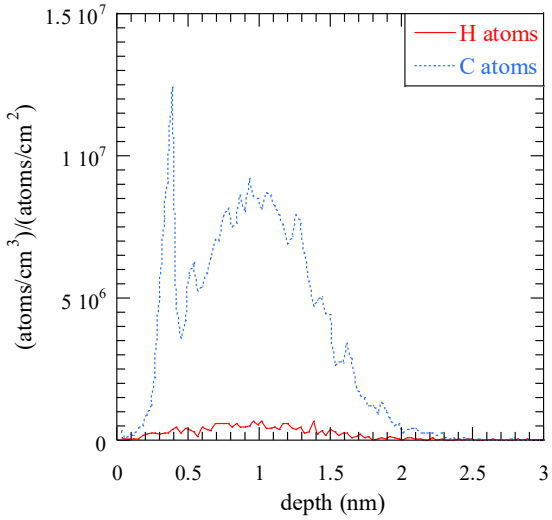

Figure 3. Original positions of sputtered atoms due to Ar ion irradiation to a-C:H films.

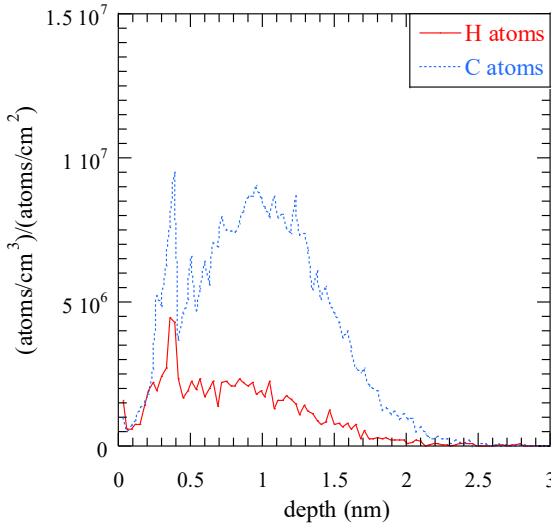

Figure 4. Original positions of sputtered atoms due to Ne ion irradiation to a-C:H films.

well as theira ration H/C for each ion irradiation. Compared to Ar ions, Ne ions tend to sputter more H atoms out than C atoms. This tendancy brings about reduction of H concentration of a-C:H fims as well as efficient structure change from sp^2 to sp^3 configuration. Eventually, harder a-C:H films are realized by Ne^+ irradiation compared to Ar^+ one.

4. Acknowledgements

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5. References

[1] J. Robertson: Phys. Status Solidi A **205** (2008) 2233.

Table 1. Sputtering yield and H/C of Ar ion and Ne ion to a-C:H films.

Ne ion	H (atom/ion)	0.0153
	C (atom/ion)	0.0060
	H/C	2.55
Ar ion	H (atom/ion)	0.0024
	C (atom/ion)	0.0015
	H/C	1.60

[2] J. Robertson: Jpn. J. Appl. Phys. 50 (2011) 01AF01.
[3] J. Umetsu, K. Koga, K. Inoue, H. Matsuzaki, K. Takenaka, and M. Shiratani: Surf. Coat. Technol. 202 (2008) 5659.
[4] J. Umetsu, K. Inoue, T. Nomura, H. Matsuzaki, K. Koga, M. Shiratani, Y. Setsuhara, M. Sekine, and M. Hori: DPS Proc. 30 (2008) 35
[5] J. Umetsu, K. Inoue, T. Nomura, H. Matsuzaki, K. Koga, M. Shiratani, Y. Setsuhara, M. Sekine, and M. Hori: J. Plasma Fusion Res. 8 (2009) 1443.
[6] T. Nomura, K. Koga, M. Shiratani, Y. Setsuhara, M. Sekine, and M. Hori, MRS Proc. 1222 (2009) DD05-16.
[7] T. Nomuta, T. Urakawa, Y. Korenaga, D. Yamashita, H. Matsuzaki, K. Koga, M. Shiratani, Y. Setsuhara, M. Sekine, and M. Hori: TENCON Proc. (2010) 2213.
[8] T. Urakawa, T. Nomora, H. Matsuzaki, D. Yamashita, G. Uchida, K. Koga, M. Shiratani, Y. Setsuhara, M. Sekine, and M. Hori: ISPC 20 Proc. POL02 (2011).
[9] K. Koga, T. Urakawa, G. Uchida, K. Kamataki, Y. Seo, N. Itagaki, M. Shiratani, Y. Setsuhara, M. Sekine, and M. Hori: PES Proc. 136 (2012).
[10] T. Urakawa, H. Matsuzaki, D. Yamashita, G. Uchida, K. Koga, M. Shiratani, Y. Setsuhara, M. Sekine, and M. Hori: Surf. Coat. Technol. 228 (2012) S15.
[11] S. Hwang, T. Okumura, . Kamataki, N. Itagaki, K. Koga, T. Nakatani, M. Shiratani, Jpn. J. Appl. Phys. 59 (2020) 100906.
[12] S. Hwang, R. Iwamoto, T. Okumura, K. Kamataki, N. Itagaki, K. Koga, T. Nakatani, M. Shiratani, Thin Solid Films 729 (2021) 138701.
[13] S.Ono, S. H. Hwang, T. Okumura, K. Kamataki, N. Yamashita, N.o Itagaki, K. Koga, M. Shiratani, J. Oh, S. Takabayashi, T. Nakatani, MRS Adv. 7 (2022)718.