Super Smoothing of Nanoscale Quartz Surface Using Amorphous Carbon Films

Abdelrahman Farghali[1], Takeharu Motokawa[2], Noriko Iida[2], Junho Choi[1]
[1] Department of Mechanical Engineering, The University of Tokyo (Japan)
[2] Institute of Memory Technology Research & Development, Kioxia Corporation (Japan)

INTRODUCTION

With the fast evolution of semiconductor technology to cope with the intense demand for more data processing and storing capabilities of electronic chips, manufacturers are obliged to minimize the design size down to the nanoscale to incorporate more transistors. As a result, surface roughness control of the end products is increasingly becoming significant as it can impact the overall performance. Amorphous carbon thin films offers a prime solution to optimize the surface roughness owing to the sp^2 and sp^3 hybridized bonding [1].

Molecular dynamics (MD) provides a deep understanding of the surface roughness evolution during amorphous carbon thin film deposition. Additionally, MD simulation offers a clear explanation regarding the growth mechanisms along with the distribution of stress at each step of the deposition [2].

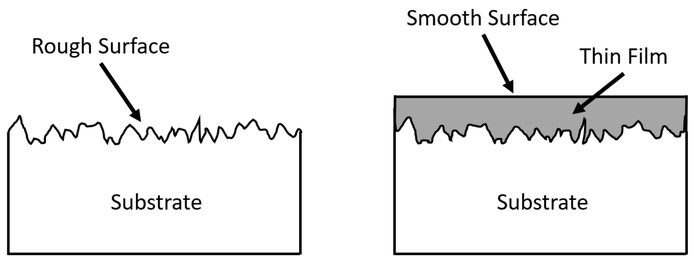

Fig. 1. Utilizing thin film technique to smooth rough surface of a substrate.

In this paper, both experimental methodologies and molecular dynamics simulation were utilized to illustrate the early stages of surface smoothing as a result of carbon atoms deposition on surface with several initial roughness.

METHODS

In this study, plasma-based ion implantation and deposition (PBII&D) was employed to a-C:H films on a quartz SiO_2 substrate with multiple surface roughness of Rq = 1.3, 1.8, and 2.5 nm to study the mechanism of surface smoothing.

Molecular dynamics simulation was employed to fully model the quartz substrate containing 13,500 silicon and oxygen atoms. The substrate was divided into three sets of layers; the bottom 11 layers (17.1 Å) were fixed, the intermediate 10 layers (15.5 Å) were subjected to a heat-bath at room temperature by Langevin equation, and the top 15 layers (23.4 Å) were free to interact with incident atoms as shown in figure 2. LAMMPS simulation package was utilized [3]

To simulate a rough surface with (Rq) of 2 Å, 4,500 argon atoms were accelerated to sputter the top free layers of quartz using Tersoff potential [4]. Next, carbon atoms were deposited on the rough surface using the (REBO) potential for C-C interactions [5]. The carbon atoms were introduced with various deposition angles, θ = 0°, 30°, 60°, and 75° with the z-axis to test the effect of deposition angle on the smoothing process.

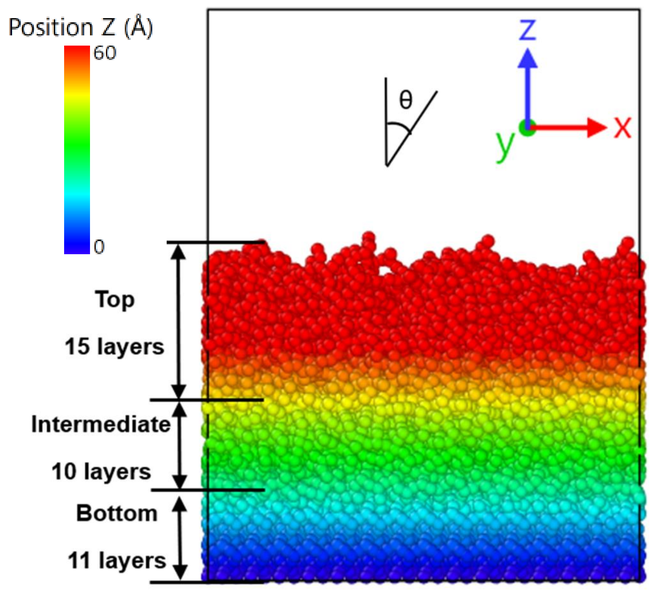

Fig. 2. Cross-section view of the simulation box after Ar sputtering with designated layers.

Experimentally, the surface roughness of a-C:H films on the quartz plates was measured by AFM. In MD simulation, the surface roughness (Rq) was calculated as follows,

$$R_q = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Z_i - \bar{Z})^2}$$

RESULTS

The smoothing process of quartz substrates pursues the same mechanism of short-term roughness decrease as shown in figure 1 (a). This is followed by an increase with a constant plateau back to the original roughness numbers and finally a continuous roughness reduction. Figure 3 (b) illustrates the changes in the surface roughness up to 2 Å after 270 nanoseconds of argon sputtering. After MD simulation of atomic carbon deposition, surface roughness follows the same fluctuation trend of the experimental results with some variations between low angle deposition (0°, 30°) and high angle deposition (60°,75°).

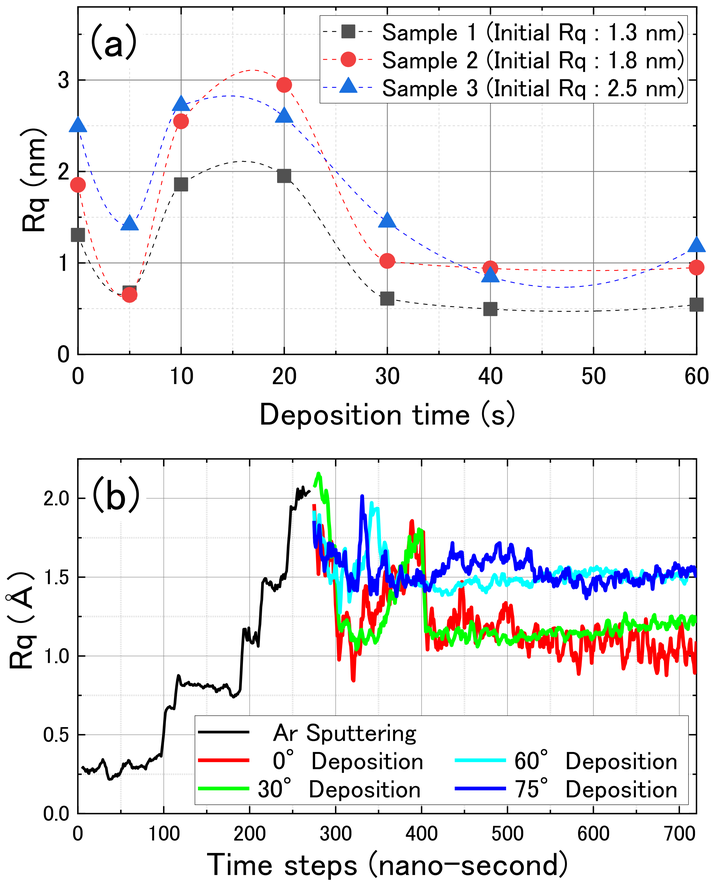

Fig. 3. (a) Roughness alterations of quartz plates after a-C:H film deposition, (b) MD simulation of roughness variations of Ar sputtering and the carbon atoms deposition.

CONCLUSIONS

Experimental results and molecular dynamics simulation data reveals a unique smoothing behavior that occurs at the early stages of carbon atomic deposition. A low surface roughness of 1.1 Å is detected at low deposition angles of 0° and 30° compared to a high surface roughness of 1.5 Å at high deposition angles of 60° and 75°. Surface irregularities of carbon islands formed due to the shadowing effect are more emphasized in the case of high angles, which is the main reason for these two surface behaviors.

REFERENCES

1. J. Robertson: Diamond-like amorphous carbon, Mater. Sci. Eng. R 37 (2002) 129-281.
2. B. Zheng, W.T. Zheng, S.S. Yu, H.W. Tian, F.L. Meng, Y.M. Wang, J.Q. Zhu, S.H. Meng, X.D. He, J.C. Han, Carbon 43 (2005) 1976–1983.
3. S. Plimpton, J. Comp. Phys. 117 (1995) 1–19; LAMMPS website: https://www.lammps.org, 2021; LAMMPS GitHub repository: https://github.com/lammps/lammps, 2021.
4. J. Tersoff, Phys. Rev. B 37 (1988) 6991.
5. J. E. Lennard-Jones, Cohesion, Proceedings of the Physical Society 43, 5 (1931) 461–482.