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Numerical Calculation on Spatial Distribution of Chemical Species in Ar Induction Thermal Plasmas with Feedstock CH_4/H_2 Injection for Diamond Film Growth considering Dissociation Reaction Rates

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1. Introduction

Diamond is a promising material for the next-generation power semiconductor devices because it has excellent properties such as extremely higher breakdown voltage, higher electron mobility, and superior thermal conductivity compared to Si or SiC. The authors' group have been investigating to apply inductively coupled thermal plasma (ICTP) to diamond film growth in experimental and numerical approaches [1,2]. For diamond growth, it is important to understand chemical species generated in the ICTP and their transport to the substrate. In this study, numerical simulation was conducted to obtain the spatial distributions of chemical species in the Ar ICTP with CH_4/H_2 feedstock gas to the substrate surface considering dissociation reaction rates, diffusive and convective transports. The model also calculated the temperature and flow velocity fields.

2. Plasma torch and calculation condition

Fig. 1 depicts a schematic diagram of the ICTP torch (z < 330 mm) and the chamber (z > 330 mm) used in our experiment and this numerical simulation. The ICTP torch is made of quartz tube and its inner diameter of 70 mm. The torch wall is cooled by cooling water. The chamber wall is made of stainless steel, which is cooled by the water. The 8-turn induction coil was placed around the torch to create the plasma in the ICTP torch. To the torch, a water-cooled feeding tube was inserted along the torch axis to supply the feedstock gas CH_4/H_2 to the plasma directly. The tip of the tube is placed at z=160 mm. A substrate was placed on the Mo substrate holder located at z=370 mm. The temperature of the tip of Mo substrate holder was fixed at 1000ºC. Argon was supplied along the torch wall as a sheath gas from z = 0 mm at a flow rate of 20 slpm in the axial direction and 20 slpm in swirl directions. The pressure in the torch and the chamber was set to 60 torr. The CH_4/H_2 gas was supplied through the feeding tube with a gas flow rate of 0.03/3 slpm as a feedstock gas.

The temperature and flow velocity fields of the ICTP was calculated by solving the mass, momentum, and energy conservation equations coupled with Maxwell's equation, and the transport equation of CH_4/H_2 gas. The spatial distributions of each chemical species were also computed by considering chemical reaction rates of 48 reactions such as dissociation reactions $CH_4+Ar \leftrightarrow CH_3+H+Ar$, $CH_3+Ar \leftrightarrow CH_2+H+Ar$ etc, and also the convective and diffusive transports of each chemical species.

3. Calculation results

Fig. 2 indicates the calculated results of spatial density distributions of (a) CH_3 and (b) C_2, which are considered important for diamond growth. The feedstock gas CH_4/H_2 gas injected from the tip of the feeding tube is dissociated thermally in the ICTP to produce CH_3, but CH_3 is also rapidly dissociated. Thus, the number density of CH_3 becomes less than 10^{11} m^{-3} along the torch axis. On the other hand, dissociation of CH_4 also produces C_2. The C_2 is produced with high densities above 10^{18} m^{-3} downstream of the torch around z=250-300 mm. This C_2 is transported by strong convection to the vicinity of the substrate holder. This convective transport of carbon radicals could play an important role for diamond growth.

References

[1] K. Hata, et al., Plasma Chem. Plasma Process. 41, 757-777, 2021

[2] K. Hata, et al., J. Phys. D: Appl. Phys., 54, 195105, 2021

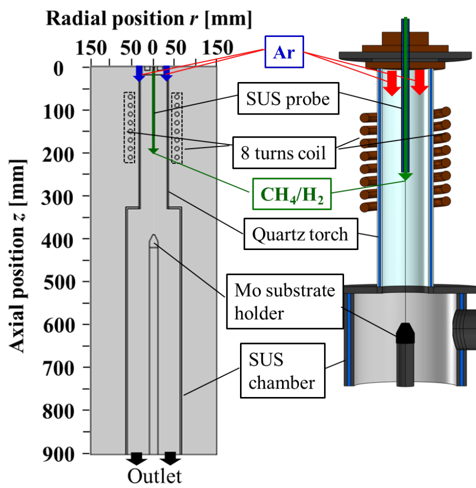

Fig.1 Plasma torch and calculation space.

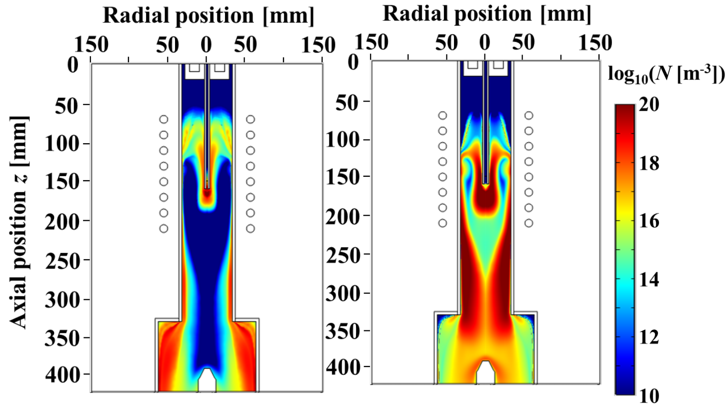

Fig.2 Spatial density distributions of (a) CH_3 and (b) C_2 in plasma torch at a pressure of 60 torr.