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Simulation of microwave plasmas concentrated on the top surface of a diamond substrate with finite thickness

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Abstract

Steady states of microwave plasma discharges have been numerically studied for chemical vapor depositions of diamonds. In the present simulations, a diamond substrate with 1 mm thick and 5×5 mm^2 areas is taken into account. It is found that distributions of plasma close to the substrate are modified by the presence of the substrate. By changing a depth of the substrate and a distance between edges of the substrate and the holder, profiles of the power density above the substrate can be varied into concave/convex distributions similar to experimentally observed surface morphologies. Clear correspondence between tendencies of these density distributions and experimentally observed surface morphologies is found.

Keywords: Plasma simulation and modeling; Microwave; CVD; Single crystal diamond

1. Introduction

Synthesizing a large single crystal diamond is an important issue for applications of diamonds in various fields. However, reported sizes of a synthesized single crystal diamond are limited still below one inch in diameter. To solve this issue, we have carried out microwave (MW) plasma chemical vapor depositions (CVDs) of thick single crystal diamonds [1,2]. To increase the growth rate of diamond CVD, many researchers have tried to find optimized reactor designs [3,4] and operating conditions [5–7]. To enhance power efficiency of the growth, we have used specialized substrate holders to achieve high growth rates [1,2]. It has been reported that continuous growth by using such holders can produce approximately 10 mm thick single crystal diamond [1].

Concave macroscopic morphologies are not desirable for continuous growth because it may cause anomalous growth along the edges of the substrate and/or defects tend to be easily created on such surfaces. By changing the types of the substrate holders, we have observed that surface morphologies can be varied into concave or convex profiles [1]. In Fig. 1, schematic views of experimentally tested substrate holders and macroscopic morphologies obtained by using those holders are shown. When the substrate is embedded into a "hole" drilled at the center of the holder top surface (Fig. 1(a), upper), the surface morphology of the substrate after depositions is usually flat or convex type (Fig. 1(a), lower). On the other hand, when side wall of the hole is far from the substrate (Fig. 1(b), upper), or when the substrate is placed on the holder without the hole, the morphology is concave type (Fig. 1(b), lower). To synthesize large and high quality single crystal diamonds, it is important to understand the mechanism which determines such surface morphologies, and to control them.

While many authors have reported simulation results of MW plasma CVD of diamonds [3–5,7–13], to the best of the author's knowledge, a diamond substrate with finite thickness has not been considered in their model. In our recent work [14], it is found that distributions of physical quantities of plasmas and gas are affected by the presence of the substrate, and the density of microwave power absorbed by plasma is high along with the edges of the substrate top surface. To elucidate correspondences between numerically predicted distributions of plasmas and experimentally obtained macroscopic morphologies as shown in Fig. 1, in this article, we have carried out

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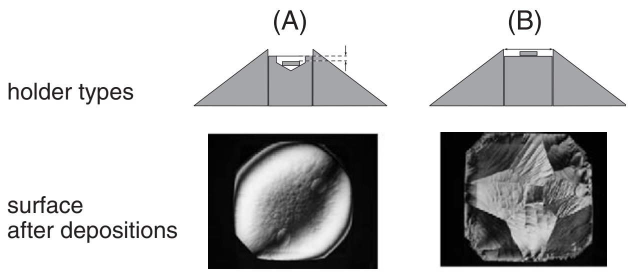

Fig. 1. Experimentally used types of substrate holders (upper column) and morphologies of top surface of the substrate obtained after deposition (lower column) by using these holders. In the case with the use of embedding type of the holder ((a), upper), convex type morphology is obtained ((a), lower). On the other hand, when the open type holder ((b), upper) is used, concave type morphology us obtained ((b), left).

simulations of MW plasma where a finite size diamond substrate placed on the various types of substrate holders are taken into account for the first time. In the next section, procedures of the simulation and the model used here are briefly summarized. In Section 3, obtained results are shown, and correspondences between those numerical results and experimental observations are discussed. The paper is summarized in Section 4.

2. Numerical modeling

Similar to the case in Ref. [14], simulation procedures are the same with those used in previous works [3,4,7]. In this paper, we shall focus on the effect of the arrangements of substrate holders and the diamond substrate. Hence, parameters included in the model are fixed throughout this paper as follows; neutral gas pressure $p_n = 160$ torr, neutral gas temperature $T_n = 10^3$ K, field strength to maintain discharges $E_m = 8 \times 10^4$ V/m, minimum electron density $n_{e\ min} = 1 \times 10^{17}$ [1/m^3], and total microwave power introduced into plasma $P_{abs} \approx 0.5$ kW. Dependence of microwave field and plasma distributions on p_n and P_{abs} are reported in other literatures [7,13]. To integrate the governing equations, a customized version of JMAG-Studio [15] is used. Fig. 2 shows a model device used in the simulations. This model device is numerically realized by using SolidWorks® [16], and corresponds to the actual experimental device, AX-5250 5 kW-MPCVD system produced by Seki Technotron Corp. [17]. A rectangular waveguide is connected to a cylindrical vessel. TE_{01} mode of microwave with a frequency of 2.45 GHz is excited at a cross section of the waveguide in the calculation. In the present simulations, except for the quartz plate and the diamond substrate, all solid materials are assumed to be perfect conductors.

A substrate holder is placed at the center of the substrate, and the diamond substrate is placed on the holder or embedded into a hole on the holder top surface. In this paper, four frustum types of substrate holders are studied. Their shapes are schematically shown in Fig. 3. In type (A), radii of the top and the bottom surfaces of this frustum are 4 and 6 mm, respectively. The height of the holder is 9 mm. A rectangular diamond substrate with 5×5 mm^2 area and 1 mm thickness is placed on the top surface of the frustum holder. In type (B), a circular hole with 4 mm radius and 1.5 mm depth is formed on the holder top surface. The diamond substrate is embedded into this hole, and the depth of the substrate top surface from the circular holder top edge is 0.5 mm in this case. In the type (C), the hole is 1.5 mm deeper than that in the case of the type (B), i.e. the depth of the substrate top surface is 2 mm. In type (D), the depth of the substrate top surface equals to that in the case of type (B), while the distance between edges of the substrate and the holder is larger than other cases. The radii of the top and the bottom surfaces of the frustums in type (D) are 8 and 12 mm, respectively. For all types of holders, the intersection point of diagonal lines of the substrate top surface coincides with the symmetric axis of the holders.

3. Results and discussions

Fig. 4 shows contours of electric field strength |**E**| (left) and electron density n_e (right) where the holder (A) (See Fig. 3(A)) is placed on the suscepter. In the figure, contours on a cross section between the suscepter and the quartz plate are shown. Amplitudes in darker (lighter) regions are larger (smaller). As shown in the figure, plasma is concentrated around the top of the substrate and the substrate holder. In the cases with the holders (B)–(D), global distributions of |**E**| and n_e far from the substrate holders are similar to those shown in Fig. 4. However, these local distributions in region close to the substrate are different from each other as described below. Local distributions of the density of the microwave power absorbed by the plasmas (power density) are summarized in Figs. 5 and 6. In Fig. 5, contours of them are shown for each type of the substrate holder. The left hand side of the figure shows results without the diamond substrate on the holders such as those in the previous work [7]. On the other hand, the right hand side shows results with the diamond substrate. In the same manner with that of Fig. 4, amplitudes of darker (lighter) regions are larger (smaller). In the case of the type (A) without the substrate, power density is high only around the top edge of the

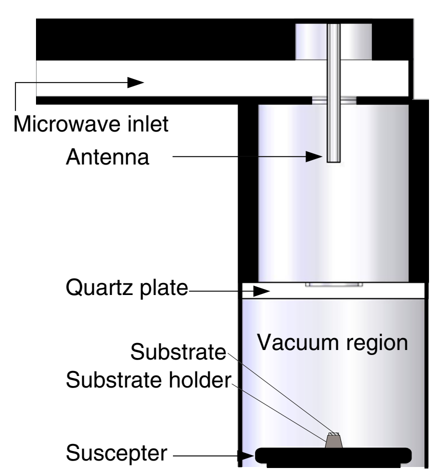

Fig. 2. Schematic view of the model device used in the simulations. At the center of the suscepter, a substrate holder shown in Fig. 3 is placed.