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Simulation with an improved plasma model utilized to design a new structure of microwave plasma discharge for chemical vapor deposition of diamond crystals

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Abstract

A new structure of microwave plasma for chemical vapor deposition of diamond crystal is proposed. The structure is designed numerically, for which an improved model given in our previous work [H. Yamada et al., J. Appl. Phys. 101 (2007), art. no. 063302.] is utilized. The experimental observations and numerical predictions agree well with each other. It is demonstrated experimentally that the proposed structure can achieve a growth rate larger than 50 μm/h over an area 1 in. in diameter.

Keywords: Plasma CVD; Diamond crystal; Simulation; Single crystal growth

1. Introduction

The growth rate and crystal size of a single-crystal diamond are smaller than those of other semiconductor materials, e.g. Si and SiC. Microwave plasma chemical vapor deposition (MWPCVD) is a method by which diamond crystals have been produced in vapor phase in a stable manner with relatively high growth rates [1–3].

To increase the power density above the substrate and the growth rate using MWPCVD [4,5], one may increase the pressure [1–3], or use a substrate holder with a specialized shape [3]. Because the shapes of the plasma generated in conventional reactors for diamond syntheses [6–8] are spherical or hemispherical, these techniques require shrinking of the area of the plasma facing the substrate as well as the plasma volume. This means that it is hard to apply these techniques to increase the growth rate for substrates with a large area, e.g. 1 in. in diameter, without a simultaneous increase in the input power.

In this article, a new design of the MWPCVD reactor, different from conventional MWPCVD reactors, is proposed in an effort to achieve a high growth rate for substrates with large area. The structure is designed numerically, for which an improved model given in our previous work [9] is utilized. It is experimentally shown that the extent of the electron number density for the generated plasma is similar to that numerically predicted, and it is confirmed that the distribution of the experimentally obtained growth rate agrees well with that of the numerically predicted power density. Furthermore, it is experimentally demonstrated that the proposed structure can achieve a growth rate larger than 50 μm/h over an area 1 in. in diameter.

2. Modeling

To design the structure of the reactor by trial and error, we have utilized a numerical simulation [4,5,9]. Recently, we have proposed an improved model which might be useful especially for this purpose. The detail of the model including the derivation of the governing equation is described in Ref. [9], and is outlined below. Under the condition of high pressure (~0.1 atm), one is able to reduce the governing equations of the microwave plasma into the following one equation:

$$\Delta n_e + \frac{1}{D_e} n_e \left[\sum_{\alpha} n_\alpha k_\alpha e^{-E_\alpha/T_e} - n_e \sum_{i} \hat{n}_i k_i e^{-E_i/T_e} \right] = 0 \qquad (1)$$

where n_e and T_e are the number density and temperature of electrons, respectively. n_α and $\hat{n}_i$ are the number densities of neutrals and ions, respectively, and are assumed to be constant. k

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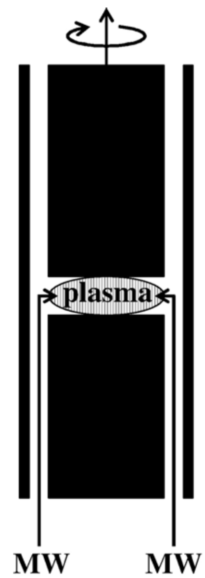

Fig. 1. Cross section of the conceptual structure proposed here. The structure is axisymmetric.

is the reaction coefficients, and E is the threshold energy of these reactions. D_e is the diffusion coefficient of electrons. In this article, Eq. (1) coupled with the Maxwell equations is solved. Parameters used in the simulation here are the same as those used in Ref. [9] unless otherwise stated. This model requires solving the Maxwell equations coupled with only one additional equation, i.e. Eq. (1). The benefit of this model is that it takes into account the effect of the plasma while the computational cost is reduced as much as possible. Furthermore, this model can be applied to the cases of plasma with large n_e where the skin effect is not negligible. Validity of the model is tested by comparing with experimental observations and numerical results given by other models. It is confirmed that the model used here is consistent with these other results in spite of the model tractability [9].

3. Concept of the proposed structure

One of the common characteristics of conventional MWPCVD reactors is that they use the cavity-resonance-mode of the microwave to transfer the power to the region above the substrate. This restricts the shape of the plasma boundary to spherical or hemispherical shapes. Therefore, in these cases, the microwave power is wasted in the region relatively far from the substrate. To maintain a high power density over a large area, the preferable shape of the plasma is flat. Fig. 1 shows the conceptual structure proposed here, which is intended to realize such plasma. There are two characteristics of the proposed structure; 1) the use of the mode of the co-axial waveguide, and 2) the method to limit the vertical extent of the plasma. A cylindrical inner conductor is disconnected at a certain position, forming a small gap between upper and lower sections of the inner conductor. The substrate is set to one of these sections. The microwave is introduced from the lower (or upper) side and propagates into the gap, and it is intended for the plasma to be generated at this narrow gap.

The advantages of this configuration are that (1) in principal, microwaves of any frequency can be transferred to the region above the substrate, while the size of the reactor must be enlarged proportionally to the wavelength in conventional cases using the cavity-resonance-mode; (2) since the thickness of the plasma is mechanically limited by the wall, the plasma shape is kept flat even for cases that the input power is relatively high, and thin concentrated plasma is produced even for the case in which the microwave frequency is low.

In the next section, it is confirmed numerically that the plasma is generated as expected under a more realistic structure that is also experimentally demonstrated in Section 5.

4. Numerical simulation

Based on the idea described in the preceding section, a numerical simulation was carried out for several configurations. This section gives numerical results for an experimental demonstration carried out in the next section. Fig. 2 shows a schematical cross-section of the tested reactor. The calculation was made for the domain enclosed by the dashed line and the structure is axisymmetric. The structure was designed for the substrate 1 in. in diameter. Conductors A and B correspond to the inner conductors in Fig. 1. Microwaves with a frequency of 2.45 GHz are introduced from the bottom passing through the side of conductor B. The distance between the bottom surface of conductor A and the top surface of the substrate is around 10 mm.

Fig. 3 shows contours of a) the strength of the electric field, b) number density of electrons, and c) power density. In this case, the input power and gas pressure are set to 2.6 kW and 19,998 Pa (150 torr), respectively. As expected, the electron number density has finite values only in the narrow gap. The plasma boundary is ellipsoidal and its aspect ratio is around 4.

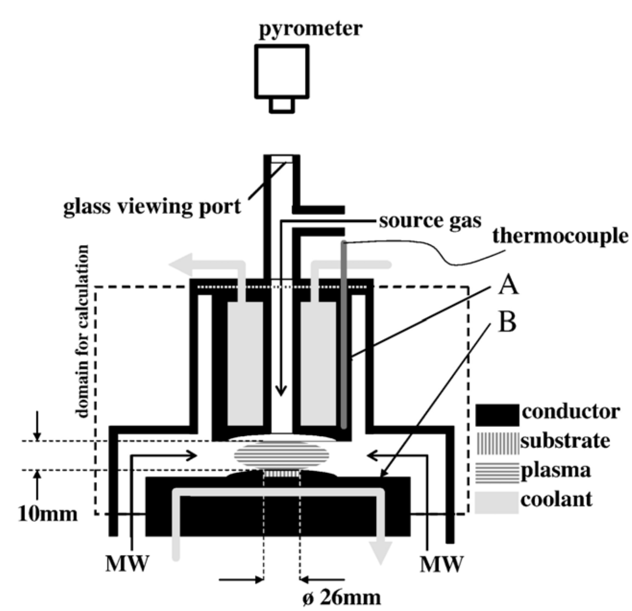

Fig. 2. Structure of the MWPCVD reactor tested in this work. While the whole of the structure is realized in experiment, the region enclosed by the dashed line represents the simulation domain.