Numericalsimulation of temperature and chemical species distributions in HFCVD for diamond film

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The hot filament chemicalvapor deposition (HFCVD) is widely used for formation of diamond film. Thetemperature distribution between the filament and substrate is most significantfactor for an excellent uniformity of formed diamond layer because thetemperature distribution has an influence on the concentration of dissociatedcarbon and hydrogen species to be deposited. Since the distance between thefilament and substrate is very narrow and the temperature gradient is extremelysharp, however, it is difficult to directly measure the temperature byexperimental method. Therefore, the 3-dimensional numerical simulation has beenconducted to estimate the temperature distribution by using a commercialcomputational fluid dynamics (CFD) code, ANSYS-FLEUNT (Ver. 17.0). Although thetemperature distribution is not measured by the experimental method, the temperatureof filament could be predicted by using the two-color pyrometer. Then themeasured temperature of filament was employed to verify the simulation result.

The temperaturedistribution in the HFCVD reactor was calculated according to the variousoperating condition. In this work, the input power and the distance between thefilament and substrate was examine as main factors. The input power wascontrolled at 12, 14, 16 and 18 kW at fixed distance between the filament and substrateas 10 mm. The distance between the filament and substrate was modulate from 6to 26 mm with 4 mm intervals at fixed 16 kW input power. The temperatures offilament were calculated from 2,512 to 2,802 K according to the input powdervariation at the fixed distance between the filament and substrate, and thosevalues were from 2,733 to 2,774 K at the fixed power of 16 kW. This results wasis in good agreement with the measured temperature by using a two-colorpyrometer within 2 % error range. At the case of the temperature of substratesurface, it was calculated from 1,009 to 1,123 K at the fixed distance betweenthe filament and substrate, and from 1,101 to 1,034 K at the fixed power.Through comparing these calculated results with actual experimental results, itis revealed that the sufficient high temperature of filament has to be achievedto increase the concentration of dissociated carbon species, and the proper temperatureof substrate surface is required to deposit uniform diamond layer. In thecondition of 16 kW and 10 mm, the most appropriate thermal environment isformed for thick and uniform diamond film. The calculated temperature of thefilament and substrate are 2,715 K and 1,088 K, respectively.

In the actualexperiments, acetone was used as the carbon source. The acetone has lowerdissociation energy and much more CH_3 radicals than a methane. TheCH_3 radicals affects positively to the quality of diamond film.According to diverse operating condition, in the numerical simulation containedthe chemical reaction of acetone, the concentration of CH_3 radical decomposedfrom the acetone was varied. It was analyzed that the influence of thetemperature distribution on the concentration of CH_3 radical andgrowth rate of the diamond on the substrate.