

DIAMOND FILM SYNTHESIZED BY MW PLASMA CVD AND COMPUTATION MODELING OF ITS OPTICAL PARAMETERS

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Abstract Diamond film was synthesized by MWPCVD. Effects of processing parameters on IR optical properties have been studied. Optical parameters of DF refractivity, thickness and surface roughness have been computed by means of mathematical model of transparency T. IR transmission curves simulated of DFs are consistent with those measured. The quality of DFs can be evaluated by comparing curves simulated and measured, and by comparing DF refractivity simulated with that of natural diamond.

1. Introduction

Since 1980s, great progress of diamond film (DF) synthesis technique has increased the quality and thickness of DF so that DF will have a vast area of application, such as optics, electronics, mechanics etc.. Particularly, DF is expected to be an attractive optical film and window materials, which is operated in harsh wear and erosion environment for its great hardness, good wearability, high infrared (IR) transparency and thermal conductivity [1].

In the present paper, DFs are synthesized by MPCVD method. The MW plasma apparatus was manufactured by ourselves. In order to use DF as optical film and window materials, and to design optical structure in infrared region, optical parameters such as transparency, refractivity, thickness, surface roughness should be measured. In fact, many tests on these parameters of DF are complex. So this work calculated several

optical parameters with computer by means of the mathematical model of transparency T. The data will be easily obtained at soon after measuring the curve of infrared transparency.

Many former studies on this subject only simulated one optical parameter of DF. And the effects of processing parameters on optical parameters could not be discussed. In this context, authors simulated several optical parameters of DF grown under different conditions, which will help us to find rules and guide the synthesising process by using MWPCVD and DF application.

2. Experiment and Computation

Diamond films were synthesized on pretreated silicon substrate under different conditions by the made-own microwave plasma apparatus; microwave power was 400 – 700w, gas pressure was 2.5 – 6.5kpa, concentration of CH₄ was 0.2 – 1.0%, deposition time was 3 – 24 hour.

IR spectra of these films were measured by IR spectrometer. By means of the mathematical model of transparency T as follows [2]:

$$T = \left| \frac{t'_{01}t'_{10}exp(-i\beta)}{1 + r'_{01}r'_{10}exp(-2i\beta)} \right|$$

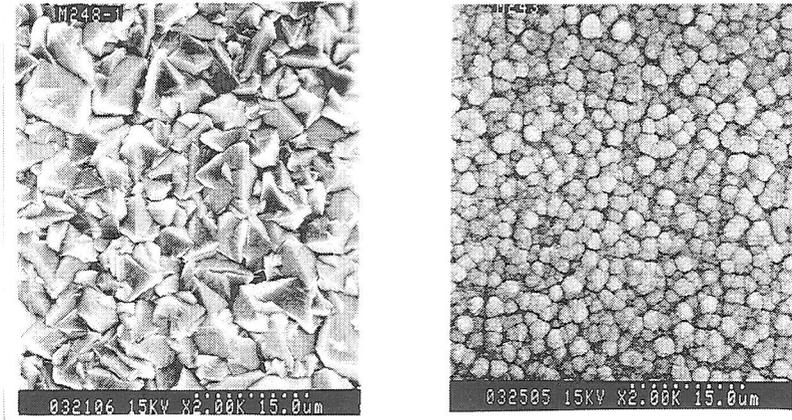
the terms t'_{01} , t'_{10} , r'_{01} , r'_{10} are the smooth surface Fresnel coefficients, the curves of IR spectra simulated and other optical parameters such as refractivity (n)、thichness (d) and surface roughness (Ra) could be calculated with computer.

3. Results and Discussion

3.1 Effects of Processing Parameters on DF synthesis

The results show that CH₄ concentration、microwave power and gas pressure are inportant factors which influnce on nucleation, growth and quality of diamond film. With increasing CH₄ concnertration, the DF morphology gets worse. At higher concentration, grains exhibit sphere without any crystal facet. With increasing microwave power and gas pressure, diamond grains show regular shape and big size. But much higher microwave power or gas pressure would result in diamond

graphitizing. Fig. 1 shows two SEM photographs of diamond films synthesized under different CH₄ concentration.



(a) CH₄ Concentration: 0.2%
 gas pressure: 5.3 KPa
 microwave power: 610W

(b) CH₄ Concentration: 1.0%
 gas pressure: 5.3KPa
 microwave power: 610W

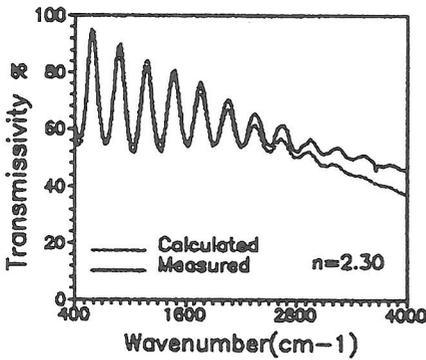
Fig.1 SEM photograph of DFs synthesized under different CH₄ concentration

3.2 Optical parameters simulated of DFs synthesized under different conditions

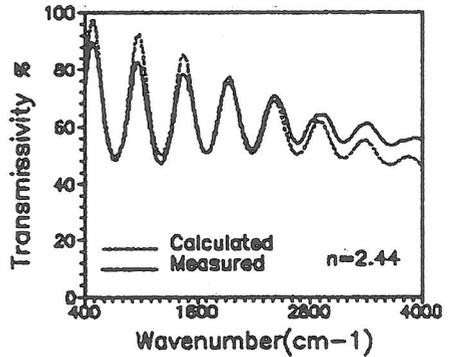
In order to increase transparency of diamond film window, its surface roughness and defects must be controlled. Surface roughness is affected by deposition time. The size of grains increase with time increasing so that surface roughness increases. The simulation curves are shown in Fig. 2, which show effects of different deposition time. And their optical parameters are listed in table 1.

Table 1 Optical parameters computed by modeling

Deposition time (hour)	21.0	13.5	8.0	6.6	3.0
Refractivity n	2.30	2.27	2.44	2.30	2.43
Thickness d (μm)	7.39	6.20	4.19	2.54	1.38
Surface roughness Ra (μm)	0.215	0.20	0.16	0.122	0.075



(a) deposition time: 8hr



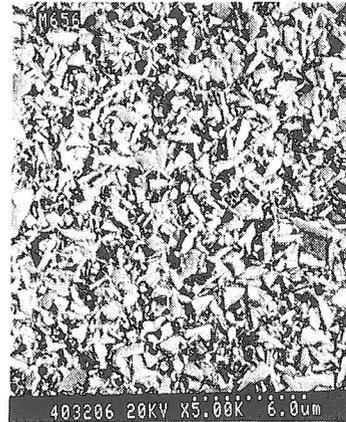
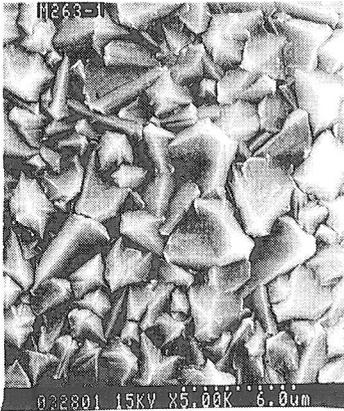
(b) deposition time: 21hr

Fig. 2 Comparison between IR transmission curves simulated and measured

The curves simulated in Fig. 2 are consistent with the curves measured, which indicate that optical parameters calculated from simulation data can be used in the practice. The data listed in table 1 prove that thickness and surface roughness increase with increasing deposition time. So smooth surface of diamond film would be grown in short deposition time. Of course, other ways such as higher nucleation density, lower substrate temperature smaller microwave power, gas pressure and grain size of grit polishing substrate etc. can decrease surface roughness, too.

On the other hand, the quality of DF can be evaluated using optical parameters calculated from simulation data. SEM photographs of DFs synthesized under two conditions are shown in Fig. 3. Fig. 3 (a) exhibits good morphology with clear surface and big grain size, while Fig. 3 (b) shows bad morphology with obscure shape, small grain size, noncrystalline component and without clear facet. And their IR transmission curves are simulated in Fig. 4, which indicates that simulation curves of DFs having high quality are much consistent with curves measured, and the refractivity of DF is much closed to that of

natural diamond ($n=2.4$). However, the bad film shows worse results, and calculated refractivity n is 2.56 which shows difference with that of natural diamond. Thus, the quality of diamond film can be evaluated using comparison between IR transmission curves simulated and measured, the refractivity calculated and ideal refractivity of natural diamond.



(a) CH_4 concentration: 0.18%
 gas pressure: 5.3KPa
 microwave power: 610w

(b) CH_4 Concentration: 0.5%
 gas pressure: 5.3KPa
 microwave power: 610w

Fig. 3 SEM photographs of DFs synthesized under two conditions

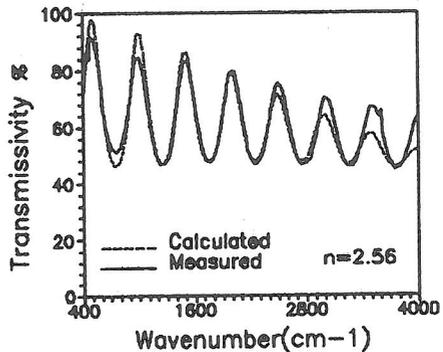
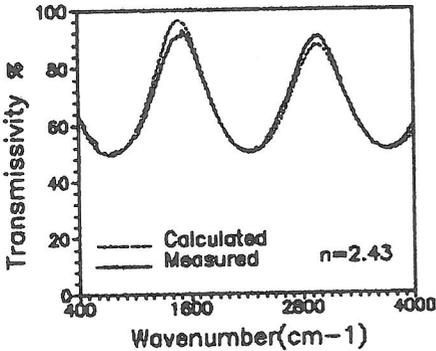


Fig. 4 Simulated and measured curves of IR transmission

4. Conclusion

(1) The quality of DF synthesized by MWPCVD varies with methane concentration, microwave power and gas pressure.

(2) The optical parameters (n , d , Ra) of DF varies with processing parameters of MWPCVD, too.

(3) By means of spectra of IR transparency of DF, its refractivity (n), thickness (d) and surface roughness (Ra) are easily computed using the mathematical model at soon.

(4) The results that simulated curves compared with measured curves and the calculated ref activity compared with that of natural diamond can evaluate the quality of DF. The smaller the differences, the better the quality of DFs.

References:

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(2) A. J. Gatesman, R. H. Giles, J. Waldman, L. P. Bourget, and R. Post, *SPIE vol. 325 Diamond Optics III*, 170—177 (1990).