THE ROLE OF BORON ON THE DEPOSITION DOMAIN FOR VAPOR PHASE SYNTHESIS OF DIAMOND FILMS

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Introduction

The feed gas compositions are typically used for predicting whether carbon precipitation from the vapor phase results in diamond, non-diamond deposition and no-deposition using an experimentally determined, ternary C-H-O diagram by Bachmann et al.[1,2] However, this diagram is not applicable for gas phase compositions containing dopant species such as Boron. Recently, Eaton and Sunkara described a C-H-O ternary phase diagram based on in-situ radical species composition for diamond deposition from the vapor phase.[3] Even this diagram was constructed for only C-H-O systems. Predictive modeling on the feed gas compositions with dopant species for diamond deposition will benefit the development of processes for obtaining quality, n-type and p-type doped diamond films from the vapor phase. In this regard, this work is focused on the question whether one can use radical species composition to predict diamond deposition when feed gas phase compositions contain dopant species such as Boron etc. The steady state gas phase computations were performed to understand how boron composition within feed gases effects the radical species compositions. The computational results were further analyzed to answer the specific questions about predictability of diamond deposition and qualitative trends.

Computations

The steady state gas phase compositions were calculated using zero dimensional, stirred reactor model using CHEMKIN III software. he reactions set for B-C-H-O gas phase chemistry is adapted from Pasternack[4] and the rest of the reactions for the C-H-O and the surface reactions are from Eaton and Sunkara.[3] A total of 154 gas phase reactions and 12 surface reactions containing 26 C-H-O and 10 B-C-H-O species were used. The computations were performed at 50 torr pressure, 1150 K temperature and a flow rate of 200 sccm. Five feed gas phase compositions are considered as shown in Figure 1. For each feed composition, the steady state compositions were computed with increasing boron concentration, i.e., B/C ratio increased from 0 to 333.

Results and discussion

The steady state computations results were analyzed by dividing the species in to two categories: participating and non-participating similar to the procedure described by Eaton and Sunkara.[3] The only difference in the procedure is that all boron containing species are also considered as non-participating species. The mole fractions for the participating species were calculated and were plotted in the C-H-O ternary diagram based on the radical species composition. Results showed that at low boron concentrations (B/C=4000ppm), the effect of boron addition is not drastic on the diamond deposition domain. At low boron concentrations, the point from the diamond deposition domain stays within the diamond domain. As the boron concentration in the feed gas is increased, the point moves toward C-H axis or into the non-diamond growth region. This is illustrated in Figure 2 with increasing boron concentration on one feed gas composition point within the diamond deposition domain. These observations are consistent with experimental observations, i.e., the quality of diamond films degrades with addition of boron in the gas phase.[5,6] The steady state compositions indicate that boron readily forms oxygenated species in the form of B_2O_3, HBO_2, and HBO and decreases the concentration of other oxygenated hydrocarbon species such as OH, O and CO. This causes the data points to locate towards the region of less O into non-diamond deposition domain within the ternary C-H-O diagram. The composition of BH, BH_2, B_2O_2, BO_2 are negligible compared to composition of other gas phase species. This behavior is consistent with all the five feed gas compositions that were considered. These results are summarized in Table 1. The feed gas compositional points from the no-growth domain shifted to the diamond growth domain and then towards the non-diamond growth region with increasing boron concentration.

Conclusions

Boron addition to feed gases affects the steady state compositions of C-H-O species, primarily the oxygenated hydrocarbons. This is because B_2O_3, HBO_2, and HBO are found to be the dominant steady state gas phase species for boron. Most important result is that the radical species compositions could be used for predictive modeling of boron containing feed gas phase compositions for diamond deposition.

Acknowledgements

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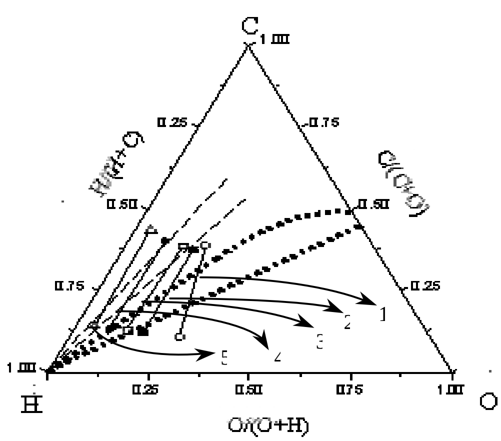

Figure 1. The position of data points with respective to feed gas composition and radical species compositions. The lens shaped region is given by feed gas compositions[2] and the upper region is described by radical species composition[3].

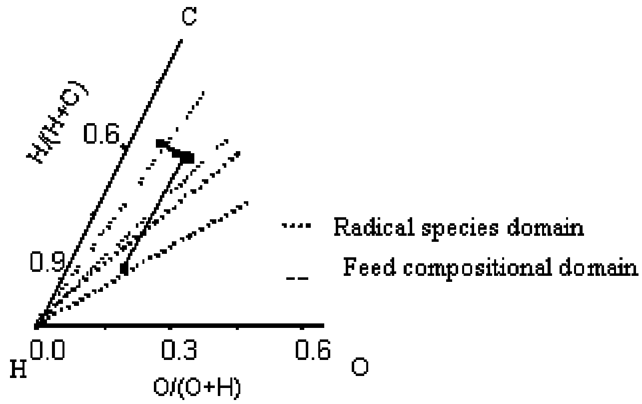

Figure 2. The effect of increasing boron concentration on the resulting radical species composition for feed gas composition located within diamond deposition domain.

Table 1. The effect of boron addition on the feed gas compositions shown in Figure 1.

			B/C					
	Bachmann		0.000	0.004	0.040	0.083	0.167	0.333
DATA PT 1	NG		NG	NG	D	D	D	ND
DATA PT 2	LB		LB	LB	D	D	D	ND
DATA PT 3	D		D	D	D	D	D	ND
DATA PT 4	UB		UB	UB	D	ND	ND	ND
DATA PT 5	ND		ND	ND	ND	ND	ND	ND

NG – No Growth, D –Diamond, ND – Non-Diamond, LB- Lower Border of Diamond Domain, UB – Upper Border of Diamond Domain