



Final Report

Surface Processes in CVD Diamond Growth  
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Executive Summary

The work performed under this contract consisted of basic research with the objective of improving our understanding of the fundamental science of diamond chemical vapor deposition. The major areas of work were

1. numerical modeling of CVD diamond growth
2. theoretical studies of growth mechanisms
3. in-situ diagnostics of gas-phase species during hot-filament diamond growth
4. *ab initio* calculations of surface migration on diamond
5. theoretical studies of transport issues and scaling law development
6. measurements of the open site fraction on a diamond surface during H exposure.

Each of these areas is described briefly below. Complete details are given in the published papers, which are attached.

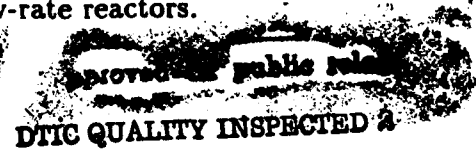
Modeling

The numerical modeling work was the first numerical model which incorporated both detailed gas-phase chemistry and transport. We first examined hot-filament reactors, and outlined the basic features of the gas-phase chemistry in this environment [1]. In a second paper, we showed that catalytic H recombination on the substrate perturbed this environment significantly, and we predicted large gradients in H concentration near the substrate (subsequently measured by others) [2]. We next modeled higher-pressure convective diamond growth methods (arcjets and combustion flames) [3]. By a detailed modeling of the reacting boundary layers in these systems, we showed for the first time that the same growth mechanism which predicted growth rates well in hot-filament systems (the CH<sub>3</sub> mechanism of Dr. Steve Harris at GM) also worked well for higher-pressure, high-growth rate methods. This provided support for CH<sub>3</sub> as the principal growth species, and was the first indication that the chemistry was the same in both high-rate and low-rate reactors.

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## Scaling Law Development

Recognizing that current diamond CVD processes must be scaled to larger areas and higher growth rates, a theoretical study was carried out to investigate the factors governing scaling for several different CVD methods [8, 9]. This work consisted both of the formulation of a simplified diamond growth mechanism, and a detailed study of atomic hydrogen transport to the diamond surface. For convective flows (arcjets, RF torches, combustion torches) optimal conditions were identified to maximize the H concentration at the substrate, and therefore the achievable growth rate.

## Open site fraction measurements

One of the critical parameters of the chemistry of diamond CVD is the fraction of surface sites which are not terminated by hydrogen during H exposure. It may be shown by simple kinetic arguments that this fraction  $f^*$  is independent of the hydrogen flux, and is fully determined by the ratio of the rate constant for H abstraction to the rate constant for sticking on open sites [8]. Values assumed in the literature for this number range from a percent or less, up to 40%. A measurement of this number would give useful information on the rate constant ratio, not obtainable in other ways.

We are currently setting up an experiment to measure this quantity, using the system shown in the figure. Elastic recoil spectrometry is being used to measure the H coverage on a single-crystal diamond surface exposed to an atomic hydrogen source created using a microwave discharge. We should have results on the open site fraction within a few months. This work is continuing under other financial support.

## References

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