

## Quarterly Report

## Analysis of Cost:

 Combustion Flame CVD Diamond DepositionContract Number: N00014-93-C2044


IBIS Associates, Inc.
55 William Street, Suite 220
Wellesley, MA 02181-4003 USA

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## Second Quarter 1994

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## Executive Summary

IBIS Associates has improved its predictive spreadsheet model of combustion flame chemical vapor deposition (CVD) diamond film fabrication. This report explains the improvements on the combustion flame deposition theory, and shows preliminary results of the economics of this CVD diamond process.

The changes to the model include the incorporation of thermal conductivity as an input to the model, allowing the user to specify the thermal properties of the diamond being formed. Also, the deposition theory in the model has been streamlined with the assistance of diamond deposition experts. Numerous inputs have been eliminated in this process, making the model easier to use.

For this report and the results contained herein, it is assumed that the transport theory model which predicts growth rates in the CVD diamond technical cost model closely predicts actual growth rates for the combustion flame technology and that the input values for variables such as the gas flow rate and substrate diameter are physically achievable.

To be investigated are alternative combustion flame deposition geometries and chemistries. Expert review has revealed that the deposition geometry assumptions (i.e. nozzle:substrate diameter ratio) in the IBIS model may not be optimal for combustion flame deposition. Suggested changes in deposition geometries involve the size, shape, and distance to substrate of the combustion nozzle, as well as higher flow rates at smaller nozzle sizes. Suggested changes in deposition chemistry include using ethylene as the carbon fuel instead of acetylene. Lastly, expert approval of the models is continually in progress.


## Combustion Flame TCM Expert Review

The combustion flame CVD diamond Technical Cost Model (in the Appendix) has been reviewed by deposition experts representing Sandia National Laboratories in both Albuquerque, NM and Livermore, CA; Stanford University; Caltech; and Lockheed. Copies of the model were transfered to these theorists along with a non-transferable site license, and all were tutored on the Technical Cost Modeling methodology. A thorough expert review of the combustion flame model was undertaken during this tutorial. In response to the model criticism that surfaced, a plan for the revision of the cost model was drafted.

The expert review of the combustion flame CVD diamond cost model produced no significant criticisms. There was a concensus among the theorists that two of the three quality measures, as reported in the first quarter report for 1994, are unnecessary. The model has been streamlined to use only one of the quality measures $(\mathrm{H} / \mathrm{CH} 3)$, which is believed to correlate the closest to thermal conductivity.

A defect-based model of CVD diamond material properties has been developed by Michael Coltrin at Sandia National Laboratories and David Dandy at Colorado State University. Inputs to this model include the hydrogen (H) and methyl radical (CH3) mole fractions at the growth surface, as well as numerous rate constants for the reactions considered at the growth surface. Outputs of this model include the growth rate and defect density, which are used to determine thermal conductivity. IBIS generated data from this model and performed regression analysis in order to find the $\mathrm{H} / \mathrm{CH} 3$ ratio as a function of thermal conductivity. As shown later in this report, the relationship assumed to exist between $\mathrm{H} / \mathrm{CH} 3$ and the thermal conductivity of the CVD diamond allows thermal conductivity to exist as an input to the cost model.

The model's shortcomings were identified by the experts as its inability to predict the effects of changing in reactor pressure, fuel chemistry, or nozzle count. The concensus was reached that a new version of the model should be developed with the ability to predict changes in these three conditions. Due to the large amount of data required to derive predictive relationships for all these processing parameters and the nonexistance of this data in the public domain, a plan for data collection from numerical models was established. As agreed, all organizations involved in the expert review with the exception of Lockheed will cooperate in the data generation.

## Sensitivity Analysis

Technical Cost Modeling permits the flexibility of performing sensitivity analyses. Using sensitivity analyses, it is possible to explore the cost implications of changing key input variables such as gas composition, production volume, material prices, product dimensions, etc. As an R\&D management tool, these analyses help set development goals for cost effective manufacturing. Further, they help in long term planning, by indicating the cost savings that may be realized through scale-up. For the purpose of these sensitivity analyses it is assumed that the transport theory model which is used to estimate the diamond growth rate closely predicts actual growth rates and that the input values for variables such as gas flow rate and substrate temperature are physically achievable. Presented in the following sections are the following analyses, all based on the assumption of thermal management quality diamond:

- Cost vs Substrate Diameter and Gas Consumption
- Cost vs Thermal Conductivity and Gas Ratio
- Cost vs Thermal Conductivity and Substrate Diameter

For all of these analyses, the ratio of substrate to duct area is held constant. This constraint is due to the geometry assumed for the combustion flame technology as modeled (i.e., a single nozzle torch). The area of the gas duct is the cross-sectional area of the flame before it is affected by the flow pattern around the substrate. For a combustion flame with a corresponding duct area impinging on an infinite plane, there will be a circular region of desirable diamond and a surrounding region of unacceptable diamond. Consider the similar case of a flame impinging on a substrate of the same area. As a substrate diameter increases while the duct diameter remains constant, there is a point at which the substrate extends into this zone of unacceptable diamond. Therefore, there is a maximum substrate:duct area ratio that should not be exceeded. Experts in CVD diamond deposition suggest that this ratio is roughly $3: 1$ for single nozzle torches. When the substrate diameter is varied in the following analyses, the duct diameter is adjusted so that the ratio of substrate to duct area is constant.

## Cost vs Substrate Diameter and Gas Consumption

Figure 1 shows the combustion flame deposition cost per square centimeter of one millimeter thick polycrystalline diamond varying with the diameter of the deposited wafer. In addition, because the duct area and gas flow rate increase with substrate area, Figure 1 shows the total gas flow rate changing with the substrate diameter. The volumetric gas flow rate must change with the duct diameter, if constant quality is to be maintained, due to the assumptions in deposition theory that are mentioned in the first quarter report of 1994. At about nine centimeters in diameter, the cost per square centimeter of combustion flame CVD diamond reaches a minimum of roughly $\$ 60$. The incorporation of the gas flow rate plot illustrates why there exists an optimum substrate diameter: as the duct area increases to


Figure 1
maintain the substrate to duct area ratio, the volumetric gas flow rate must also increase to sustain the same strain rate parameter (same quality diamond). Therefore, the economy of scaling the substrate diameter peaks at about nine centimeters, above which the required gas flow increases the cost.

## Cost vs Thermal Conductivity and Gas Ratio

The effect of quality, in terms of thermal conductivity, on CVD diamond deposition cost at different gas ratios can be seen in Figure 2. The reason for the rise in cost with thermal conductivity relates to the correlation between purity and thermal conductivity. For this simulation, the purity of diamond is assumed to depend on the ratio of atomic hydrogen to methyl radicals at the growth surface; this model predicts that thermal conductivity will increase with this ratio. Increasing the ratio of atomic hydrogen to methyl radicals, while keeping the proportion of acetylene to oxygen flow constant, requires an increase in the flow rate of the inlet gases. As shown in Figure 1, increasing flow rates leads to rising costs. From Figure 2, higher thermal conductivity diamond ( 1,000 to $1,500 \mathrm{~W} / \mathrm{mK}$ ) should be grown at lower ratios of acetylene to oxygen, dropping the cost by a factor of four when lowering this ratio from 1.10 to 1.02 at $1,500 \mathrm{~W} / \mathrm{mK}$. Also shown in Figure 2 is the cost of thermal conductivity. CVD diamond grown to achieve $1,000 \mathrm{~W} / \mathrm{mK}$ thermal conductivity costs about an order of magnitude less than diamond with $1,500 \mathrm{~W} / \mathrm{mK}$ thermal

Deposition Cost Vs. Thermal Conductivity and Subatrate Diamoter


NOTE: This graph is the result of current diamond deposition
theory, which relies on numerous simplifying assumptions.

Figure 3

## Conclusions

IBIS Associates has improved its predictive spreadsheet model of combustion flame chemical vapor deposition (CVD) diamond film fabrication. This report explains the improvements on the combustion flame deposition theory, and shows preliminary results of the economics of this CVD diamond process.

The changes to the model include the incorporation of thermal conductivity as an input to the model, allowing the user to specify the thermal properties of the diamond being formed. Also, the deposition theory in the model has been streamlined with the assistance of diamond deposition experts. Numerous inputs have been eliminated in this process, making the model easier to use.

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## Appendix

| PRODUCT SPECIFICATIONS Revision Date: 6/30/94 |  |  |  | gas database |  |  |  | Price <br> \$/SCM | No. of sunt/Mo Carbons SCM |  | Mo.Tank Rental | Price Update |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| Part Name 6 in | h. substr |  | Name | 0 | None |  |  | \$0.00 | 0.00 | OE+00 |  |  |
| Wafer Diameter | 15.24 | cm | DIAM | 1 | .19 Hydrogen | Alrco | 99.9981 | \$0.34 | 0.00 | 3E+04 | \$2,070 | 1/93 |
| Finished Wafer Thickness | 1,000 | um | THIK | 2 | .19 Hydrogen | Airco | 99.998\% | \$0.32 | 0.00 | 4E+04 | \$2,970 | 1/93 |
| Thermal Conductivity | 1,000 | W/mK | THERMCON | 3 | .1q Hydrogen | Airco | 99.9984 | \$0.30 | 0.00 | 1E+05 | \$4,500 | 1/93 |
|  |  |  |  | 4 | Liq Argon | Airco | 99.998\% | \$1.41 | 0.00 | 8E+03 | \$590 | 1/93 |
| Annual Production Volume | $1.0$ | (000/yr) | NUM | 5 | Liq Argon | Airco | 99.998\% | \$1.32 | 0.00 | 2E+04 | \$820 | 1/93 |
| Length of Production Run | $5$ | yrs | PLIfe | 6 | Liq Argon | Airco | 99.9984 | \$1.29 | 0.00 | 3E+04 | \$1,300 | 1/93 |
|  |  |  |  | 7 | Hydrogen | MG Ind. | 99.99994 | \$29.86 | 0.00 | OE+00 |  | 1/93 |
| process related factors - surface preparation |  |  |  | 8 | Ilydrogon | MG Ind. | 99.99964 | \$10.61 | 0.00 | OEtOO |  | $1 / 93$ |
| Process in Use? | 1 | [1-Y 0-N] | USE1 | 9 | Hydrogen | MG Ind. | $99.999 \%$ | \$10.28 | 0.00 | OE+00 |  | 1/93 |
| Dedicated Investment | 0 | [1-Y 0-N] | DED1 | 10 | Hydrogen | Air Prod. | 99.954 | \$1.59 | 0.00 | OE +00 |  | 1/93 |
| Process Yield | 95.0\% |  | YLD1 | 11 | Argon | MG Ind. | 99.99994 | \$33.09 | 0.00 | OE +00 |  | 1/93 |
| Average Equipment Downtime | 20.0\% |  | DOWN1 | 12 | Argon | Air Prod. | 99.99974 | \$37.33 | 0.00 | OE+00 |  | 1/93 |
| Direct Laborers Per Station | 0.50 |  | NLAB1 | 13 | Argon | Air Prod. | 99.9998 | \$11.74 | 0.00 | OE+00 |  | 1/93 |
|  |  |  |  | 14 | Argon | Alr Prod. | 99.9974 | \$2.03 | 0.00 | OE+00 |  | 1/93 |
| Substrate Material | 11 | [menu ] | MATLI | 15 | Methane | Alr Prod. | 99.994 | \$21.99 | 1.00 | OE+00 |  | 1/93 |
| Pleces Per Batch Process Time | 20 | pcs/batch | PCS 1 | 16 | Methone | Alr Prod. | 99* | \$13.76 | 1.00 | OE+00 |  | 1/93 |
|  | 60.00 | $\mathrm{min} / \mathrm{batch}$ | PTIME1 | 17 | Methane | Air Prod. | 934 | \$4.93 | 1.00 | OE+00 |  | 1/93 |
| Building Space Requirement | 250 | sqft/sta | FLR1 | 18 | Acetylene | Air Prod. | 99.64 | \$9.70 | 2.00 | OE+00 |  | 1/93 |
|  |  |  |  | 19 | Acetylene | Alr Prod. | 98.54 | \$5.30 | 2.00 | 0E+00 |  | 1/93 |
| process related factors - deposition |  |  |  | 20 | Acetylene | Pipeline | 98.54 | \$2.00 | 2.00 | OE+00 |  | 1/93 |
| Process In Use? | 1 | [1-Y 0-N] | USE2 | 21 | Hellum | Alr Prod. | 99.99954 | \$15.90 | 0.00 | OE+00 |  | 1/93 |
| Dedicated Investment | $0$ | [1-Y 0-N] | DED2 | 22 | Hellum | Air Prod. | 99.995\% | \$4.77 | 0.00 | OE +00 |  | 1/93 |
| Process Yield | 87.58 |  | YLD2 | 23 | Nitrogen | Air Prod. | 99.99964 | \$45.50 | 0.00 | OE+00 |  | 1/93 |
| Average Equipment DowntimeDlrect Laborers | 15.08 |  | DOWN2 | 24 | Nitrogen | MG Ind. | 99.9998 | \$9.23 | 0.00 | OE+00 |  | 1/93 |
|  | 0.40 | /sta | NLAB2 | 25 | Nitrogen | Alr Prod. | 99.9984 | \$1.24 | 0.00 | OE+00 |  | 1/93 |
|  |  |  |  | 26 | Liq oxygen | Alr Prod. | 99.54 | \$0.21 | 0.00 | 1E+00 | \$350 | 1/93 |
| Machine Power | 2 | kW | POW2 | 27 | oxygen | Air Prod. | 99.54 | \$0.58 | 0.00 | 0E+00 |  | 1/93 |
| Machine Load/Unload Time | $120$ | min/batch | PTIME2 |  |  |  |  |  |  |  |  |  |
| Available Deposition Time | 8,640 | hrs/yr | DAYHR2 |  |  |  |  |  |  |  |  |  |
| Heat Removal via Substrate Coolant Temp. Rise | $50.04$ | of total | hTRMV2 |  |  |  |  |  |  |  |  |  |
|  | $50$ | C | TEMP 2 |  |  |  |  |  |  |  |  |  |
| Heat Capacity of Coolant | 1.0 | cal/g/c | CP2 |  |  |  |  |  |  |  |  |  |
| Building Space Requirement | 1,500 | sqft/sta | FLR2 |  |  |  |  |  |  |  |  |  |
| Acetylene:Oxygen Ratio (R) $\begin{array}{r}\text { Oxygen } \\ \text { Acetylene }\end{array}$ | 1.05 | [1.02<x<1.1] | GRATIO2 |  | TRATE DATABA Substrate | Source | $\begin{gathered} \text { Price } \\ \text { s/ea } \end{gathered}$ | Thick um | Diam cm | $\begin{array}{r} \text { Etch } \\ \text { um/min } \end{array}$ | Life uset | $\begin{aligned} & \text { Price } \\ & \text { Update } \end{aligned}$ |
|  | 26 | [menu \%] | gasaz |  |  |  |  |  |  |  |  |  |
|  | 20 | [menu \$] | GASB2 | 0 | None |  | \$0.00 | 1 | 1.00 | 1.00 | 1.00 |  |
|  |  |  |  | 1 | silicon | S1-Toch | \$2.65 | 1270.00 | 5.08 | 20.00 | 1 | 1/93 |
| Oxygen Recycle Rate | 0.04 |  | RECYC2A | 2 | Silicon | Si-Tech | \$3.50 | 1270.00 | 7.62 | 20.00 | 1 | 1/93 |
| Gas Recycle Equipment Cost | 0.04 |  | RECYC2B | 3 | sillcon | S1-Tech | \$6.25 | 1270.00 | 10.16 | 20.00 | 1 | 1/93 |
|  | \#N/A | total | MCH2A | 4 | S1licon | Si-Tech | \$9.70 | 1270.00 | 12.70 | 20.00 | 1 | 1/93 |
|  |  |  |  | 5 | silicon | Si-Tech | \$18.60 | 1270.00 | 15.24 | 20.00 | 1 | 1/93 |
| Growth Correction Factor (f) | 0.50 |  | GCF2 | 6 | Silicon | Si-Tech | \$57.95 | 1270.00 | 20.32 | 20.00 | 1 | 1/93 |
| Substrate:Duct Area Ratio | 3.00 | $[1<x<-4]$ | SUBDUC2 | 7 | Silicon | Si-Tech | \$4.35 | 3810.00 | 5.08 | 20.00 | 1 | 1/93 |
| Substrate Distance:Duct Diam | 1.00 | [0<x<-10] | L:D2 | 8 | Silicon | Sl-Tech | \$8.15 | 3810.00 | 7.62 | 20.00 | 1 | 1/93 |
|  |  |  |  | 9 | silicon | 51-Tech | \$14.50 | 3810.00 | 10.16 | 20.00 | 1 | 1/93 |
| process related factors - etching |  |  |  | 10 | silicon | Si-Tech | \$22.65 | 3810.00 | 12.70 | 20.00 | 1 | 1/93 |










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| Average Inspection Time Percent Inspection Machine Cost | $\begin{gathered} 15.00 \\ 100 \\ \$ 50,000 \end{gathered}$ | min/batch /sta | $\begin{aligned} & \text { PTIME6 } \\ & \text { INSP6 } \end{aligned}$ MCH6 |
| :---: | :---: | :---: | :---: |
| Machine Power | 0.10 | kw | Pow6 |
| Building Space Requirement | 50 | sqft/sta | FLR6 |
| process related factors - inspection - thermal conductivity |  |  |  |
| Process In Use? | 1 | [1-Y 0-N] | USE7 |
| Dedicated Investment | 0 | (1-Y $0-N$ ) | DED7 |
| Process yield | 95.04 |  | YLD7 |
| Average Equipment Downtime | 5.04 |  | DOWN7 |
| Direct Laborers Per Station | 1.00 |  | nlab7 |
| Average Inspection Time | 15.00 | min/batch | PTIME7 |
| Percent Inspection | 1004 |  | INSP |
| Machine Cost | \$50,000 | /sta | мсн7 |
| Machine Power | 0.10 | kW | POW7 |
| Building Space Requirement | 50 | sqft/sta | FLR7 |
| OPTIONAL INPUTS |  |  |  |
|  | override | est1mate |  |
| Surface Preparation |  |  |  |
| Machine Cost | so | \$65,774 | /sta |
| Machine Power | 0.0 | 19.2 | kw |
| Deposition |  |  |  |
| Duct Area | 0.00 | 60.80 | sqcm |
| Total Gas flow Rate | 0 | 2,743 | s 1 m |
| Deposition Rate | 0.00 | 1.14 | $\mathrm{g} / \mathrm{hr}$ |
| Deposition Equipment cost | so | \$71 | ks/sta |
| Etching |  |  |  |
| Process Cycle Time | 0.00 | 0.18 | hrs |
| Chemical Requirement | \$0 | \$5.00 | /pe |
| Laser Trimming |  |  |  |
| Process Cycle |  |  |  |
| Lapping |  |  |  |
| Lapping Time | 0.00 | 111.11 | hrs |
| Lapping Plate Cost | so | \$869 | /ea |
| Lapping Machine Cost | so | \$11,939 | /sta |
| Lapping Machine Power | 0.00 | 4.2 | kW |
| exogenous cost factors |  |  |  |
| Direct Wages | \$13.33 | /hr | wac |
| Indirect Salary | \$50,000 | /yr | salary |
| Indirect:Direct Labor Ratio | 1.00 |  | ilab |
| Benefits on Wage and Salary | 35.08 |  | BENI |
| Working Days per Year | 360.00 |  | DAYS |
| Working Hours per Day (*) | 8.00 | /hr | HRS |
| Capital Recovery Rate | 104 |  | CRR |
| Capital Recovery Period | 5.00 | yrs | ELIFE |
| Building Recovery life | 20.00 | yrs | BLIFE |
| Working Capltal Period | 3.00 | months | WCP |








