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Economical Analysis and Optimization of a Low Pressure Chemical Vapor Deposition (LPCVD) Reactor

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Abstract: An economical analysis of the LPCVD hot wall tubular reactor functioning is presented including equipment amortization, clean room location, supplies, maintenance, labor, gas and energy consumption. From a technical point of view, CVD1 model is used to characterise the phenomena involved during polysilicon deposition, linking growth rate distribution to operating conditions. An optimization is then realized in three different cases with and without a temperature profile. By this study the main costs of CVD operation such as gases consumption and equipment amortization are identified, and the total cost has been drastically reduced by using a temperature profile.

1. INTRODUCTION

To realize thin layers for electronic components, the most widely used technique is chemical vapor deposition (CVD). From a general point of view, a CVD reactor always appears, more or less, as an enclosure in which convenient gases are put into contact with hot substrates.

Two kinds of CVD reactors are commonly used to deposit thin layers from reactive gaseous sources: the hot-wall reactor and the cold-wall reactors. The most interesting type for an economical analysis is the hot wall reactor because this geometry presents the highest capacity with more than one hundred wafers and constitutes the more often used apparatus in the microelectronics industries.

Many kinds of thin layers are elaborated in this type of equipment: pure polysilicon, in situ boron doped polysilicon, in situ phosphorus doped polysilicon, semi insulating polysilicon and silicon nitride. To develop a first economical analysis of CVD process, we have chosen the simplest case of pure polysilicon deposition.

In this paper, the model used to represent the phenomena involved in a CVD reactor during pure polysilicon deposition is firstly presented. In the second part, the different costs involved in a CVD operation are estimated and an economical criterion is defined. Lastly, an economical analysis of a CVD process is made and the main costs are put in evidence. An economical optimization is then realized.

2. INDUSTRIAL PROCESS MODELING

A complete CVD operation is not limited to the deposition phase (figure 1), it also includes preliminary steps (wafer loading, gas pumping, temperature stabilization) and final steps (bleeding, get back to atmospheric pressure, unloading). All these different steps have been considered to estimate the global cost of a CVD operation. But, except for deposition step, they have been all taken as constant periods and only the energy and the gas consumed during these steps have been estimated.

For the deposition step, geometry parameters and operating conditions are taken into account to estimate the silicon growth rate on each wafer, by using the CVD1 [1] model described below. A schematic view of the hot-wall tubular reactor is proposed in figure 2 and the main characteristics of reactor geometry are collected in table 1.
From a modeling point of view, in such a reactor, the substrates temperature can be considered to be imposed by the three zone furnace and even if independent of the operating parameters. Such a situation remains relatively simple, inasmuch no thermal phenomena have to be taken into account [1,2], and only the mass transport problem has to be solved.

For pure polysilicon deposition from silane, the overall stoichiometry of the reaction can be expressed as follows:

$$\text{SiH}_4(g) \rightarrow \text{Si}(s) + 2\text{H}_2(g)$$  \hspace{1cm} (1)

Experimental studies and previous modeling works [1,3] have clearly demonstrated that the deposit does not present noticeable radial non uniformities due to the fact that surface reactions are the rate-controlling factor of a convenient LPCVD regime, so it is not necessary to take into account the radial variation of the concentrations. As a consequence, the concentrations of the gaseous species can be considered uniform in every interwafer space. This explain why the LPCVD reactor has been considered as a series of continuously stirred tank reactor (CSTR), in which the gases are perfectly mixed, each reactor or cell being constituted by an interwafer space (figure 3), the corresponding internal wall of the tube and by the corresponding part of internal elements (wafer supports).
In each cell, silane consumption by reaction (1) results in silicon deposition on three places: on the tube wall, on the wafer carrier boat and on the wafer surface, the total surface is noted $S_T$. The equations describing the behaviour of the gas phase in the $i$th cell are the following:

- **Mass conversion of the $j$th species**:
  
  $$ F_{j,i} = F_{j,i-1} - R_{S_{j,i}} S_T $$

- **Molar fraction definitions**:
  
  $$ y_j = \frac{F_j}{\sum F_j} $$

- **Kinetic equations (consumptions)**:
  
  $$ R_{S_{j,i}} = f(y_{j,i}, T, P) $$

Several expressions for the polysilicon growth rate are available in the literature, the expression most frequently considered being that established by Wilke et al [4].

$$ R_S = \frac{K P_{SiH_4}}{1 + K_h P_{H_2} + K_s P_{SiH_4}} $$

With the corresponding rate constants:

- $K = 3.2 \times 10^{-3} \exp\left(\frac{-6800}{T}\right)$
- $K_h = 4.8 \times 10^{-8} \exp\left(\frac{-10000}{T}\right)$
- $K_s = 0.82 \times 10^{-10} \exp\left(\frac{-18000}{T}\right)$

This equation allows the calculation of the production or consumption terms for every species, the complete algebraic system is solved by an iterative method and the growth rate evolution along the wafer boat is calculated.

### 3. COST ESTIMATION AND CRITERION DEFINITION

The first step of this economical analysis has been devoted to an estimate of the various costs involved in a complete CVD operation. Three kinds of costs have been distinguished:

- **Constant costs** which are independent of functioning conditions and of yearly production. They consist in equipment amortization estimated by the straight line method (CAM) on five years and clean room cost which is proportional to occupied surface area (CEMP)

$$ C_{\text{constant}} = \text{CAM} + \text{CEMP} $$
Semi-variable costs which are independent of the operating conditions but dependent on the operation number per year ($N_{cycle}$). They are constituted by quartz costs (reactors tube, thermocouple tube, wafer boat) and preventive maintenance costs (cleaning of quartz tube, supplies and corresponding labor costs). To establish these expressions, the quartz and preventive maintenance costs have been summed on a year. The quartz cost, supposed to be directly proportional to the cycle number, has then been reduced to a cost per year. On the contrary, the preventive maintenance costs are not directly proportional to the cycle number, because preventive maintenance is realized systematically every twenty cycles with a constant cost per intervention.

\[ C_{\text{semi-variable}} = C_{\text{quartz}} + C_{\text{main}} \]

\[ C_{\text{semi-variable}} = a_1 N_{cycle} + a_2 \text{integer}\left[\frac{N_{cycle}}{20}\right] \]

- Variable costs depending directly on operating conditions, including labor (CMD), energy (CEN), gas consumption (CG) and non satisfactory wafers. The labor costs involve the human intervention on the one hand for wafer loading and unloading which are proportional to the wafer number, and on the other hand, for the process supervision which is only proportional to the cycle number. The energy cost is proportional to the heating power (temperature dependent), the heating time (remained constant) and the kWh cost. For gas consumption three different contributions have been distinguished corresponding to three different states (loading and unloading (CG1), pressure changes (CG2) and deposition (CG3). In all cases, the cost is proportional to the total gas flow used for each step, the step duration, the gases cost and the cycle number.

\[ C_{\text{variable}} = \text{CMD} + \text{CEN} + \text{CG} \]

\[ \text{CMD} = [a_3 N_w + a_4] \text{sho} N_{cycle} \]

\[ \text{CEN} = \text{Pch} \cdot \text{tch} \cdot C_{kw} \]

\[ \text{CG} = \text{CG1} + \text{CG2} + \text{CG3} \]

\[ \text{CG1} = Q_{N_2}^1 \text{tch} \cdot \text{CG}_{N_2} \]

\[ \text{CG2} = \sum_{i=\text{step}} \left[ Q_{N_2}^i \Delta i \text{time} \cdot \text{CG}_{N_2} \cdot N_{cycle} \right] \]

\[ \text{CG3} = \left( O_{\text{SiH}_4}^0 \cdot \text{CG}_{\text{SiH}_4} + Q_{N_2}^0 \cdot \text{CG}_{N_2} \right) \cdot \text{tdep} \cdot N_{cycle} \]

For non satisfactory wafers covered by a too thin or too thick layers $N_w$, a penalty function is added to the total cost.

Finally, the economical criterion has been defined as the summation of the different costs detailed above, divided by the yearly production of convenient wafers.

\[ \text{criterion} = C_{\text{deposition}} = \frac{C_{\text{total}}}{[N_w - N_k] N_{cycle}} \]

To illustrate the present study, a particular CVD unit has been chosen in a microelectronic industry plant. All the costs have been estimated as follows:
4. OPTIMIZATION PROCEDURE

The economical criterion previously defined has been minimized by using a commercial code of IMSL library called subroutine D2ONF. Some constraints have been applied to the operating variables to maintain them in LPCVD conditions commonly used for undoped polysilicon deposition: pressure between 0.1 and 1.0 Torr, temperature between 823.0 and 923.0 K, total gas flow rate between 50.0 and 1000.0 sccm and deposition time between 5.0 and 180.0 minutes. For the temperature profile along the wafer boat, three cases have been studied: a constant profile, a linear profile with a positive slope limited to 10 K, and a free linear profile without limitation.

These constraints on operating parameters insure a polycrystalline silicon deposit without powder formation in the gas phase, according to the experimental studies reported in the literature [5].

From a technical point of view, another constraint has been added to distinguish convenient wafers from others. For a satisfying wafer, the layer thickness must be between 5700 Å and 6300 Å.

In the second case, the restriction of the thermal gradient along the wafer boat to 10 K, ensures the silicon layers to present nearly the same crystalline structure and so electrical properties.

5. RESULTS AND DISCUSSIONS

For the three different types of thermal profile along the wafer boat, the economical criterion has been minimized considering that the total yearly production of convenient wafers is free, and that number of operation per year is deduced by dividing the total time allowable in one year by the time needed for a CVD operation. The different parameter values obtained for the optimum criterion are collected in table 2. The detail of the different costs are also summarized in table 3.

<table>
<thead>
<tr>
<th>Pressure (Torr)</th>
<th>Temperature (K)</th>
<th>Temperature slope (K/m)</th>
<th>Silane flow rate (sccm)</th>
<th>Deposition time (min)</th>
<th>criterion (F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>case 1</td>
<td>1.0</td>
<td>871.9</td>
<td>0.0</td>
<td>596.33</td>
<td>55.26</td>
</tr>
<tr>
<td>case 2</td>
<td>1.0</td>
<td>887.5</td>
<td>15.79</td>
<td>588.43</td>
<td>33.42</td>
</tr>
<tr>
<td>case 3</td>
<td>1.0</td>
<td>886.5</td>
<td>29.45</td>
<td>502.43</td>
<td>32.24</td>
</tr>
</tbody>
</table>

Table 2: Values of the operating parameters obtained for the optimum criterion.

<table>
<thead>
<tr>
<th>Ncycle/year</th>
<th>CAM</th>
<th>CEMP</th>
<th>Quartz</th>
<th>Cmaint</th>
<th>CMO</th>
<th>CEN</th>
<th>CG</th>
</tr>
</thead>
<tbody>
<tr>
<td>case 1</td>
<td>3132</td>
<td>360</td>
<td>30</td>
<td>140.94</td>
<td>143.41</td>
<td>245.33</td>
<td>31.42</td>
</tr>
<tr>
<td>case 2</td>
<td>3723</td>
<td>360</td>
<td>30</td>
<td>167.56</td>
<td>170.33</td>
<td>291.44</td>
<td>33.08</td>
</tr>
<tr>
<td>case 3</td>
<td>3758</td>
<td>360</td>
<td>30</td>
<td>169.11</td>
<td>171.9</td>
<td>294.14</td>
<td>33.31</td>
</tr>
</tbody>
</table>

Table 3: Detail of the different costs included in a CVD operation.

The first interesting result is that in all cases, the optimum pressure value is the upper boundary 1 Torr imposed for operating pressure. It means that a high pressure is suitable from a kinetic point of view.

The optimum values obtained for the other variables have been found to be intermediate between the lower and upper limits selected.

If we compare now the different kinds of cost, for example in the case of an isothermal operation, we can note that the major costs are the equipment amortization (26%), labor (18%) and gas consumption (32%). As a first concluding remark, the reduction of gas consumption can be considered as the first way of the total cost reduction (figure 4).

When a temperature profile is possible for CVD operation, in the two different cases studied, the criterion is drastically reduced (more than 15%). This result can be firstly surprising if we only consider that the mean temperature has been increased of 15 K (figure 5), increasing also the partial cost of energy, but in the same time, the deposition time has been strongly reduced. If we look at the evolution of the silicon layer along the wafer boat illustrated by figure 6, we can observe that the continuous decrease of the thickness for isothermal case is no longer valid for thermal profile cases. The natural depletion of silane along the wafer boat is balanced by an increase of the temperature (and of course of the silicon growth rate)
at the end of load. For nearly same values of total gas flow rate for cases 1 and 2, the deposition time is drastically reduced traducing a better use of the silane gas flow rate. So the number of CVD operations is increased (3132 to 3723) and the yearly production also.

If we consider now the non isothermal cases, some small changes appear. As previously, the criterion value is reduced by a reduction of the deposition time and by a better use of total silane flow rate but the number of CVD operations is slightly changed (from 3723 to 3758). On the contrary the corresponding needed gradient of temperature is enough high (15 K), conducing us to prefer the second case to maintain nearly the same crystalline structures for all thin layers deposited.

Fig. 4: Different costs of silicon CVD deposition (case 1)

Fig. 5: Temperature profile in three studied cases.

Fig. 6: Evolution of the silicon layer thickness along the wafer boat.
6. CONCLUSION

In this paper, a first economical analysis has been made to estimate the total cost of a CVD operation. Among the various costs taken into account, the main costs for polysilicon deposition as equipment amortization and gases consumption have been put in evidence. To reduce the partial costs linked to gases consumption, a technical and economical optimization of the hot wall reactor functioning has been made by using CVD1 model. For a free yearly production, an important reduction of total cost has been obtained by using a temperature profile along the wafer boat. The better employment of the total gas flow rate of silane by a temperature increase along the wafer boat, reduces the time deposition and allows to treat a large number of wafers per year.

**List of symbols**

- $a$: Temperature profile slope (K/m)
- $t_{dep}$: Deposition time (minutes)
- $N_w$: Total number of wafers per cycle
- $P$: Pressure (Torr)
- $T$: Temperature (K)
- $Q$: Gaz flow rate (sccm)
N_{cycle} Total yearly cycle number
P_{ch} Heating power (kW)
\tau_{ch} Heating time (h)
Sho Labor cost (kF/h)
C_{kw} Electrical energy cost (kF/kWh)
N_w Number of non satisfactory wafers
\Delta t_{me} Step duration (minutes)

References