XFACT : a furnace analysis and characterization tool

Citation for published version (APA):

Kumar, R. C. K., & Pineda de Gyvez, J. (1995). XFACT : a furnace analysis and characterization tool. *IEEE Transactions on Semiconductor Manufacturing*, 8(1), 84-87. <https://doi.org/10.1109/66.350761>

DOI:

[10.1109/66.350761](https://doi.org/10.1109/66.350761)

Document status and date:

Published: 01/01/1995

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

[Link to publication](#)

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license above, please follow below link for the End User Agreement:

www.tue.nl/taverne

Take down policy

If you believe that this document breaches copyright please contact us at:

openaccess@tue.nl

providing details and we will investigate your claim.

Correspondence

XFACT: A Furnace Analysis and Characterization Tool

Ravi C. K. Kumar and Jose Pineda de Gyvez

Abstract—The diffusion furnace is one the most important and complex process equipment in the process line and efforts towards characterizing it will be well worth the effort. A CAM package for wafer temperature map reconstruction using only a few sampled data points is proposed. The software is completely generic and has no affiliation to any make of furnace. The data required for simulation can easily be obtained from the actual piece of equipment. Interpolation techniques with high accuracy are used for developing the temperature contours inside the furnace using a modified version of the Lagrange's interpolation technique.

I. INTRODUCTION

High temperature processes in VLSI manufacturing have always posed problems to process engineers. The cylindrical furnace, popularly referred to as the "diffusion furnace", is one of the most important pieces of equipment for any VLSI process. For a pictorial display of a typical cross section of the furnace the reader is referred to Fig. 1 [1]. Knowledge of temperature distributions can enlighten the process engineer in several areas, including maximum heating and cooling rates, the relevant control algorithm to be applied, and the parameters for the algorithm. Several attempts have been made to model the furnace temperature distribution [1]–[3]. These works are highly theoretical, model specific, and many times loss of generality has made their utility difficult.

The critical importance of temperature non-uniformity has already been recognized as a decisive factor in process equipment like RTP furnaces and several attempts have been made to characterize these non-uniformities [4], [5]. Yet diffusion furnaces have not received the same attention, primarily because it is extremely difficult to non-invasively measure temperature. The temperature distribution at several points in the furnace is different due to a number of factors. The furnace is cooler at the ends. The temperature is also higher closer to the quartz walls than along the axis. The distribution constantly changes over time due to variations in gas flow and introduction of wafers, etc. Also, due to the temperature, the quartz tube sags so that wafers are closer to the heating element at one point and further away from them at other points. The wafers are mounted on a boat which will have a significant impact on the distribution inside the furnace. The first wafer to enter the furnace is likely to experience a different temperature distribution. For all these reasons the process outcome on one wafer will never be the same as another kept at a different point or for a different duration.

An important consideration in the simulation is the collection of temperature samples from within the furnace. Temperature samples can be collected as part of routine maintenance operations on the furnace. To obtain a comprehensive characterization, a sampling of the temporal and spatial data of the temperatures inside the furnace is needed. An obvious advantage of this approach is that the data includes all the environmental disturbances—such as thermal flow and temperature gradient—embedded in the furnace's chamber.

Manuscript received October 6, 1993; revised February 27, 1994.

The authors are with the Department of Electrical Engineering, Texas A&M University, College Station, 77843 TX USA.

IEEE Log Number 9405233.

Fig. 1. Data reconstruction process. (a) First stage. (b) Second stage. (c) Interpolation approach.

To properly simulate the effect of environmental conditions on a given wafer in the chamber, at least two temperature maps must be available. Interpolated maps can be built up for any point required using these data and used to determine the outcome of the process. Naturally, from any temporal/spatial map obtained, temperatures for each isothermal surface element can then be taken and be used to model a given process step across the entire surface of the wafer.

Fig. 2. Several phases of the wafer map reconstruction technique. (a) Initial set of points. (b) After first stage interpolation. (c) After second stage interpolation. (d) Example using actual temperature values.

For XFACT the samples in each set must be collected at points equidistant from the center of the wafer. Hence all data points fall on a set of concentric circles on the wafer surface. There is no limit on the maximum number of data sets; the more used, the better the samples. However, the theoretical minimum limit is two sets of data, with two samples in each set. The upper limit is defined by the number of samples one can extract from the furnace without appreciable error.

II. TEMPERATURE RECONSTRUCTION BASED ON WAFER MAPS

The wafer is modeled as a set of isothermal surface elements that follow a grid-like structure. For simulation purposes the depth of the wafer is not important. Temperature samples taken from the furnace are inserted into the grid model of the wafer and used as starting points to derive the wafer's temperature map. In XFACT, data is built using a two stage interpolation technique. The first stage is built up directly from the data samples. This stage creates newly interpolated points concentric with the initial samples. The second stage uses points obtained from the first stage and reconstructs the temperature of the entire furnace cross section. Temperature profiles for any location in the furnace can be obtained either by direct extraction of samples at the location or by interpolating with profiles obtained in the neighborhood of the desired location. Similarly either samples taken at the actual time, or taken at nearby time intervals can be used for developing the profile for a given time instance. Hence it is possible to explore any spatial/temporal location within the furnace.

Interpolation is a common procedure in numerical analysis. The goal is, given a set of values $(T_0, d_0), (T_1, d_1), \dots, (T_n, d_n)$, satisfying a relation $T = f(d)$, where the nature of $f(d)$ is not known or is too complicated, find a value for T given the corresponding d . Several numerical techniques exist for this purpose, such as Newton's forward

and backward formulas, Stirling's central difference formulas, and Lagrange's interpolation technique [6], [7]. We adopt the latter procedure since the intervals are nonuniform.

In the first stage interpolation, the values of all points on the same concentric position are computed from the given samples. This is illustrated in Fig. 1(a) for first order interpolation. The relation between any point and the sample points in this case is given by

$$T_r = \sum_{i=0}^{n-1} T_i \prod_{j=0, j \neq i}^{n-1} \frac{\theta_r - \theta_j}{\theta_i - \theta_j} \quad (1)$$

where T_i are temperatures equidistant from the wafer center, making angles θ_i w.r.t. the horizontal axis. T_r represents all points between them on the same circle. In the second stage, all the points between zones are interpolated using the points obtained from the first stage. This is illustrated in Fig. 1(b). For every remaining point on the grid, an array of points is created for interpolation. There is one point from each zone in this array, with the same angle as the test point. An anchor is a point on this array immediately behind the test point along the direction of interpolation. Similarly, tail points are the n points on the array which follow the test point. The direction of interpolation is governed by the maximum length of the tail-points array. The equation here is similar to (1)

$$T_r = \sum_{i=0}^{n-1} T_i \prod_{j=0, j \neq i}^{n-1} \frac{d_r - d_j}{d_i - d_j} \quad (2)$$

The distances of points from the center of the wafer are represented by d_i . The accuracy of the interpolated map depends critically on the order of interpolation. For lower orders the accuracy would be limited. Higher order interpolations give better accuracy up to a point.

Fig. 3. CPU time complexity.

But they are computationally expensive and need more data points. The latter factor is crucial, since it is limited by the technology available for drawing the temperature from the furnace. In XFACT, the order for the first stage interpolation can be arbitrarily large since the sample distribution is circular and the $(n+k)^{\text{th}}$ point of the array would correspond to the k^{th} point. However, for the second stage, interpolation is a function of the number of zones. The maximum possible order of interpolation is equal to the number of data points available after the point in question. For a linear array this goes on decreasing, and so the maximum interpolation possible is different for different points. For interpolation in the reverse direction however, higher orders of interpolation are possible for points coming later, since here the maximum interpolation order is defined by the number of data points prior to a point. In other words, the maximum order of forward interpolation linearly decreases for all points while the order for reverse interpolation linearly increases. Since the accuracy of interpolation is independent of the interpolation direction, it can be so chosen that a minimum nonsingular order can be assured for all points when the interpolation contains at least three points. The procedure we adopted ensures at least an order of $n/2$ given n points. This is illustrated in Fig. 1(c). For all points until the n^{th} point, at least $n/2$ order is assured. For the points between $n/2$ and $n/2 + 1$, the maximum possible order is $n/2$. Beyond this reference, interpolation can be performed in the reverse direction. This can assure $n/2$ points. The direction is always outward from the wafer center for points inside the smallest zone, but the procedure involves extrapolation since there can be no computed points within the inner most zone. The anchor will be the first point of the interpolation array, and the tail-points will be the next n points. Similarly for all points outside the largest zone, extrapolation proceeds towards the wafer center. The actual results of a typical interpolation process are shown in Fig. 2(a)–(c). A full scale interpolation is possible with only two points per zone and two zones, *i.e.*, with 4 points. But obviously the truncation error would be very large. This error, if known would be useful in finding the order required for the simulation. Higher orders need not necessarily imply greater accuracy. Mathematically the error is given to be

$$\varepsilon_n = \frac{f^{n+1}(d)}{(n+1)!} (d-d_1)(d-d_2) \cdots (d-d_{n+1}). \quad (3)$$

Here f represents the equation which describes the curve describing the distribution of temperature; f^n represents the n^{th} derivative of this equation. A few rules of thumb can be derived on inspecting the equation. If the samples indicate a very large range or steep variations, a higher order would be justified since the error would be large because of the large value of the derivative function at that point. A simulation for estimating the error due to interpolation yielded a simple truth. If the order of the function f is known or at least estimable, an interpolation of the same order will yield negligible error if f is a pure quadratic. But if f is a mixed quadratic, one would have to determine the highest significant order, going by the assumption that higher orders have lesser weight, and then use the same order for simulation. Higher orders would not improve simulation results. A couple of observations are outlined next. i) If the functional relationship of the values is a n^{th} pure quadratic, then an n^{th} order interpolation is guaranteed to yield zero errors. Lesser orders will yield errors. ii) If the function is a mixed quadratic, then the order to be chosen is a compromise between the accuracy required and the computation affordable. Higher orders contribute less to accuracy, and so by defining a cutoff at order n , accuracy is guaranteed till the cutoff by choosing an interpolation order of n . iii) Offsets in a function have no effect on the interpolation results; accuracy is independent of the direction of interpolation. A trial and error approach is required to obtain the optimum interpolation order in XFACT. However since most temperature relations involve the fourth order, it would be safe to assume an order of at least 4. This would require at least 5 zones of 5 data points each.

III. SIMULATION RESULTS

Measured temperature values are used for illustration purposes [8]. In this case, interpolation was conducted for the wafer on position 3 using wafers at positions 1 and 6 as reference. Simulated results are presented in Fig. 2(d).

In XFACT, the number of isothermal surfaces or the granularity of the simulation is user defined. The finer the required resolution the more the granularity. But the quantization error has the same relation in the inverse sense. The simulation time has an $O(n^2)$ complexity, where n is the resolution specified. The cost of higher resolutions in terms of computational intensity is demonstrated in Fig. 3. The timings refer to simulations conducted on a SPARC II workstation.

IV. CONCLUSION

A generic simulator to characterize a diffusion furnace has been outlined. The simulator can handle most kinds of furnaces. The simulator fills a need for knowledge in between the area of process modeling and equipment control. The central idea of collecting spatial data to characterize furnace eccentricities can be employed with almost any process model for which the furnace is used, *e.g.*, annealing or diffusion.

REFERENCES

- [1] B. J. Van Schravendijk *et al.*, "Modeling and control of the wafer temperature in a diffusion furnace," *J. Appl. Phys.*, vol. 61, p. 1620, 1987.
- [2] Mokuya Kinji *et al.*, "Characteristics of the transient wafer temperature distribution in a furnace for semiconductor fabrication processes," *Electron. Telecomm. Jpn.*, vol. 70, no. 12, p. 59, 1987.
- [3] ———, "Transient model of wafer temperature in a furnace for semiconductor fabrication process," *Electron. Telecomm. Jpn.*, vol. 70, no. 12, p. 59, 1987.
- [4] H. A. Lord, "Thermal and stress analysis of semiconductor wafers in a RTP oven," *IEEE Trans. Semicond. Manuf.*, vol. 1, no. 3, Aug. 1988.
- [5] S. Wood *et al.*, "Pyrometer modeling for rapid thermal processing," *SPIE Rap. Ther. and Rel. Proc. Techs.*, vol. 1393, p. 337, 1990.
- [6] V. Rajaraman, *Computer Oriented Numerical Methods*, 2nd edn. India: Prentice-Hall, 1990.
- [7] A. Ralston, *A First Course in Numerical Analysis*, 1st edn. New York: McGraw-Hill, 1965, p. 339.
- [8] T. A. Badgwell *et al.*, "In situ measurements of wafer temperatures in a low pressure chemical vapor deposition furnace," *IEEE Trans. Semicond. Manu.*, vol. 6, no. 1, p. 65, Feb. 1993.