Applications of Natural Exponential Functions in Semiconductor Processes

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Abstract

Semiconductor IC fabrication involves many different processes, such as dielectric film deposition, metal film deposition, photolithography, etch, implant, CMP (Chemical Mechanical Polish), etc. To achieve a consistent process, either tools or wafers or both require preconditions. Although these processes are entirely different, those pre-conditions have a common goal of reaching a stable status. Understanding this procedure of reaching a stable status is important in process optimization for both quality and cycle time point of views. In this paper, two universal natural exponential functions are discussed for simulating a stabilization procedure of process pre-conditions and processes which have similar characteristics.

INTRODUCTION

Semiconductor IC fabrication involves many different processes, such as dielectric film deposition, metal film deposition, photolithography, etch, implant, CMP (Chemical Mechanical Polish), etc. There are many research publications and books [1], [2] which introduce these processes. There are also different process simulation tools or software which can describe and predict an individual process and process integration. However, to achieve a consistent process, either tools or wafers or both require preconditions. For instance, a metal target of PVD (Physical Vapor Deposition) needs to be pre-sputtered to certain KW-hours (Kilowatt hours) before running production wafers. A wafer needs to be heated to a certain temperature before CVD (Chemical Vapor Deposition) film deposition can be started. There is lack of literature which discusses these preconditions. Although these processes are entirely different, those pre-conditions have a common goal of reaching a stable status. To understand this procedure of reaching the stable status is important in the process optimization for both quality and cycle time point of views. In this paper, two universal natural exponential functions are discussed for simulating the stabilization procedure of process pre-conditions and processes which have similar characteristics.

NATURAL EXPONENTIAL FUNCTIONS

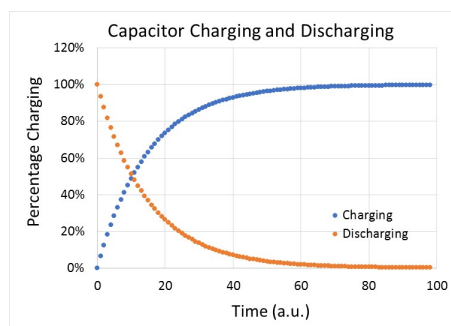
The simplest exponential function is e^x which has many applications with different forms in science, engineering, and manufacturing. One of the most famous or common formulas is the one used for describing phenomena of capacitor charging or discharging as the equations in Eq. (1) and Eq. (2).

$$Y = (Y_f - Y_i) * (1 - e^{-(t-t_0)/\tau}) + Y_i \quad (1)$$

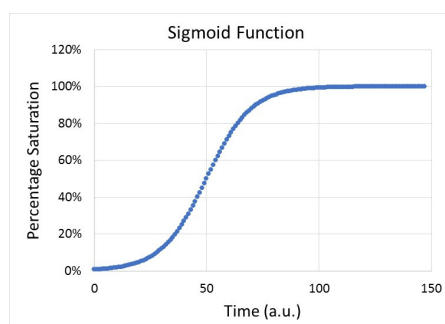
and

$$Y = Y_f + (Y_i - Y_f) * e^{-(t-t_0)/\tau} \quad (2)$$

Where Y_i is the initial status of a pre-condition procedure, Y_f is the final equilibrium status, τ is the time constant, t is the time and t_0 is the time off set.



(a)



(b)

Fig. 1. (a) Capacitor charging and discharging curves; (b) Sigmoid curve

The other useful exponential function is the Sigmoid function as in Eq. (3).

$$Y = \frac{1}{1 + e^{-(t-t_0)/\tau)}} \tag{3}$$

Figure 1a shows the curves of both the charging and discharging procedures with $|Y_f - Y_i| = 1$ and Figure 1b is the curve of a Sigmoid function. The common signature of the curves is Y approaches an equilibrium status with time. The difference of the curves is at the beginning section of the curves, thus they can be used for simulating different pre-condition procedures.

APPLICATIONS

Direct application of the exponential charging or discharging function in semiconductor process is wafer heating or cooling, because of the similarity of electrical and thermal circuitries. This was discussed previously in Ref. [3], [4]. In this paper, we will discuss applications of the exponential functions in other process areas.

Case 1: Moisture Absorption

Moisture absorption is a diffusion phenomenon which can be described by Fick's second law of diffusion [1], [2]. The renowned application of Fick's second law of diffusion is the dopant pre-dope and drive-in diffusion in semiconductor doping process. In dopant diffusion, it is with either a limited or a constant source assuming an infinite substrate volume as the conditions. The function solution is a dopant distribution in a substrate at time t.

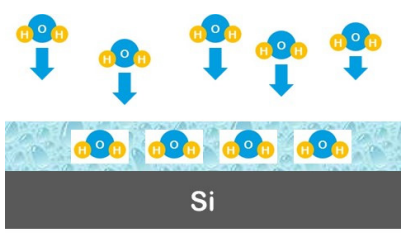


Fig. 2. Diagram of polymer film on a Si substrate

This is not the case for film moisture absorption, because there is a limited volume which moisture can be diffused in as shown in Figure 2. Also, what we are interested in is total moisture absorbed at different times, which requires an integration over the entire distribution at each time t. This makes the solution even more complicated. Practically for simplification, what we want is to use a simple formula to describe the moisture absorption in a film. In this situation, water molecules diffuse into a film from the surface by filling the micro pores. There will be a distribution gradian from the film surface to the interface of the film and Si substrate. The molecules will stop further moving once they arrive at the interface. Since there are only certain pores in the film available for moisture molecules, eventually all the micro pores will be filled with water molecules and the absorption will reach an equilibrium status. Figure 3 shows results (blue dots) of an experiment of moisture absorption and time dependence. This dependence can be well fitted with a natural exponential function (red line) similar to the electrical charging function, as what is also shown in the figure. From this dependence, we can determine how long material can be left in a room environment without significant moisture absorption.

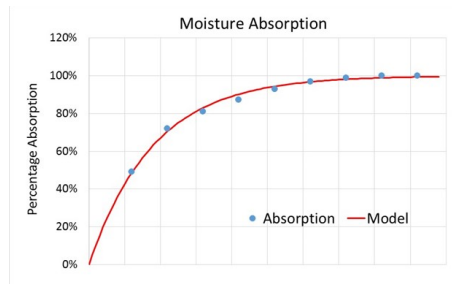


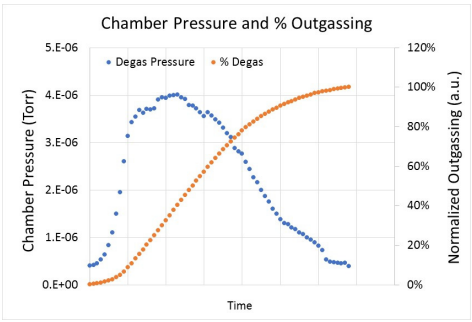
Fig. 3. Time dependence of moisture absorption experiment (blue dots) fitted with an exponential function model (red line)

Case 2: Outgassing

Outgassing is an opposite physical phenomenon from moisture absorption. It is important to know how long outgassing will take if a material is fully absorbed with moisture. There are many different methods to measure this outgassing. One is called Pressure-Time method [5] as described in Eq. (4).

$$P(t) = \frac{k}{S} R(t) + P_0 \tag{4}$$

P(t) is the pressure at time t, P_0 is the baseline pressure, R(t) is the outgassing rate at time t, S is the pumping speed, and k is a constant. The curve with blue dots in Figure 4(a) is the experimental outgassing pressure as a function of time. With Eq. (4), the outgassing amount at time t in a vacuum environment can be calculated with the integration of the area under the curve of P(t) ~ t. The normalized integration result is shown as red dots in Figure 4(a) also. Figure 4(b) has three curves. The blue dot curve is the normalized experimental outgassing result. The red dot-bar curve is a fitting with an exponential function Eq. (1). The short green bar curve is a fitting with Sigmoid function Eq. (3). Although Sigmoid function is not the direct solution of Fick's second law of diffusion, it has a very good fit over the entire time range. The exponential function has its weakness of fitting the beginning section, but the fitting above 40% outgassing is very good, which is the region we are more concerned about regarding to the outgassing procedure.



(a)

(b)

Fig. 4. (a) Chamber pressure and normalized outgassing. (b) Normalized experimental outgassing result (blue dot) with fitting of both exponential charging function (red dot-bar) and Sigmoid function (green bar)

Case 3: Optical Measurement Error Rate

Optical measurement is one of the important metrology methods widely used in semiconductor process. Figure 5 is a simplified diagram of an optical metrology tool. There is a light source, which can be either a laser source or a light bulb. The emission light shoots on a sample. The reflected or diffracted light from the sample is collected by a detector and analyzed with a signal analyzer. Error rate is an important criterion for an optical metrology tool. The error rate can be time dependent, especially at the beginning stage after each time turned on. This is because the laser or light bulb source requires warming up. This warming up is a heat procedure, which should follow the exponential charging function [3], [4]. A similar time dependence of the error rate should be expected and is shown in Figure 6. The blue dots are experimental data. The red line is the fitting with an exponential discharging function as in Eq. (2). A "zero" error rate can be achieved after a certain time of light source stabilization. Warm up for all tools should follow the similar model here.

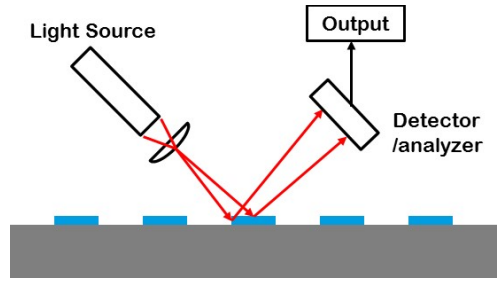


Fig. 5. A simplified diagram of an optical metrology tool

Fig. 6. Time dependence of measurement error rate of an optical metrology tool.

Case 4: CMP Polish Rate

In addition to process preconditioning, other processes can also be described with the exponential functions. CMP, a surface planarization process, is one of them. Figure 7 shows a diagram of the CMP process schematic. A wafer is mounted on a rotating head with pressure pushing down. The wafer surface faces down touching the slurry and polish pad, which are on a rotation station. For a flat surface like a monitor wafer, polish rate is a function of slurry type, polish pad type, rotational speeds of both head and station, etc. However, once these are fixed in a process, the polish rate then only depends on the pressure added. However, this is not true for a real production process.

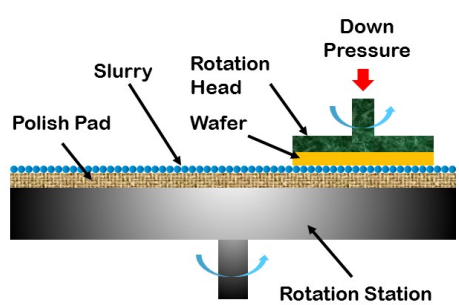


Fig. 7. A diagram of CMP process schematic

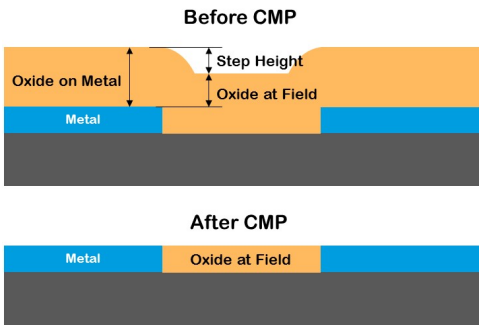


Fig. 8. A schematic of a production wafer before and after CMP polish

Figure 8 is a schematic of a production wafer before and after the CMP process. There is a step height between oxide on metal and oxide at field area, which will be removed with CMP process. This is because the pad pressure on the oxide above the metal area is higher than that in the field area due to the step height difference. The oxide above the metal will be polished faster than the oxide in the field area. Eventually, the step will be polished away. The polish rate of the oxide on the metal area is a function of the step height or the polish time as shown in Figure 9. The experimental results are the blue dots. This time dependence can be also simulated with an exponential discharge function (red line).

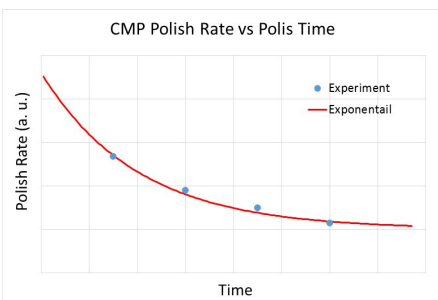


Fig. 9. CMP polish rate with a topology surface

Time Constant:

Beside the four cases discussed above, there are many other processes which have similar characteristics and can be simulated with an exponential function, such as a deposition rate changing with number of precondition wafers run in a CVD process, a photo CD as a function of develop time, etc.

The most important parameter of the simulation with an exponential charging function is the time constant . Mathematically, the time constant is the time of the change reaching 63% of an equilibrium status and 2 is the time of reaching 86%. Physically, time constant is related to change rate.

Time constant depends on multiple parameters in a process. In moisture absorption, it is a function of humidity, temperature, and pressure. Therefore, to change the moisture absorption, we need to change one of these three conditions. In the case of a CMP process, it is a function of pad type, rotational speed, slurry type, substrate material, pattern density, etc. In a real production situation, substrate material and pattern density are not changeable. Therefore, to shorten a process time or time constant, pad type, rotational speed, or slurry type must be adjusted.

Theoretically, an equilibrium status cannot be reached and only be infinitely close. So, practically we need to know when it can reach a status which a process can tolerate. The balance of the time and process quality is what we pursue.

CONCLUSIONS

In this paper, we discussed the applications of the different natural exponential functions in different semiconductor process areas including metrology measurement. This exponential model fitting and/or simulation can help the optimization between process cycle time and product quality.

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REFERENCES

[1] Y. Nishi, et al, *Handbook of Semiconductor Manufacturing Technology*, 2000

[2] S. Wolf, et al, *Silicon Processing – for the VLSI Era, Volume 1 – Processing Technology*, 1986

[3] X. Huang, et al, *Thermal Property of WNiSi Thin Film Resistor*, CS MANTECH, 2014

[4] X. Huang, et al, *A Simulation of Wafer Temperature-Time Profile in PVD Process Using an Exponential Model and Its Applications*, CS MANTECH, 2015

[5] P. Chiggiato, *Outgassing*, TS-MME Coating, Chemistry, and Surfaces CERN, 2006

ACRONYMS

CMP: Chemical Mechanical Polish
CVD: Chemical Vapor Deposition
PVD: Physical Vapor Deposition
CD: Critical Dimension