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Heat transport in cold-wall single-wafer low pressure chemical-vapor-deposition reactors

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A model is formulated to understand and predict wafer temperatures in a tungsten low pressure chemical-vapor-deposition (LPCVD) single-wafer cold-wall reactor equipped with hot plate heating. The temperature control is usually carried out on the hot plate temperature. Large differences can occur between the susceptor and the wafer temperature, especially at the typically low pressures for LPCVD systems. Verification of the model was done by measurements of the true wafer temperatures as a function of total pressure, gas composition, gas flow, and coatings of wafer and susceptor. A good agreement between model and measurements was found by considering the heat transport by radiation and gas conduction.

I. INTRODUCTION

The heat transport in a tungsten (W) low pressure chemical-vapor-deposition (LPCVD) cold-wall system has been described previously by Schmitz, Suijker, and Buiting.¹ In that work large differences in temperature between susceptor and wafer were reported. The aim of the present work is to model the heat transport in cold-wall reactors and validate this model with measurements. In that way it may be possible to gain more insight in what wafer temperatures can be expected for certain circumstances. We will focus on a W LPCVD system, but the results can be generally adapted to other cold-wall systems.

Knowledge of the true wafer temperature in the case of W LPCVD is important because a temperature difference between wafer and susceptor can cause selectivity loss (i.e., deposition on susceptor). Further, for experimental work it is important to know what the wafer temperature will do if process conditions are changed. The knowledge of the wafer temperature behavior in these cold-wall reactors will lead to a better understanding of the influence of process parameters on, for example, growth rate.

It will be shown that the temperature difference between wafer and susceptor can be minimized by adapting the wafer and susceptor coatings, gas compositions, and the total pressure; but even after minimizing the temperature difference effect, there will remain a considerable temperature difference between the wafer and susceptor. This is inherent to this type of reactor.

II. THEORY

The heat transport in cold-wall reactors can be described by four mechanisms; these are radiation, gas conduction, gas convection, and solid-solid conduction. As will be shown, in LPCVD conditions, the convective heat transfer due to the gas flow is of minor importance. In our

reactor the wafer is not clamped against the susceptor, so there is no real solid-solid contact, and thus the solid-solid conduction between susceptor and wafer is small. Therefore in the model only the heat transport by (i) radiation and (ii) gas conduction is considered.

A. Radiation

The emissive power of a grey body is described by the Stefan-Boltzmann equation, given by

$$E_r = \epsilon \sigma T^4, \quad (1)$$

where E_r is the radiation energy, ϵ the emissivity of the surface at the temperature T , and σ is the Stefan-Boltzmann constant. For two infinite flat surfaces A_1 and A_2 facing each other, the energy flux per unit area due to radiation from the hot (temperature T_1 and emissivity ϵ_1) to the cold surface (temperature T_2 and emissivity ϵ_2) can be calculated as is indicated in Fig. 1,

$$\begin{aligned} E_{r,1 \rightarrow 2} &= \epsilon_1 \epsilon_2 \sigma (T_1^4 - T_2^4) \sum_{i=0}^{\infty} [(1 - \epsilon_1)(1 - \epsilon_2)]^i \\ &= \sigma (T_1^4 - T_2^4) \left(\frac{\epsilon_1 \epsilon_2}{\epsilon_1 + \epsilon_2 - \epsilon_1 \epsilon_2} \right). \end{aligned} \quad (2)$$

For calculating the radiation of two bodies of arbitrary geometry at different temperatures, the so-called view factor has to be considered. The view factor F_{12} represents the fraction of radiation leaving surface A_1 that is directly intercepted by surface A_2 . For two grey surfaces the net heat flow $Q_{r,1 \rightarrow 2}$ from surface A_1 to A_2 is given⁴ by the equation

$$\begin{aligned} Q_{r,1 \rightarrow 2} &= \sigma (T_1^4 - T_2^4) \left[\frac{1}{A_1 F_{12}} + \frac{1}{A_1} \left(\frac{1}{\epsilon_1} - 1 \right) \right. \\ &\quad \left. + \frac{1}{A_2} \left(\frac{1}{\epsilon_2} - 1 \right) \right]^{-1}. \end{aligned} \quad (3)$$

FIG. 1. Schematic drawing showing the radiative coupling between two parallel surfaces, showing what happens with the radiation leaving surface 1.

For two infinite parallel grey surfaces of the same area and $F_{12} = 1$, the net heat flow per unit area between these two surfaces equals Eq. (2). Because our W LPCVD cold-wall reactor is an axisymmetric system the heat transfer is modeled containing three coaxial disks, consisting of the susceptor (surface 1), the wafer (surface 2), and the cold-wall (surface 3); see Fig. 2. The view factor from the susceptor to the wafer F_{12} for a susceptor wafer distance much smaller than the wafer diameter is approximately equal to unity. The view factor from wafer to the cold wall F_{23} is also set to unity, because almost all of the radiation leaving the wafer surface is intercepted by the cold wall.

In vacuum the temperature of the wafer is only determined by radiation and one can calculate the wafer temperature, if the emissivities of the surfaces and the wall and susceptor temperature are known. When not operating at vacuum conditions, the heat transfer by gas particles has to be considered also.

B. Gas conduction

The second mechanism for heat transfer is gas conduction. Smoluchowski² has described the thermal gas conduction for two parallel surfaces at a distance d . The energy flux per unit area may be represented by the relation given by

FIG. 2. (a) Scheme of the cold-wall reactor geometry, and (b) the setup used for the wafer temperature modeling.

$$E_c = \frac{k_m(T_1 - T_2)}{d + 2g}, \quad (4)$$

where k_m is the mean thermal conductivity over the range $T_1 - T_2$. The distance between the two plates is d , and the coefficient g is as shown by Kennard² equal to

$$g = \frac{2 - \alpha}{\alpha} \frac{9\gamma - 5}{2(\gamma + 1)} \lambda, \quad (5)$$

where α is the thermal accommodation coefficient, γ is the ratio of the specific heat at constant pressure C_p to that at constant volume C_v , and λ is the molecular mean free path. Thus, for calculating the gas conduction one first has to know the thermal accommodation coefficient, the thermal conductivity, and the molecular mean free path. These three subjects will be considered in Secs. II B 1–II B 3

1. The thermal accommodation coefficient

The thermal accommodation coefficient α is a parameter that relates the temperature belonging to the incident and the temperature of the reflected gas streams from a solid surface. It is assumed that the molecules of the incident gas stream and the solid surface are hard spheres, and that binary collisions result in a net exchange of energy depending on the molecular mass ratio. The thermal accommodation coefficient is defined^{2,3} as the fractional extent to which molecules that collide with a solid surface and are reflected have their mean energy adjusted toward the temperature of the wall. The reflected molecules from the hot surface possess a mean energy which corresponds to a temperature lower than the surface temperature. According to general dynamic considerations,^{2,3} the constant α should be determined by the relation

$$\alpha = \frac{4mM}{(m + M)^2}, \quad (6)$$

where M is the mass of the gas molecules striking the surface and m is the molecular mass of the surface molecules. For two different surfaces the accommodation coefficient has the value

$$\alpha = \frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2 - \alpha_1 \alpha_2}, \quad (7)$$

where α_1 and α_2 are the values of the accommodation coefficients for the two surfaces, respectively. In practice, deviation from the calculated accommodation coefficients in Eq. (6) can occur compared to the observed values. As far as the accommodation coefficients were not given in literature,¹⁻³ they were calculated according to Eqs. (6) and (7).

2. The thermal conductivity

For calculating the heat transfer by gas conduction, the ratio γ of the specific heat at constant pressure C_p to that at a constant volume C_v has to be known, [see Eqs. (4) and (5)]. This ratio is tabulated in Ref. 2 for different gases, $\gamma = \frac{5}{3}$ for monoatomic gases and approaches 1 for polyatomic gases.

FIG. 3. Thermal conductivities for the gases of interest for W LPCVD as a function of the temperature.

According to Eq. (4), for the calculation of the heat transport by gas conduction, the thermal conductivity has to be known. This thermal conductivity k_T at temperature T is, according to Eucken in Refs. 2 and 4, equal to

$$k_T = \frac{15}{4} \frac{R}{M} \mu \quad (\text{for monoatomic gases}), \quad (8a)$$

$$k_T = (C_p + \frac{5}{2}R) \frac{\mu}{M} \quad (\text{for polyatomic gases}), \quad (8b)$$

where M is the molecular mass of the gas, R is the gas constant, and C_p is a function of temperature and can be written as

$$C_p/R = A + BT + CT^2 + DT^3. \quad (9)$$

The values A, B, C , and D are tabulated in the literature, (see, e.g., Ref. 2). R is the universal gas constant. The viscosity μ in Eqs. (8a) and (8b) can be written as

$$\mu = 2.6693 \times 10^{-8} \cdot \frac{\sqrt{MT}}{\delta^2 \Omega_\mu}, \quad (10)$$

where δ is the molecular collision diameter and Ω_μ is a slowly varying function of the dimensionless temperature kT/ϵ ; ϵ/k can be obtained from the tabulated Lennard-Jones parameters.⁴ The function Ω_μ may be interpreted as the deviation from the rigid sphere behavior.

From Eqs. (8)–(10) and the appropriate tables the thermal conductivity can be calculated as a function of the temperature. In Fig. 3 the thermal conductivities of the gases of interest for tungsten LPCVD are shown as a function of the absolute temperature. In the temperature range of tungsten LPCVD these thermal conductivities are linear with the temperature on a log–log scale. The thermal conductivity of gas mixtures may⁴ be estimated by

$$k_{\text{mix}} = \sum_{i=k}^n \frac{x_i k_i}{\sum_{j=1}^n x_j \phi_{ij}}. \quad (11a)$$

FIG. 4. Comparison of the heat transport by radiation E_r and by gas conduction (E_c argon or E_c hydrogen) as a function of the pressure for two infinite surfaces at a distance of 100 μm having both an emissivity of 0.5.

The x_i values are the mole fractions, and k_i the thermal conductivities of the species i . The values of the coefficients ϕ_{ij} are given by

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_i}{M_j} \right)^{1/4} \right]^2. \quad (11b)$$

The values of μ_1 can be calculated from Eq. (10), and M_i stand for the molecular weights of the gas components.

3. The mean free path

Gas particles undergo frequent collisions. The distance between two successive collisions is the free path of a particle. The average distance of all the molecules is the mean free path λ . The mean free path depends on the molecule collision diameter and the number of molecules per cubic meter n , and can be written as²

$$\lambda = \frac{1}{\sqrt{2} \pi n \delta^2}, \quad (12a)$$

where n depends on the pressure and δ can be found by the previously mentioned Lennard-Jones parameters.⁴ For the mean free path of molecules A and B in a binary mixture the following relations have been derived²:

$$\frac{1}{\lambda_A} = \sqrt{2} \pi n_A \delta_A^2 + \pi n_B \left(\frac{1}{2} (\delta_A + \delta_B) \right)^2 \left(1 + \frac{M_A}{M_B} \right)^{1/2}, \quad (12b)$$

$$\frac{1}{\lambda_B} = \sqrt{2} \pi n_B \delta_B^2 + \pi n_A \left(\frac{1}{2} (\delta_A + \delta_B) \right)^2 \left(1 + \frac{M_B}{M_A} \right)^{1/2}. \quad (12c)$$

Since all the parameters of interest for the heat transfer by gas conduction can be calculated from Eqs. (4)–(12), and with the use of the proper tabulated data, the heat transfer can be calculated.

If two disks are at a distance d of 100 μm , the heat flux as a function of the pressure can be calculated. In Fig. 4 the calculated heat transfer as a function of the pressure in

hydrogen and in argon is shown, assuming a temperature difference of 100 K and emissivities of 0.5 for both disks. It can be seen that the amount of heat transport by radiation is equal to the conductive heat transfer at a pressure of about 150 Pa. At 1000 Pa the contribution to the heat transport by radiation is only 7.5% of the conductive heat transport by hydrogen, but in argon this is still 24%. Note that the transition from radiative to conductive heat transport in Fig. 4 is at a pressure that is typical for LPCVD.

III. MODEL DESCRIPTION

The heat transport between coaxial disks according to Fig. 2(b) can be calculated by four fluxes of heat. These are as follows:

- (i) net radiation from susceptor to wafer, $Q_{r,1 \rightarrow 2}$;
- (ii) gas conduction from susceptor to wafer, $Q_{c,1 \rightarrow 2}$;
- (iii) net radiation from wafer to the wall, $Q_{r,2 \rightarrow 3}$;
- (iv) gas conduction from wafer to the wall, $Q_{c,2 \rightarrow 3}$.

In thermal equilibrium the heat flux to the wafer is equal to heat flux leaving the wafer, or

$$Q_{r,1 \rightarrow 2} + Q_{c,1 \rightarrow 2} - Q_{r,2 \rightarrow 3} - Q_{c,2 \rightarrow 3} = 0. \quad (13)$$

Thus, by making use of Eqs. (2) and (4), Eq. (13) can be solved and the temperature of the wafer can be found. However, these equations are highly nonlinear and many of the parameters themselves depend on the wafer temperature and are not easy to calculate. The wafer temperature could be found by estimating the wafer temperature falling between susceptor and wall temperature as a starting value followed by repeatable substitution in Eq. (13), using a simple zero-point algorithm.

A. Model assumptions

The simple model suffers from some approximations; these are as follows.

(i) The model is one dimensional and assumes three disks at different temperatures. In reality the reactor is not one dimensional and the reactor wall is not a disk as is indicated in Fig. 2.

(ii) The accommodation coefficients are not exactly known. As far as they were not tabulated in the literature they were calculated using Eq. (6).

(iii) Emission coefficients in the literature are not very suitable, since they depend on several material properties, e.g., a change in roughness can result in a different effective emissivity. Moreover the emissivities often depend on temperature and wavelength. For the materials of interest the emissivities, as given in Table I, were found in the literature.

Table I shows that the emissivity of the different materials can vary much. To obtain correct values for the modeling, the emissivities of silicon wafers with or without different tungsten and silicon-dioxide coatings were measured using a pyrometer operating at 3.45 μm wavelength; for further details the reader is referred to Secs. IV and V.

At temperatures below 1000 K lightly doped silicon is more or less transparent for wavelengths between 1.5 and 15 μm . This results in a temperature- and wavelength-

TABLE I. Literature emissivity values of the materials of interest.

Material	Emissivity (ϵ)	Reference
Graphite	0.7–0.8	8
Silicon ^a	0.05–0.72	1,5,6,10
Silicon dioxide ^b	0.70–0.90	1,8,10
Tungsten	0.05–0.15	1,8
Stainless steel	0.35–0.80	4,8
Aluminiumoxide	0.20–0.30	4,8

^aSilicon emissivity (wavelength = 1–15 μm) is a strong function of the carrier concentration.

^bEmissivity of silicon dioxide on Si wafer (0.02 $\Omega\text{ cm}$) at a certain wavelength is a periodical function of the thickness.

dependent emissivity.⁵ To obtain a constant (i.e., temperature and wavelength independent) emissivity, highly doped (0.02 $\Omega\text{ cm}$) epiwafers were used in the experiments.⁶

B. Model calculations

Using the model, a calculation can be made of the true wafer temperature as a function of pressure and gas composition. In Figs. 5(a) and 5(b) the temperature of a Si wafer (assuming $\epsilon_{\text{Si}} = 0.55$) is calculated as a function of the pressure and gas composition for the case of an uncoated Si wafer [Fig. 5(a)] and a tungsten (assuming $\epsilon_{\text{W}} = 0.15$) front-side-coated wafer [Fig. 5(b)]. In these figures large differences between susceptor and wafer temperature can be observed. In the case of a silicon wafer without front-side coating Fig. 5(a) shows that this temperature difference can be as large as 90 K for a susceptor temperature of 800 K. The dip in wafer temperature at about 20 Pa is due to the fact that the net loss of heat by conduction from the wafer front side is larger than the gain of heat of the wafer back side. This dip is more pronounced in the case of a gas having a higher gas conductivity, such as hydrogen. At pressures above 20 Pa, an increase in wafer temperature can be seen with increasing pressure. This is because the conduction between susceptor and wafer increases faster than the conduction from wafer to the wall. At very low pressures the contribution by conduction to the heat transfer can be neglected and the wafer temperature depends only on the emissivities of susceptor, wafer (back and front side), and reactor wall. The difference between Figs. 5(a) and 5(b) illustrates that in the case of a low wafer front-side emissivity, the heat transport from wafer to wall is also lower resulting in a higher wafer temperature.

In our W LPCVD reactor there is no clamping of wafer to the susceptor and the wafer rests freely on the susceptor; therefore there will always be a temperature difference between the susceptor and the wafer. This temperature difference depends on various parameters and can be reduced by choosing the proper processing conditions. The dependence of the wafer temperature on the pressure as a function of several parameters will be discussed below.

FIG. 5. Wafer temperature as a function of pressure for (a) a silicon wafer and (b) a wafer coated by tungsten on the front side at a susceptor temperature of 800 K. Curves are calculated assuming $\epsilon_{Si} = 0.55$ and $\epsilon_W = 0.15$.

1. Emissivity of the susceptor

The influence of the emissivity of the susceptor ϵ_1 on the wafer temperature is shown in Fig. 6(a) where ϵ_1 is varied from 0.1 to 1.0. From this figure it is clear that a high emissivity of the susceptor reduces the temperature difference between wafer and susceptor. If the emissivity of the susceptor is only 0.1 the temperature difference is as large

as 225 K, for a susceptor emissivity of 1.0 this is "only" 75 K. In our reactor the initial graphite susceptor was coated with Al_2O_3 , which has an emissivity of only 0.2–0.3.^{4,8} By removing this coating the susceptor emissivity could be increased to 0.7–0.8.⁸ This should result in a smaller temperature difference between susceptor and wafer.

2. Emissivity of the wafer back side

From the above it should be clear that the influence of a coating on the back of the wafer on the temperature difference is important. The effect of the wafer back-side coating on the wafer temperature as function of the pressure is calculated and these results are shown in Fig. 6(b). In order to diminish the temperature difference, the wafer back-side emissivity ϵ_2 should also approach one.

3. Emissivity of the wafer front side

If the emissivity of the front of the wafer ϵ_3 changes, it has an effect on the wafer temperature. This is shown in Fig. 6(c), where the emissivity of the front side changes from 0.1 to 1.0. It can be seen that the temperature difference between susceptor and wafer decreases by reducing the wafer front-side emissivity.

4. Emissivity of the reactor wall

The effect of the emissivity of the reactor wall ϵ_4 on the wafer temperature is shown in Fig. 6(d). The wafer temperature is calculated for three emissivities of the reactor wall. The difference between wafer and susceptor will be minimal for a low emissivity of the reactor wall (i.e., a highly reflective reactor wall).

5. Wafer-to-wall distance

Although the distance from the wafer to the cold wall L is fixed, it is interesting to know the effect of L on the wafer temperature as a function of the pressure. In Fig. 7(a) the results of the wafer temperature as a function of pressure is

FIG. 6. Calculated wafer temperatures as a function of the hydrogen pressure. (a) Emissivity of the susceptor ϵ_1 varying from 0.1 to 1.0. (b) Wafer temperature for different emissivities of the wafer back side ϵ_2 ranging from 0.1 to 1.0. (c) Wafer temperature for different emissivities of the wafer front side ϵ_3 ranging from 0.1 to 1.0. (d) Wafer temperature as a function of the emissivity of the reactor wall ϵ_4 going from 0.1 to 1.0. Other parameters are shown in the insets.

FIG. 7. (a) Wafer temperature vs the hydrogen pressure for different distances L from the wafer to the wall. (b) The same for different distances between the wafer and the susceptor.

calculated for three different distances between wafer and the cold wall. Figure 7(a) shows that by decreasing the wafer-to-wall distance the dip in the wafer temperature versus pressure increases. To avoid such a temperature dip the reactor dimensions should be large. Our reactor has an average distance between wafer and the cold wall of about 15 cm. This is rather large for this type of reactor implying that the dip in temperature will be not that large. Another effect by decreasing the wafer-to-wall distance is a shift of the wafer temperature minimum to a higher pressure [see Fig. 7(a)].

6. Distance susceptor to the wafer

Since the wafer is not clamped to the susceptor, there will always be a distance d between the susceptor and the wafer, which will be increased additionally by wafer bending or a bad wafer positioning. Figure 7(b) shows that the effect of an extra spacing between the wafer and the susceptor on the wafer temperature is small and only significant at the "higher" pressures.

IV. EXPERIMENT

Experiments were performed in the W LPCVD cold-wall reactor. Temperatures of the susceptor could be measured by means of a series of thermocouples. The wafer temperature was measured with a dual-beam pyrometer, at wavelengths of 2.1 and 2.3 μm . Because of the dual wavelength the temperature measurements are independent of the emissivity; this is only true for bodies having the same emissivity at wavelengths of 2.1 μm as well as at 2.3 μm . In general this is the case, but some materials, such as tungsten and high-ohmic silicon, do not satisfy this demand. Temperature measurements of these kind of materials do need an extra calibration. This calibration was done at atmospheric pressure in a nitrogen ambient by clamping the wafer to the susceptor. For these conditions the wafer temperature is equal to the susceptor temperature, and the pyrometer could be calibrated. Calibration was done for

the Si wafers with or without specific coatings in a temperature regime of 573–873 K (300–600 °C).

The temperature of a Si wafer (0.02 Ω cm) was measured as a function of the pressure with and without different coatings on the back and front side. The wafer coatings used in these experiments were LPCVD tungsten and thermally grown silicon dioxide.

Measurements using a single-wavelength pyrometer, operating at 3.45 μm , were used to obtain the emissivity values of the Si wafer with and without the different coatings. This was done by clamping the wafers to a thermocouple temperature-controlled susceptor. By knowing the exact susceptor temperature and the pyrometer readout the emissivity of the different coatings could be determined.

V. MEASUREMENTS

A. Emissivity measurements

Emissivities were measured as a function of temperature, applying the pyrometer operating at 3.45 μm wavelength. The results of these measurements are presented in Fig. 8. The emissivity of the highly doped silicon epiwafer is constant over the measured temperature range and has a value of 0.71 ± 0.01 . This emissivity value was reported also by Maex in Ref. 6 for this type of silicon at approximately the same wavelength. The silicon wafer coated with 0.7 μm SiO_2 revealed a constant emissivity of 0.85 ± 0.03 . One has to note that this value is dependent on SiO_2 thickness and wavelength; but, in the considered temperature range radiation mainly occurs around wavelengths of 4 μm . This means that the measured emissivity is valid in the temperature range from 575 to 875 K, and only for the applied silicon epiwafer coated with the 0.7- μm -thick SiO_2 layer.

Tungsten-coated Si wafers showed an emissivity slightly increasing with temperature. The thickness of the tungsten coating hardly influences the emissivity (see Fig. 8). This can be explained by the fact that the roughness of these

FIG. 8. Measurements of the emissivities of Si wafers with or without different coatings.

LPCVD tungsten films is much smaller than the wavelength of $3.45 \mu\text{m}$, meaning that the emissivity will not be influenced by this roughness. The roughness of W LPCVD films has been shown to be linear with the film thickness. For these types of films the roughness has a value of 6.4% of the total thickness.¹¹ For the $0.8\text{-}\mu\text{m}$ -thick tungsten film this results in a roughness of $0.05 \mu\text{m}$, which is indeed much smaller than the wavelength. The emissivity of the tungsten-coated Si wafers was 0.13 ± 0.02 in the measured temperature range.

These measured emissivity values will be used in the model calculations when comparing the measurements with the proposed model. The value of the cold-wall emissivity could not be measured and was set to 0.40. This value is consistent with values reported in literature, (see Table I). Moreover, this value resulted in a good fit between the model calculations and the measurements. In Table II the employed emissivities for the model calculations of the different materials are summed up.

B. Influence of flow rate on the wafer temperature

Intuitively one would expect that an increase of a gas flow will decrease the wafer temperature. Previously Schmitz and co-workers¹ showed that the influence of flow rate had little effect on the wafer temperature in their cold-wall reactor. For our reactor the effect of heat transport by forced flow is examined in a flow range from 100 to 5000 sccm at a H_2 pressure of 13, 67, and 133 Pa. The temper-

TABLE II. Emissivity values used for wafer temperature modeling.

Material	Emissivity (ϵ)
Graphite	0.75
Silicon	0.71 ± 0.01
Silicon + $0.7 \mu\text{m SiO}_2$	0.85 ± 0.03
Tungsten	0.13 ± 0.02
Stainless steel	0.40
Aluminiumoxide	0.25

TABLE III. Influence of flow rate on wafer temperature.

H_2 flow (sccm)	T_{wafer} (K)		
	$p\text{H}_2 = 13 \text{ Pa}$	$p\text{H}_2 = 67 \text{ Pa}$	$p\text{H}_2 = 133 \text{ Pa}$
100	649	661	669
1000	650	659	669
5000	...	659	668

ature measurements were performed on a Si epiwafer and the susceptor temperature was fixed at 728 K. Results of these measurements are presented in Table III.

The data in Table III show that the influence of the flow rate is insignificant for the wafer temperature in the flow regime generally used in LPCVD applications. To understand this, one has to consider that the ratio of the heat flow by gas conduction and the heat transport by convection. This ratio is equal to $\text{Pr} \times \text{Re}$, where Pr is the so-called Prandtl number equal to $C_p \cdot (\mu/k)$, and Re is the Reynolds number, equal to $L'v(\rho/\mu)$ where L' is the characteristic length of a system, v the average speed of the gas, and ρ is the density of the gas. For our reactor the Reynolds number varies from 0.5 to 10.⁹ The Prandtl number is about 0.7 for all gases. This means that the heat transport by convection is comparable with the contribution by conduction. In the W LPCVD regime of the reactor the net heat flow from wafer to the cold wall is dominated by radiation rather than conduction and convection. Thus, although the heat transport by forced convection is comparable to the conductive heat transport, the contribution of both to the total heat flow from wafer to the wall is small. This explains that the flow rate increase did not decrease the wafer temperature.

C. Solid-solid heat transfer from susceptor to wafer

The calculations as presented do not incorporate the solid-solid heat transfer from the susceptor to the wafer. Because the wafer is not clamped on the susceptor there is no real solid-solid contact. The calculations, ignoring the solid-solid heat transfer, showed that the distance d from susceptor to the wafer did not influence the wafer temperature in the low-pressure regime. The influence of the solid-solid heat transfer is examined by intentionally increasing the susceptor-to-wafer distance. The temperature of a Si wafer was measured versus pressure with and without an extra spacing between wafer and susceptor. The temperature as function of pressure for both cases is shown in Fig. 9. The extra spacing was about $500 \mu\text{m}$. Differences between the two curves can be observed only at pressures where gas conduction becomes important. These observations differ somewhat from those reported by Schmitz and co-workers.¹ They found a difference in temperature at low pressures, too, when intentionally increasing the distance between the susceptor and the wafer. This may be attributed to the fact that their experiments were performed in a much smaller reactor, and the wafer-to-wall distance was much smaller than in our reactor. In that case temperature differences can become more pronounced. The observed

FIG. 9. Measurements of the silicon wafer temperatures as a function of the argon pressure, with (Δ) and without ($\bullet$) an extra spacing between susceptor and the wafer. The lines are the model calculations assuming emissivities as presented in Table II.

temperature differences at pressures above about 100 Pa do support the observations of Schmitz and co-workers.¹ Figure 9 also shows the good match between the calculated curves and the measurements. The calculated curves were obtained using the measured emissivities summed up in Table II. From the above-described observations one can conclude that ignoring the solid–solid heat transfer did not, as expected, introduce a great inaccuracy in the calculations.

D. Effect of gas composition on wafer temperature

In general for tungsten LPCVD argon or hydrogen is used in excess; therefore, the measurements and calculations of the wafer temperature are performed for these gases. Another reason is that by introducing WF_6 in the reactor all kinds of reactions occur giving a nonstationary situation, which makes these wafer temperature measurements impossible. In Fig. 10(a) the temperature of a sili-

con wafer is shown as a function of the pressure, for 100% H_2 , 100% Ar, and 50% H_2 + 50% Ar. In Fig. 10(b) this is shown for the silicon wafer with a 0.35- μ m-thick tungsten coating on the front side. From these figures we see that the calculated curves do match the measurements. The model accurately predicts the observed trends. The absolute values are within 10 K correct in the measured pressure regime from 1 to 1000 Pa. In Figs. 10(a) and 10(b) the calculated curves for gas mixtures are also presented. Although free mean paths and thermal conductivities can be calculated for gas mixtures (semiempirical formula of Wilke⁴), for the accommodation coefficient no data is available for gas mixtures. Thus, in Figs. 10(a) and 10(b) the 50% H_2 + 50% Ar line is calculated using the semiempirical relations of Wilke for the thermal gas conductivity [Eq. (11)] and a general relation for binary mixtures for the mean free path of the molecules [Eq. (12)]. The accommodation coefficients were estimated being the mean value of hydrogen and argon for the different surfaces.

Another phenomenon that can be observed in Figs. 10(a) and 10(b), is that during a blanket tungsten deposition on, e.g., a Si wafer, the temperature of the substrate changes because of a decreasing emissivity of the wafer front side. This wafer temperature change depends on the deposition pressure, gas composition, and the change in emissivity. In Figs. 11(a) and 11(b) wafer temperatures are calculated for different wafer coatings as a function of the total pressure in either argon [Fig. 11(a)] or hydrogen [Fig. 11(b)]. Additionally some measured values are plotted in Figs. 11(a) and 11(b), showing again the agreement between the model and the measurements.

The substrate temperature increase during the tungsten deposition on Si can be as large as 46 K at a hydrogen pressure of 10 Pa and a susceptor temperature of 773 K. When a tungsten deposition is carried out at a much higher

(a)

(b)

FIG. 10. Measurements and the model calculations of wafer temperatures vs the pressure for different gas compositions (100% H_2 , 100% Ar, and 50% H_2 + 50% Ar) and for different front-side coatings: (a) silicon wafer and (b) silicon wafer with 0.35 μ m LPCVD tungsten. Temperature of susceptor is 723 K. Note the difference in Y-axis scaling.

FIG. 11. Model calculations and some measurements of the wafer temperatures as a function of pressure for different front- and back-side coatings. Susceptor temperature is 773 K. (a) Gas composition is 100% argon and (b) 100% hydrogen.

hydrogen pressure, e.g., 1000 Pa, the temperature change is less, but still 17 K [see Fig. 11(b)].

E. Effect of susceptor coating on the wafer temperature

Model calculations indicated that a susceptor emissivity approaching one is favorable for minimizing the temperature difference between wafer and susceptor, as was shown in Fig. 6(a). Wafer temperature measurements were carried out on a Si wafer having a tungsten front-side coating that was placed on a graphite susceptor with and without an Al_2O_3 coating. Results of these measurements are shown in Figs. 12(a) and 12(b). The susceptor temperature was fixed at 823 K for both cases. The curves of Figs. 12(a) and 12(b) were calculated assuming an emissivity of 0.25 for the Al_2O_3 coating. This is a reasonable value because the tabulated emissivity values for Al_2O_3 range from

0.2 to 0.3.^{4,8} The wafer temperature deviation for the two different susceptor coatings can be as large as 35 K at low pressures.

VI. CONCLUSIONS

Model predictions and measurements showed that in cold-wall reactors the true temperature of the wafer can differ significantly from the susceptor temperature. Moreover during processing the wafer temperature varies widely with pressure and gas composition, and is also dependent on susceptor and or wafer coatings. In processing one should be very alert to these effects since otherwise wrong conclusions can easily be deduced.

FIG. 12. Temperature of silicon wafer with a LPCVD tungsten front-side coating vs the pressure for three gas compositions and a susceptor temperature of 823 K. The influence of the susceptor coating is shown by comparison of (a) an Al_2O_3 -coated susceptor and (b) a graphite susceptor.

The heat transport in the W LPCVD reactor could be successfully modeled by considering only the heat flow by radiation and gas conduction. The model predicts the wafer temperature as a function of: (i) gas composition; (ii) pressure; (iii) coatings of wafer and susceptor; (iv) distances between wafer and the cold wall and, between wafer and susceptor, respectively.

From the model calculations one may conclude that the temperature difference between susceptor and wafer in the W LPCVD cold-wall reactor is minimal for: (i) high emissivity of susceptor and wafer back side; (ii) low emissivity of wafer front side; (iii) high total pressure; and (iv) low emissivity of the reactor wall. The dip in wafer temperature will be minimal by the choice of the right carrier gas composition (i.e., argon) and a large wafer-to-wall distance.

The measurements were in good agreement with all the trends predicted by the model. The absolute wafer temperatures were accurately predicted in the entire pressure range from 1 to 1000 Pa within 10 K.

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