MODELING OF THE RADIATION ENVIRONMENT IN THE LOWER CHAMBER OF RAPID THERMAL PROCESSING FURNACES

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ABSTRACT

A cold shield concept has been proposed to increase the effective emissivity of a silicon wafer seen by the radiometer in a rapid thermal processing (RTP) tool. This was done in order to reduce the uncertainty of the temperature measurement by radiation thermometry. A simple enclosure model based on two parallel, isothermal, and diffuse-gray surfaces cannot account for the temperature non-uniformity or the edge and side effects; therefore a detailed enclosure analysis model was developed. Furthermore, the simple model cannot take inputs of radiative properties, which can be wavelength dependent, and of reflectance data of the silicon wafer which can be specular, diffuse, or somewhere in between. Therefore, this paper presents an analysis of the radiation environment of the lower chamber of the RTP test bed at the National Institute of Standards and Technology (NIST) using the classical enclosure theory method. A Monte Carlo method is also presented that in the future may include parameters that the enclosure method cannot handle.

Parametric studies are presented in order to evaluate the effect that the radiative properties, temperature, and geometric arrangement, have on the effective emissivity and heat flux distribution of the chamber. The models predict that the effective emissivity of the chamber will be greatly increased from the wafer emissivity 0.65 to about 0.90. This increase will minimize the sensitivity of radiation thermometers to variations in the emissivity of the silicon wafer. This work will help researchers to gain a better understanding of the radiation heat transfer in RTP systems and to improve radiation temperature measurements in those systems.

INTRODUCTION

The main hurdle in the implementation of RTP for mainstream manufacturing applications has been accurate temperature measurement accuracy and control (Roozeboom, 1991, 1993 and 1996; Timans, 1996; Vandenabeele, 1994). One way to improve the accuracy of the temperature measurement by radiation thermometry (RT) is to construct a cavity that simulates a blackbody (DeWitt et al., 1997). This has been done to the NIST RTP platform by adding reflective surfaces in the lower chamber (see Figure 1).

Previously, a simple two surface model was used to predict the effective emissivity of such chambers (DeWitt et al., 1997). These simple models are useful in preliminary studies to validate the theory but are unable to give accurate results that will fit the data. Specifically, this model cannot account for the edge effects or temperature gradients that are routinely encountered in the wafers inside RTP chambers. This paper presents a classical enclosure theory model that has been developed to expand the capability of the simple two surface model. This model gives a representation of the radiation environment in this chamber. Using the data obtained from the model, the spectral temperature read by the RT can be corrected to give the true temperature of the wafer.

The classical enclosure theory models that are presented cannot account for non-diffuse and non-gray optical properties of the materials that are used in the RTP chamber; therefore, a preliminary Monte Carlo models was developed. Monte Carlo models can be used to represent surfaces that emit and reflect non-diffusely and specularly. This allows more accurate modeling of the radiating surfaces inside the furnace and provides a more realistic representation of the radiation environment inside the chamber.

The lower chamber of the RTP tool consists of the area enclosed by the bottom of the wafer, a guard ring, a guard tube, and a cold reflective shield. All of the surfaces in the chamber with the exception of the wafer are highly reflective in order to simulate a blackbody enclosure. The first method used to model the chamber is the classical enclosure theory method, which consists of performing energy balances on each surface and obtaining their radiosities. In this method, the walls of the chamber are presumed to be diffuse-gray and have known temperatures. The method is then expanded to include a specular bottom surface (cold plate). Using this method the effect of various parameters on the effective emissivity of the chamber are studied. The second model is the Monte Carlo model, which is a statistical method used to represent physical phenomena. This method is used first to simulate the same conditions that were modeled using enclosure theory and the results are the same. Later, the method is expanded to include non-diffuse surfaces.

THE CLASSICAL ENCLOSURE THEORY MODEL

A number of models were developed to try to gain a better understanding of the important parameters involved in the lower chamber of the RTP platform. The lower chamber consists of the wafer, guard ring, guard tube, and cold plate (see Figure 2). These models are based on classical enclosure theory, are for gray-diffuse surfaces, and can be extended to diffusely emitting and spectrally reflecting surfaces. Classical enclosure theory is based on performing energy balances on the surfaces to be modeled. A detailed derivation of the equations used is found in the book by Incropera and DeWitt (1996).

When an energy balance is performed on a surface of an enclosure, the resulting equation after some mathematical manipulation and application of the definitions of view factor and radiosity, is

$$\frac{E_{bi} - J_i}{(1-\varepsilon_i)/\varepsilon_i A_i} = \sum_{j=1}^{N} \frac{J_i - J_j}{(A_i F_{ij})^{-1}}, \qquad (1)$$

where, E_{bi} is the blackbody emissive power, J_i is the radiosity of the surface, J_j is the radiosity of the other surfaces of the enclosure, ε_i is the surface emissivity, A_i is the surface area and F_{ij} is the view factor from the surface to each surface of the enclosure. From the prescribed temperatures and geometrical and material properties, Eq. (1) can be used to set up an equation for each surface of the enclosure. This will set up a matrix of equations for the enclosure. This matrix equation is solved for the radiosities of the surfaces, and an effective emissivity ε_{eff} is defined as the radiosity over the blackbody emissive power. Later, this effective emissivity is used to correct the temperature measured by the radiometer by using the measurement equation.

The preceding derivation was performed for diffuse gray surfaces, but it can be applied to non-gray surfaces. By replacing ε_i with $\varepsilon_{\lambda i}$ and E_{bi} with $E_{\lambda b,i}$ and performing the same derivations as before, Eq. (1) becomes

$$\frac{E_{\lambda\,b,i} - J_{\lambda\,i}}{(1-\varepsilon_{\lambda\,i})/\varepsilon_{\lambda\,i} A_i} = \sum_{j=1}^{N} \frac{J_{\lambda\,i} - J_{\lambda\,j}}{(A_i F_{ij})^{-1}} \tag{2}$$

which can be solved for $J_{\lambda i}$, where $\varepsilon_{\lambda i}$ is the spectral emissivity, $E_{\lambda b,i}$ is the spectral emissive power, and $J_{\lambda i}$ is the spectral radiosity. The spectral emissive power is defined by Planck's law multiplied by π, i.e. πL_{λ}. Then, the spectral effective emissivity is

$$\varepsilon_{\lambda,\mathrm{eff}} = \frac{J_{\lambda\,i}}{E_{\lambda\,b,i}} \tag{3}$$

When total properties are used, the model mimics the use of a radiometer that measures all wavelengths, but when spectral properties are used, a single-wavelength radiometer is simulated.

For gray surfaces Eq. (2) can be integrated to obtain Eq. (1) but the opposite is not true; also even if ε_i is the same as $\varepsilon_{\lambda i}$, ε_{eff} does not have to be the same as $\varepsilon_{\lambda,eff}$. While Eq. (1) can only be used for gray surfaces, Eq. (2) can be used with any surface to obtain the spectral effective emissivity at a particular wavelength.

These equations were set up and solved for the case of the lower chamber of the NIST RTP furnace using the commercial software MathCad. After entering the dimensions of the chamber, the number of surfaces, the optical properties, and the temperatures, the program calculates the surface areas, emissive powers and the view factors for all the surfaces. Later, the matrix with Eq. (1) is solved for the radiosities of all the surfaces. From this point, the program calculates the effective emissivity, the spectral temperature and the heat flux of the surfaces. These results can be plotted graphically by the software.

The models that were first developed using classical enclosure theory consisted of simplified enclosures with diffuse emitting and reflecting surfaces. These models were used to gain experience in developing these kinds of codes and to get an idea of the important parameters that affect temperature measurement in RTP. Later the models were expanded to include a specularly reflecting bottom plate. This was done to better simulate the actual chamber, since the bottom plate of the chamber is coated with nickel, a very specular reflector.

To model the specular bottom surface, the method presented by Siegel and Howell (1992) was used. This method consists of calculating new view factors for the surfaces using virtual surfaces, when the surface is reflected specularly. In this method, if a surface is viewed indirectly through reflection, a specular view factor is calculated, taking into account the new geometry and the specular reflectivity of the surface that is reflecting it.

THE MONTE CARLO METHOD

Monte Carlo is a name given to a family of modeling methods that uses the statistical characteristics of real processes to simulate physical events. In the case of radiative heat transfer, the model consists of surfaces that emit bundles of energy; these bundles are then traced around the cavity until they are absorbed by one of the surfaces. The emission, reflection and absorption of these bundles at the surfaces must mimic the behavior of the real surfaces being modeled. The derivation of the Monte Carlo method for radiative heat transfer can be found in Howell (1998), Kalos and Whitlock (1986) and Yang et al. (1995).

A FORTRAN program was used to develop a Monte Carlo model that represents the radiation environment inside the lower chamber of the RTP furnace. Due to the complexity of modeling the vertical surface of the chamber, only two surfaces were modeled. These are the silicon wafer with the guard ring and the cold plate. The vertical surface is modeled as a zero K blackbody; therefore, any energy bundle that would strike the vertical surface is lost. The input data to the model consist of the diameters of the two concentric disks and the distance that separates them, the temperature distribution (T_1, T_2, etc.) of each disk, the number of surfaces, the optical properties of each surface, and the number of bundles to emit.

The program calculates the radius of each sub-surface by dividing the total surface into equal areas. The energy flux from the first sub-surface is

$$q_{e,1} = \varepsilon_1 A_1 E_{\lambda b,1} \tag{4}$$

then, the energy of each bundle emitted by the sub-surface is

$$w = \frac{q_{e,1}}{N_1} \tag{5}$$

where N_1 is the number of bundles emitted by the wafer at sub-surface 1. The number of energy bundles emitted by the other sub-surfaces is then

$$N_i = \frac{q_{e,i} N_1}{q_{e,1}} \tag{6}$$

where $q_{e,i}$ is the energy flux from surface i, and is defined as

$$q_{e,i} = \varepsilon_i A_i E_{\lambda b,i} \tag{7}$$

With all the necessary information calculated, four random numbers between 0 and 1 are selected. These determine the place of emission from the surface and the direction of this emission. A radius r and an angle φ define the place of emission, while the direction is defined by a directional angle θ and a rotation angle ϕ.

The place where the emitted bundle hits the second surface is calculated using the following relations

$$x = L \tan\varphi \cos\theta + r \cos \tag{8}$$

$$y = L \tan\varphi \cos\theta + r \sin \tag{9}$$

where L is the distance between the plates. Then the radius and angle of impact on the second disk are converted from Cartesian to cylindrical coordinates. If the radius of impact is larger than the radius of the second surface then the bundle is lost and another is emitted. Otherwise, a random number is selected. If this random number is smaller than the absorptivity of the surface, then the bundle is absorbed; otherwise, the bundle is reflected. For a diffuse reflection the same procedure as that used for the emission of a bundle is followed, i.e. random numbers are chosen to determine the direction of reflection. For a specular reflection, the direction of incidence determines the direction of emission. The bundle is traced around the cavity until it is absorbed by a surface or lost. Then another bundle is emitted until the specified number of bundles is emitted by all the surfaces. The effective emissivity of a surface is the number of emitted and reflected bundles from the surface divided by the number of bundles that a blackbody at the same temperature would emit. For a diffuse surface the effective emissivity of a spot is calculated by adding the number of emitted and reflected bundles from the spot that the radiometer sees (see Fig. 3) and dividing by the number of bundles that a blackbody at the same temperature would emit.

One of the advantages of the Monte Carlo method over the classical enclosure method is that it permits a refinement of the definition of the effective emissivity. For surfaces that are non-diffuse, the effective emissivity can be defined as the number of bundles that were emitted and reflected from the spot towards the radiometer, divided by the number of bundles that a blackbody at the same temperature would emit towards the radiometer. This definition of the effective emissivity will more accurately reflect the energy that the radiometer sees from the wafer. While this definition mightdescribe a more realistic situation, the Monte Carlo code will require more bundles to be emitted by the surfaces in order to maintain an acceptable accuracy.

RESULTS

All of the results that are presented here start from the base case summarized in Table 1. The geometric dimensions of the chamber are those of the NIST RTP platform. The parameter that is varied is the only one that is not set to the base case value, while the others remain constant. This method will identify the parameters that affect the effective emissivity and how much they affect it. Figure 4 gives a guide of the temperature errors that the radiometer will encounter with different effective emissivities. The silicon wafer emissivity at 800 °C is about 0.65 and will result in a radiometer reading that is 30 °C lower than the thermocouple reading. If this emissivity is enhanced to 0.95, this error can be lowered to about 5 °C.

Table 1 Base case values

	T_w	T_c	ε_w	ε_c	r_w	r_c	L
Value	800 °C	25 °C	0.65	0.2	0.1 m	0.135 m	0.0125 m

The features that have the biggest effect on the chamber effective emissivity are the emissivities of the wafer and cold plate. The wafer emissivity is not a variable that can be controlled in the day to day application of RTP, but the cold plate and guard ring emissivitiescan be modified in the NIST facility. If the cold plate emissivity is maintained very low, then the temperature error will be reduced greatly. Figure 5 also underscored the importance of accurately knowing the value of the wafer emissivity, it shows that a 5% error in the value of the wafer emissivity can cause a 2% to 3% in the value of the effective emissivity. Figure 5 also shows the benefits of the blackbody chamber when the emissivity of the guards and cold plate is very small. For a very reflective cold plate, a 5% error in the value of the wafer emissivity will only cause a 0.05% error in the value of the effective emissivity.

Figures 6 and 7 demonstrate that for this particular wavelength the spectral radiometer would be much more insensitive to changes in the temperatures of the wafer or the cold plate. This result assumes that the optical properties remain constant with changes in temperature. From Planck's law, the maximum amount of energy emitted by a blackbody at 800 °C is approximately at 2.7 µm. The spectral radiometer used in the analysis has a wavelength receiver of 0.95 µm, therefore, it is much less vulnerable to changes in temperature. Furthermore, the amount of energy available at this wavelength is less than that available at the maximum wavelength.

Figure 7 shows the effect of treating the bottom cold plate as a specular surface. The figure shows that the effective emissivity will follow the same pattern as if the surface was treated as diffuse, but the value of the effective emissivity will be about 0.016 lower. This pattern is repeated for both figures, and furthermore it is seen in all the parametric analyses that were performed. It can be noted that the same applies to the spectral and diffuse cases. Note that for two infinite parallel surfaces, the effective emissivity is the same with either the diffuse or the specular cold plates. With the guard ring and guard tube, however, the effective emissivity depends on the specularity of the cold plate. This result suggests that directional properties may have non-negligible influence on the effective emissivity in the actual RTP chamber.

After all the radiosities have been calculated for the surfaces, Eqs. (2) or (3) can be used to calculate the heat fluxes to the surfaces. The first study that was performed using these fluxes was to verify the effect that the radiometer opening might have on the temperature uniformity of the wafer. Figure 8 shows the results of these tests. For the tests the radiometer opening was modeled as a blackbody when present and as a normal part of the cold plate otherwise, and the wafer was divided into ten surfaces of equal radius. It is clearly seen that the radiometer opening will cause heat flux non-uniformity in the wafer, resulting in temperature non-uniformity. Therefore, the radiometer opening should be as small as possible. This figure also shows the effect that the cold guards have on the edge of the wafer. The cold guards cause the heat fluxes at the edge of the wafer to be diminished introducing more temperature non-uniformity.

Figure 9 shows the heat flux experienced by the wafer when the guard rings are cold (298 °C) and warm. For the warm condition, the guard ring is assumed to be at 600°C and the guard tube is assumed to be at 400 °C. It can be seen from the figure that the heat flux of the wafer becomes more uniform with the warm guard rings.

These findings have been experimentally verified at NIST and have been responsible for the redesign of the RTP test bed. Studies like this one shed light on the causes of wafer temperature non-uniformity inside an RTP chamber. They also help researchers improve the design of future chambers. Further research should be done to investigate the effect of guard ring and guard tube temperature and emissivity on the heat flux distribution. The effect of directional dependent radiative properties can be studied using the Monte Carlo method.

The model that was developed using the Monte Carlo method was a general model, which could later be modified to include situations that are more detailed. In other words, it was a general model capable of performing analyses of simple diffuse-gray surfaces or could be used to model surfaces with angle and/or wavelength dependent properties. In order to confirm the model, it was used with the same parameters that were used to confirm the classical enclosure theory model. Table 2 shows the result of these tests.

For these tests, the enclosure model was used without a guard ring and the guard tube was modeled as a 0 K blackbody. The results of these tests agree well. The Monte Carlo model is not expected to give the exact answer for a particular situation, because it is a statistical method that uses random numbers the answers change a little with every run. Furthermore, the answers are expected to vary with the number of energy bundles selected for each run of the program.

Table 2 Validation of the Monte Carlo Model

	Enclosure Theory Avg. Eff. Emis.	*Monte Carlo Avg. Eff. Emis.*	*Standard Deviation*
Two Infinite Surfaces	0.9033	0.9054	.003698
Diffuse Cold Plate	0.8850	0.8844	.002089
Specular Cold Plate	0.8800	0.8769	.001935

Being a statistical method the model can be used a number of times and a standard deviation can be found for the average of the effective emissivities from the total number of sample tests. Table 3 shows typical average effective emissivity values obtained with the model and their standard deviations. It also shows the advantage in running the model with more emitted energy bundles. This advantage is tempered by the fact that the calculation time involved in running the model with a grater number of emitted energy bundles is greatly increased. For the values of the table, each run was divided into ten runs where the number of emitted bundles by the first surface is the number in the first column.

Table 3 Average values with Standard Deviation and Number of Bundles Emitted

Number of Emissions	*Average Eff. Emis.*	*Standard Deviation*
100,000	0.88312	0.005647
500,000	0.88328	0.003017
1,000,000	0.88449	0.002089

In order to demonstrate the usefulness of the Monte Carlo model, a simple analysis that cannot be accomplished with the enclosure theory model is presented in Fig. 10. This figure shows the variation of the effective emissivity with the percentage of specularity of the wafer. For this simulation, the emissivity of the wafer is 0.65, but the reflectivity is modeled as a surface that is between a completely diffuse surface and a completely specular surface. In other words, the reflectivity of the wafer is always 0.35, but can be partially diffuse and partially specular. This kind of simulation can represent a real surface better, and is impossible to accomplish with the enclosure model.

The Monte Carlo method shows great promise in modeling optical parameters that are impossible to model with any other methods, but the guard ring and guard tubes need to be incorporated into the model in order to obtain accurate results. The Monte Carlo method is also capable of modeling properties with spectral, angular and temperature dependencies. These modifications need to be incorporated into the model in order to take advantage of the full potential of this method.

CONCLUSIONS AND RECOMMENDATIONS

The enclosure theory model was used to perform parametric studies of the enclosure and to determine the effect of the different parameters. These studies were performed using the total wavelength spectrum as well as the single wavelength method. The studies shows that wafer temperature and emissivity as well as cold plate temperature and emissivity all have a role in the effective emissivity of the wafer. This suggests that in order to achieve accurate temperature measurements using a radiometer these variables need to be well known. The results also show that the single wavelength measurements at $\lambda = 0.95$ μm are largely insensitive to temperature variations in both the wafer and cold plate in this temperature range.

The enclosure method was also used to study the heat flux of the wafer under different conditions in the chamber. The effect of the radiometer opening was studied and it was found that the opening causes temperature non-uniformities on the wafer. The studies also suggest that the cold ring temperature and emissivity can be appropriately selected to provide wafer temperature uniformity. More studies of these phenomena are needed to quantify the effect of these variables, and experimental results are required to verify the findings.

The Monte Carlo model was verified against the enclosure theory model by placing them both under the same conditions. Although these results were statistically similar, the lack of a guard ring and guard tube on the Monte Carlo model makes it hard to conduct studies that can approach reality. This model needs to be expanded to include these guards, and to include spectral properties. The Monte Carlo method was also used to simulate a wafer with partially diffuse and partially specular reflectance. This cannot be accomplished by the enclosure theory method and demonstrates the potential of the Monte Carlo method.

In order to exploit the full potential of the Monte Carlo method the geometry of the chamber needs to be modeled fully. This means that the guard ring needs to be included in the next phase of modeling. The model also needs to be improved by gathering real emissivity data of silicon wafers as a function of angle and wavelength and incorporating these into the model. This may be accomplished by measuring the bi-directional reflectance distribution functions of the wafers and substituting these for the directional-hemispherical properties currently employed by the model.

ACKNOWLEDGEMENTS

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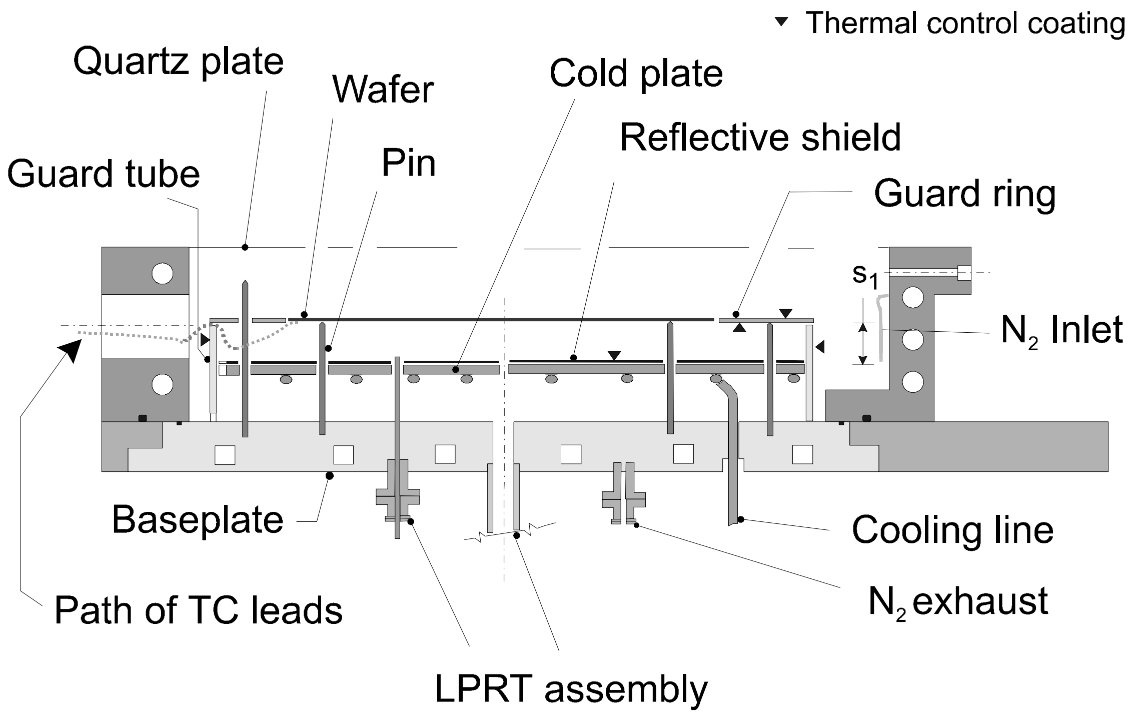

Figure 1 The NIST RTP radiation chamber

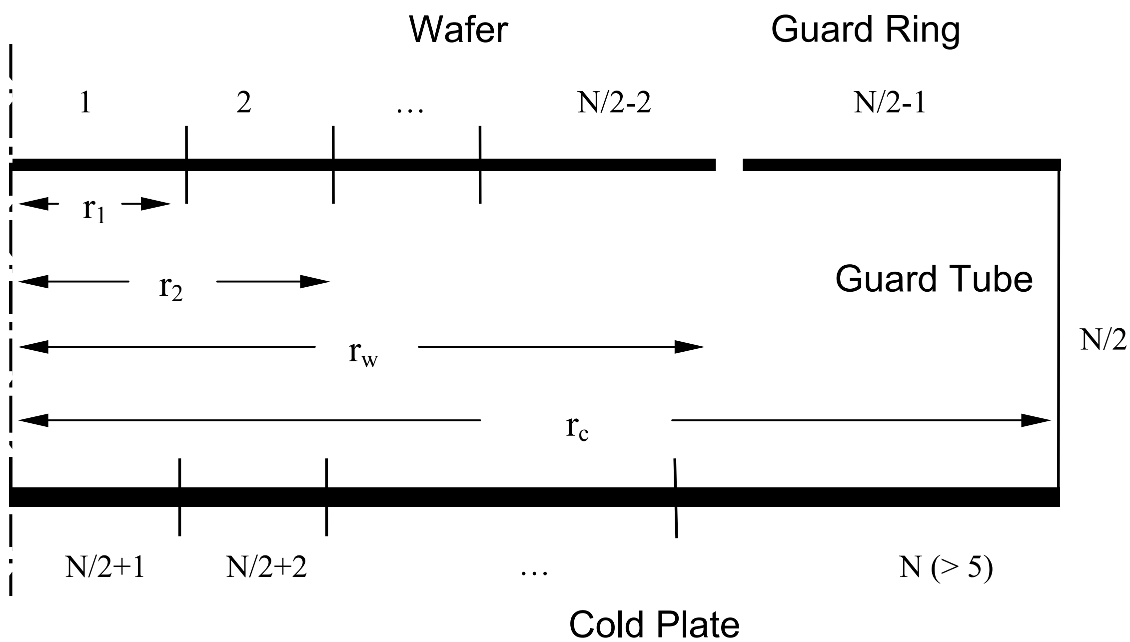

Figure 2 Axisymmetric schematic of the enclosure model

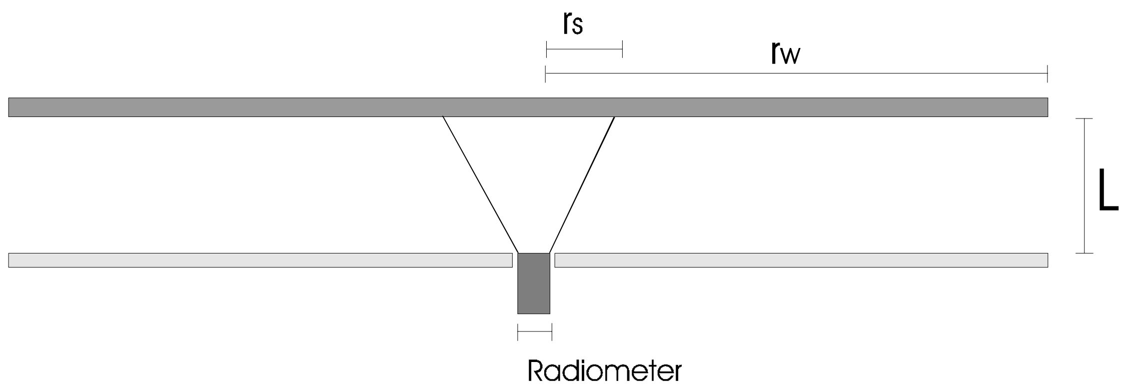

Figure 3 Radiometer and spot size inside the RTP chamber

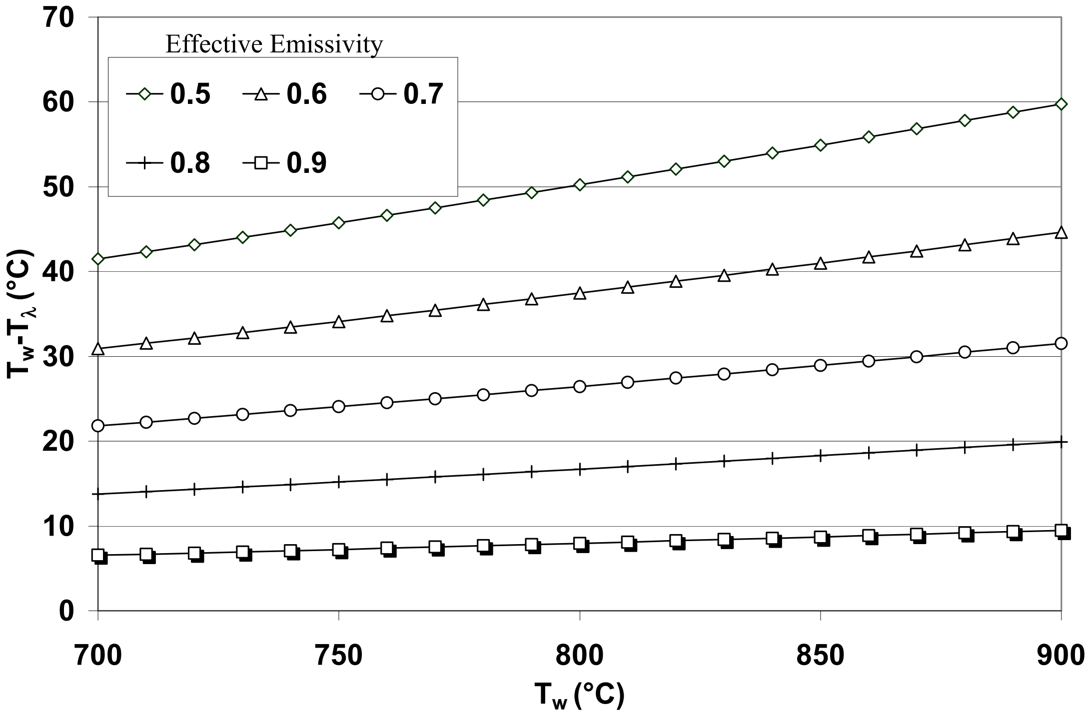

Figure 4 Variation of temperature error with effective emissivity

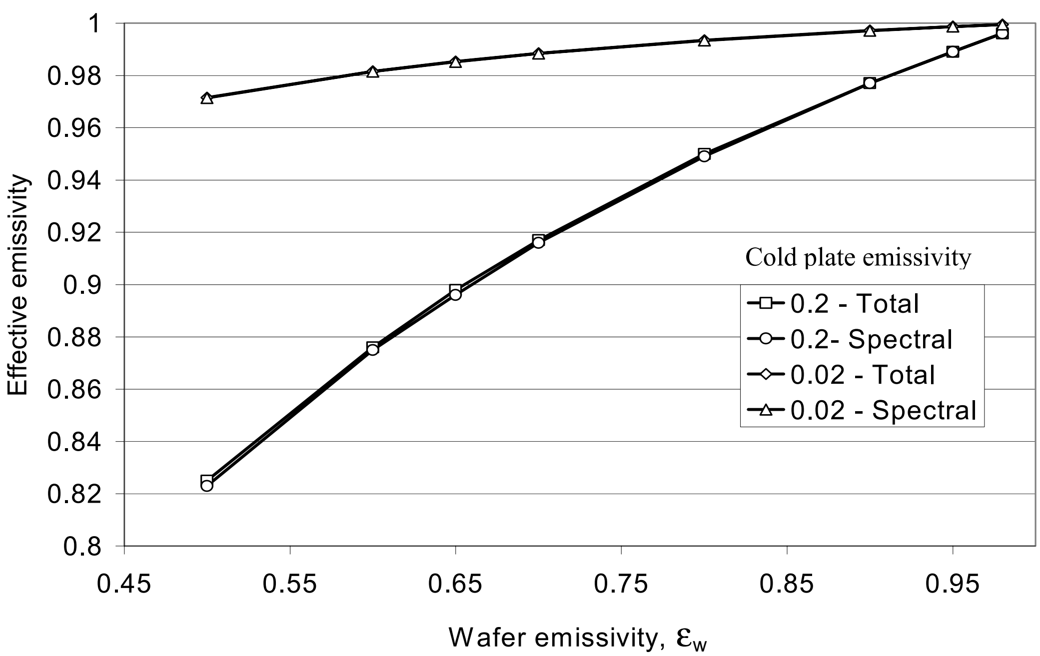

Figure 5 Variation of effective emissivity with wafer emissivity

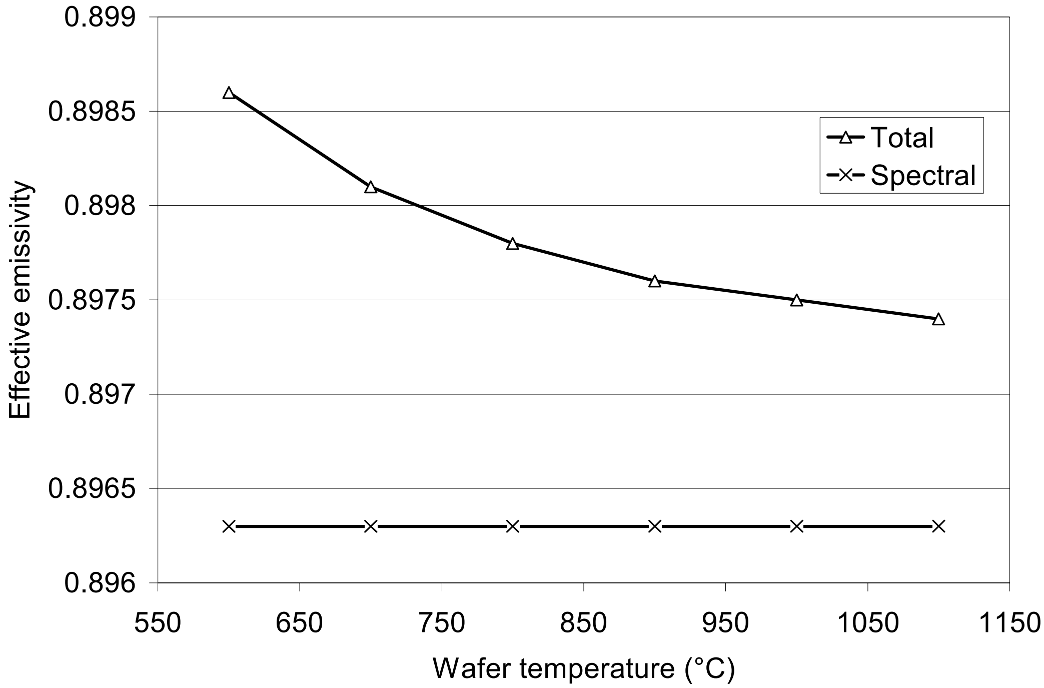

Figure 6 Variation of effective emissivity with wafer temperature

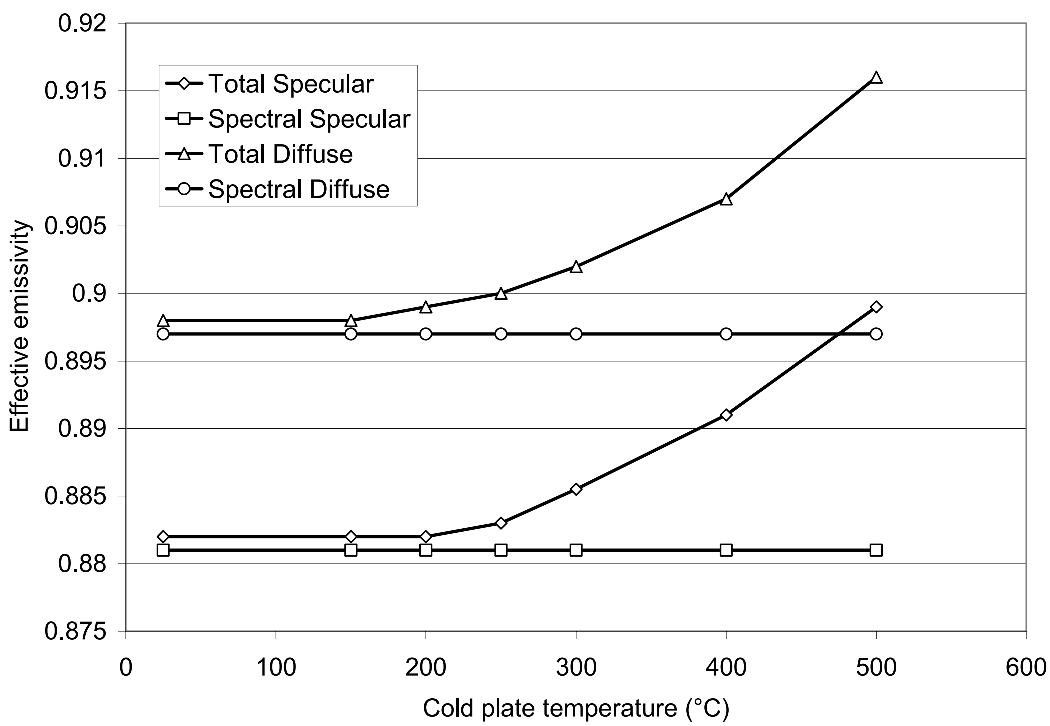

Figure 7 Variation of effective emissivity with cold plate temperature with specular or diffuse bottom surface

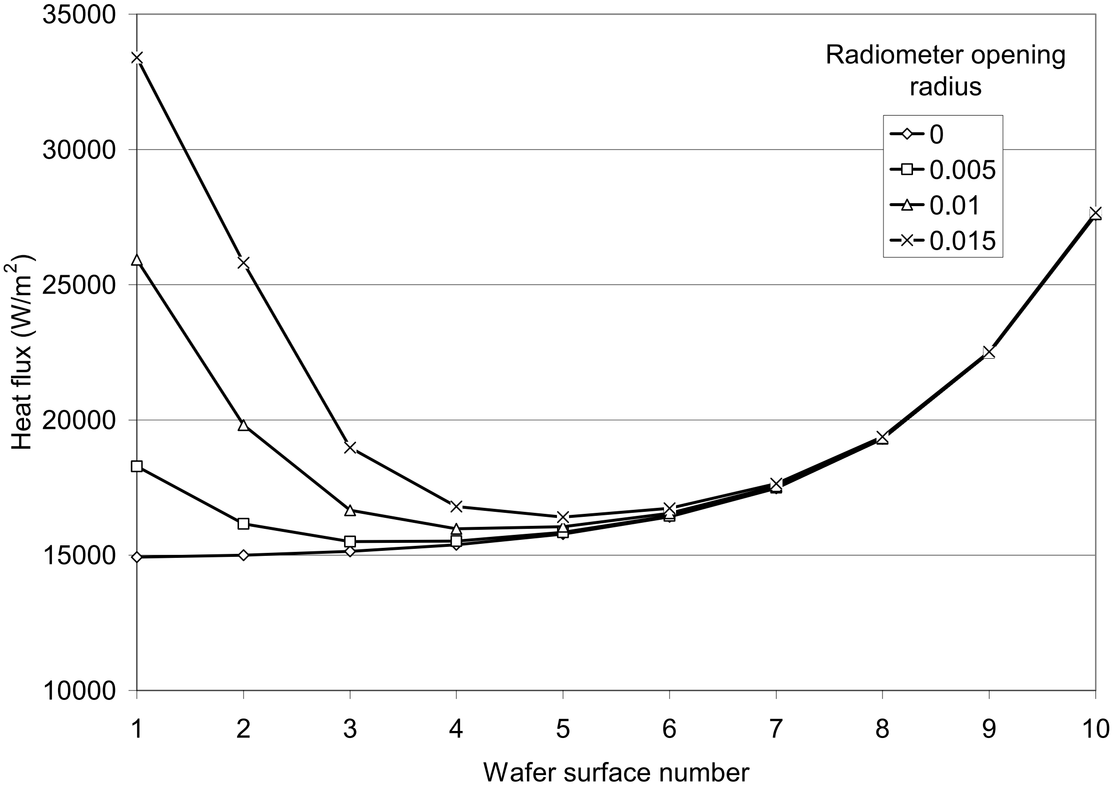

Figure 8 Heat flux of the wafer as a function of radiometer opening size

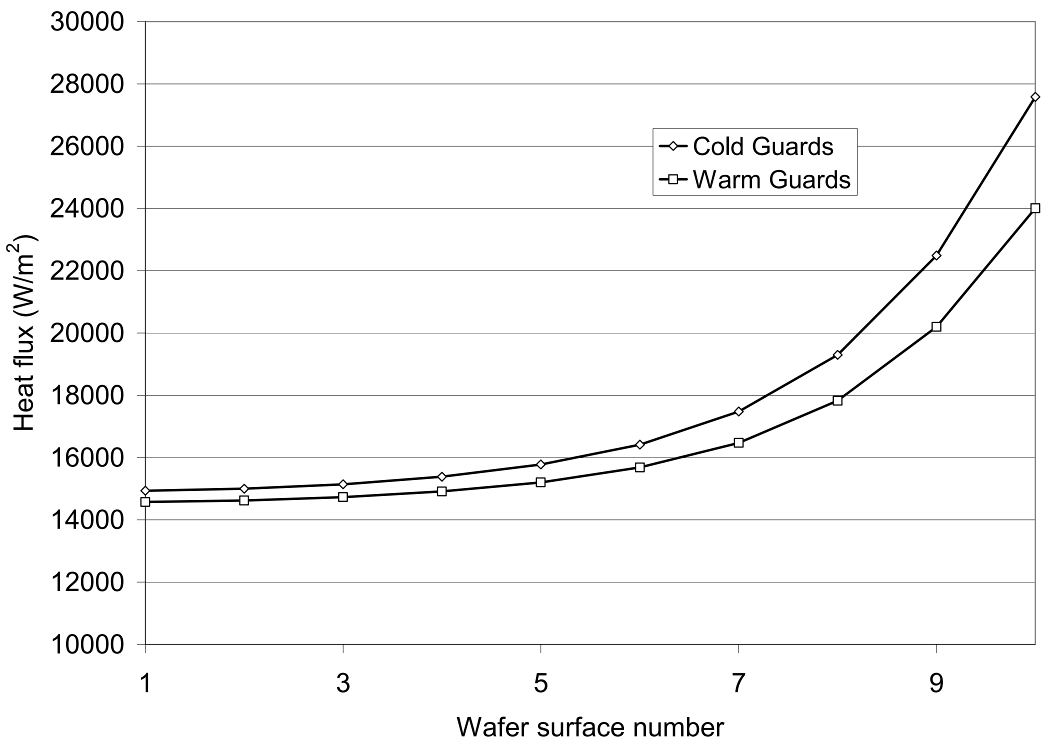

Figure 9 Effect of the guard temperature on the heat flux of the wafer

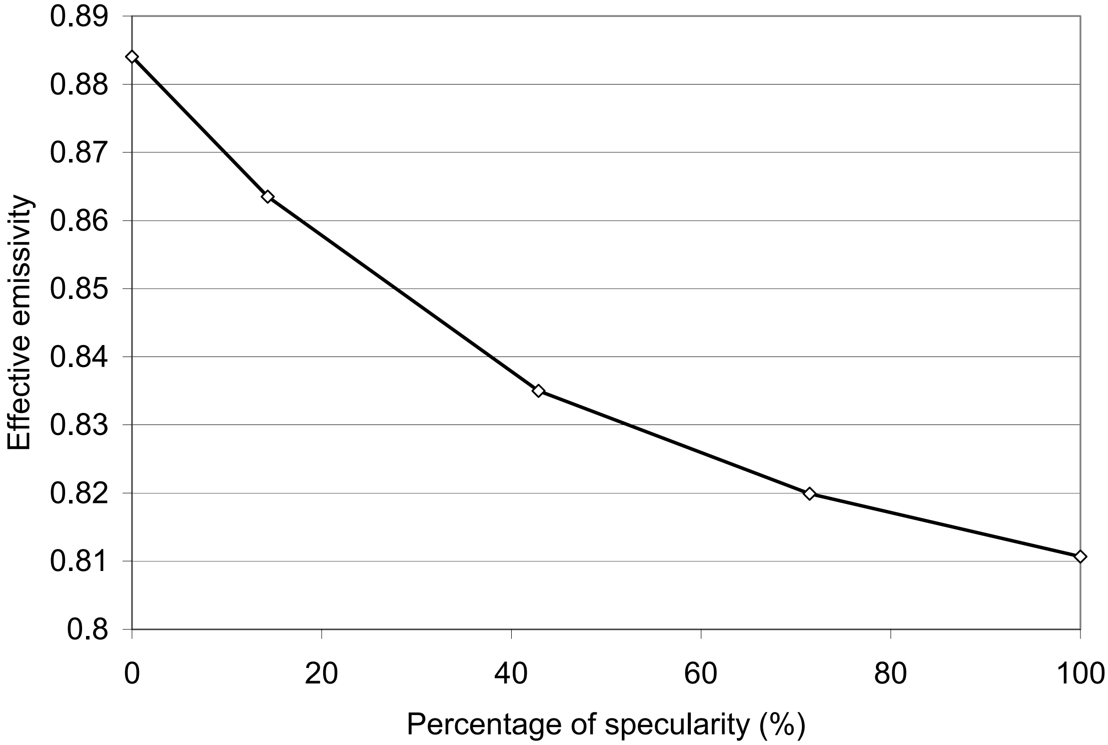

Figure 10 Variation of effective emissivity with wafer specularity