SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES Vol. 5
Edited by S. Selberherr, H. Stippel, E. Strasser - September 1993

Radiative Heat Transfer with Quasi Monte Carlo Methods

A. Kersch and W. Morokoff†

Corporate Research and Development, Siemens AG
Otto-Hahn-Ring 6, D-81739 München, GERMANY
†IMA, University of Minnesota
206 Church Street S.E., Minneapolis, MN 55455, USA

Abstract

Monte Carlo simulation is often used to solve radiative transfer problems where complex physical phenomena and geometries must be handled. Slow convergence is a well known disadvantage of this method. In this paper we demonstrate that a significant improvement in computation time can be achieved by using Quasi-Monte Carlo (QMC) methods to simulate Rapid Thermal Processing.

1. Introduction

Monte Carlo simulation is an indispensable tool for modeling Rapid Thermal Processes (RTP) with an accuracy of a few degrees. Only this method allows very detailed modeling of the physical processes and geometrical complications which arise in real applications involving radiation transport. A well known disadvantage of this method is slow convergence, which has prohibited wide spread usage. In this paper we demonstrate that a significant improvement in computation time can be achieved by using Quasi-Monte Carlo (QMC) methods to simulate radiative heat transfer.

The QMC method [1] involves using deterministic, quasi-random sequences in place of random numbers in a Monte Carlo calculation. One well known example of such a sequence is the Halton sequence. While the idea of quasi-Monte Carlo is almost as old as the Monte Carlo approach itself, these methods have rarely been used in real world engineering problems. This may be attributed to the fact that many Monte Carlo problems are high dimensional, and quasi-random sequences tend to lose their advantage as dimension increases [2][3]. Also, great care must be taken to avoid problems arising from the fact that the quasi-random numbers are not independent.

As the following results show, however, a considerable advantage can be won by applying quasi-random sequences to the modeling of the radiative heat transfer from the heater to the wafer inside Rapid Thermal Processing equipment. Figure 1 shows the draft of the cylinder symmetric projection of a typical single wafer reactor.

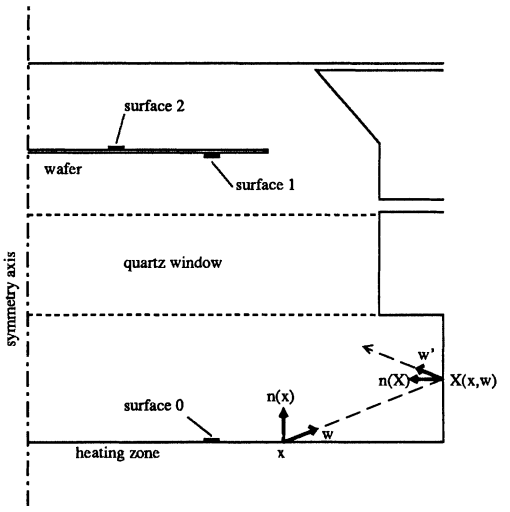

Figure 1: Geometry of the reactor and position of specific surface elements.

2. Description of Radiation Exchange

The radiative energy transfer inside the reactor can be described mathematically by an integral equation for the spectral radiation intensity. The solution of the integral equation leads to a problem of multidimensional integration.

Let D be the interior surface of the reactor, x be a point on D and n_x the interior normal. Let ω be the direction of a radiation bundle and Ω^+ be the half sphere of directions oriented toward the reactor interior. The optical surface properties are described by $a_{\lambda,T}(x,\omega)$, the spectral absorptivity (= emissivity), $r_{\lambda,T}(x)$ the spectral reflectivity and $P_x(\omega \leftarrow \omega')$ the (normalized) probability that a bundle coming from direction ω is reflected into direction ω'. $T(x)$ is the temperature distribution of the surface. $X(x,\omega)$ describes the target of a bundle on the surface starting at x with direction ω. We restrict ourselves to opaque surfaces.

The iterative solution of the integral equation leads to a series expression for the distribution E_λ of radiation intensity impinging on the surface, $E_\lambda = \sum_{k=1}^{\infty} E_\lambda^{(k)}$, where

$$E_\lambda^{(k)}(x) = \int_{[D]^k} \int_{[\Omega^+]^k} a_{\lambda,T}(x,\omega) r_{\lambda,T}(y_{k-1}) \dots r_{\lambda,T}(y_1) P_{y_{k-1}}(\omega \leftarrow \omega_{k-1}) \dots P_{y_1}(\omega_1 \leftarrow \omega_0)$$

$$\delta(x - X(y_{k-1}, \omega_{k-1})) \dots \delta(y_1 - X(y_0, \omega_0))\, a_{\lambda,T}(y_0, \omega_0) I_{\lambda,T}^{BB}(y_0)\, (d\omega)^k (dy)^k$$

The series may be truncated such that the remaining terms are smaller than the desired accuracy. The dimension of integration is $2k + 2 + 1$ in the k-th step (2 dimensions for the initial position, one dimension for the spectral distribution). In case of specular reflection, $P_x(\omega \leftarrow \omega') = \delta(\omega - \omega' + 2(n_x \cdot \omega')n_x)$ and the path is determined completely by the initial direction. The dimension of integration in this case is only 2+2+1. The above procedure is the fractional absorption method. When a probability for a complete absorption is introduced, we can call it a discrete absorption method. This method introduces one more dimension of integration for every discrete process.

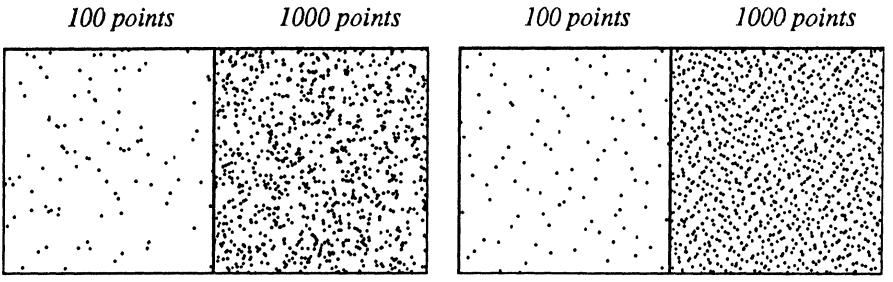

Figure 2: Points with pseudo-random sequence, with quasi-random sequence

3. The Computational Experiment

The goal of the experiments was to determine the accuracy of the amount of heat transfer between surface elements as a function of computation time. We show here the results for specularly reflecting surfaces. The first step towards this goal was to compute error size as a function of N, the number of rays emitted from the source. This error size was determined by calculating results for an ensemble of 30 experiments for every choice of N and taking the standard deviation. In a typical experiment, N rays were emitted from a surface or point source located at *surface 0*. The initial direction was sampled using Lambert's Law, which means that the elevation angle was sampled from a cosine distribution, while the azimuthal angle was sampled from a uniform distribution on $[0, 2\pi]$. The sampling was done using one point from a multi-dimensional quasi- or pseudo-random sequence, such that two angles were assigned separate dimensions. A further dimension was used to sample the initial energy of the ray from Planck's black body distribution.

In the standard Monte Carlo method in which a pseudo-random sequence is used as the source of integration nodes, the expectation of the integration error for the integral $\int f(\mathbf{x})d\mathbf{x}$ is

$$\epsilon(f, N) = \sigma(f)N^{-\beta} \tag{1}$$

with $\beta = 0.5$. For many problems, quasi-random sequences [4] significantly outperform random sequences in the range of practical N. The convergence rate is generally between $\beta = 0.5$ and $\beta = 1.0$. The best way to predict performance for a specific type of problem is to analyze the results for a test problem, as is done below. Figure 2 shows the coverage of the 2-D cube with points generated from a pseudo-random sequence and a Halton sequence.

4. Results

In Figure 3 we show results using the fractional energy absorption method and specularly reflecting surfaces.

Figure 3 shows the expected relative error $\epsilon(N)$ as a function of the number of emitted rays N for the Halton sequence and a pseudo-random sequence using the fractional absorption method with a constant surface absorptivity of 0.4. Results are given for *surface 1* and *surface 2* on the wafer. The plotted points are the calculated errors for various N (averaged over 30 runs), while the lines are a least squares fit of the data to the functional form (1).

Figure 3 illustrates a clear advantage of using a quasi-random sequence over a pseudo-random sequence in the calculation, both in error size and in convergence rate (i.e., β). The error in calculating the energy transfer to *surface 1* with $N = 100000$ is over a factor of three smaller if the Halton sequence is used than if a random sequence is used.

In our computational experiments we studied several factors like surface absorptivity, position of wafer surface to heat source, and choice of quasi-random sequence. A comparison of the fractional and discrete absorption methods was also made. Results show accelerated convergence and improved accuracy of QMC over the standard Monte Carlo approach, and indicate when the fractional and discrete absorption methods should be used to obtain optimal results.

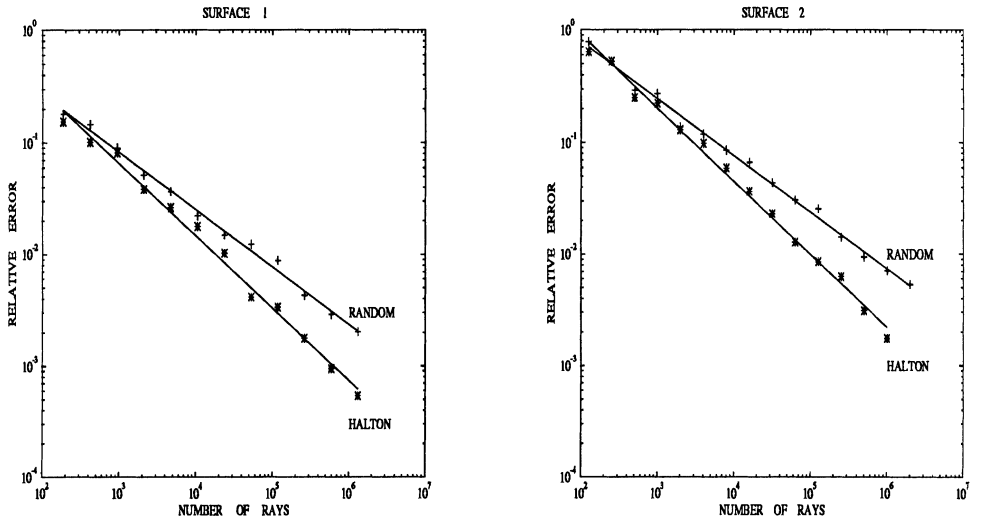

Figure 3: Comparison of random and quasi-random sequences using the fractional absorption method with absorptivity = 0.4.

References

[1] J.H. Halton, *On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals*, Numer. Math. 2, 84-90, 1960.

[2] W.J. Morokoff and R.E. Caflisch, *Quasi-random sequences and discrepancy*, SIAM Sci. Comp. (to appear).

[3] W.J. Morokoff and R.E. Caflisch, *Quasi-Monte Carlo Integration*, submitted to J. Comp. Phys. (1991).

[4] H. Niederreiter, *Random number generation and quasi-Monte Carlo methods*, SIAM Regional Conference Series in Applied Mathematics, CBMS-NSF 63, 1992.