

A numerical simulation method for the laser-induced temperature distribution

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A numerical simulation approach for the evaluation of temperature distribution in a substrate during the laser processing is developed. The explicit finite-difference solution of the heat (diffusion) equation is chosen as the starting point in order to simply retain general nonlinearity, physical transparency, and flexibility of the procedure. The method is tested with a simulation of silicon substrate irradiated by cw argon laser, and the results are compared with those from experiments and exact analytical results, where available. Deficiencies due to the omission of the nonlinearity, i.e., the temperature dependency of the material properties, in the results of approximative analytical approaches are discussed.

I. INTRODUCTION

Laser processing has become a widely used tool in a variety of technical applications. This is mainly due to the high spatial resolution it offers, precision in spatial control, and flexible use of the different beam parameters and power. The spatial resolution is limited mainly by the wavelength and beam divergence, and technically the submicrometer accuracy is attainable with a standard optical setup. Therefore, laser processing has found a large field of applications in microelectronics.^{1,2}

Most of the laser processing applications are based on the energy absorption in the form of heat, locally at the spot of the laser beam. Typical applications in microelectronics are annealing, cutting, joining, etching, and pyrolytic chemical vapor deposition. In development and design of the processing techniques understanding of the basic phenomena involved is needed. The spot temperature, which primarily depends on the laser power and beam width, and the properties and structure of the substrate, plays a central role. Basically, the whole temperature distribution in the substrate is of interest as the underlying driving force in the surface and bulk chemical processes. Furthermore, the temperature distribution in the substrate should be carefully controlled in the post-processing of circuit containing structures to avoid their thermal damage. For these reasons the temperature distribution and its time evolution have been extensively examined using analytical models,³⁻⁶ numerical calculations,⁷⁻¹² and experimental methods.¹³ The *in situ* experimental methods are, however, relatively few and limited, leaving many open questions to be investigated.

A numerical simulation is a straightforward approach for tracing the important factors and values of key parameters without too many limiting approximations, even in the case of the most nonlinear system. Therefore, it provides a rapid and cheap aid for solving instantaneous technical problems, too. A simulation composed of well-known elementary processes may also be a comprehensible starting point for higher level models, or it may be a completing realization of an analytical approach.

In this paper we report a simulation procedure, which is simple and therefore general, without the usual limitations

of analytical approaches. It is numerically based on the finite-difference solution of the heat conduction equation and physically composed of the elementary processes. Therefore, the procedure is physically transparent and the inclusion of other temperature-driven processes like etching, deposition, diffusion of dopants, etc., becomes straightforward. Furthermore, the inclusion of temperature dependence in heat conductivity, adsorption coefficient, surface reflectivity, and heat capacity, which we have found essential, is easily accomplished. We have tested the procedure for the cw argon laser-irradiated silicon substrate, with a reference to the results of experiments and analytical approaches, which usually omit most of the temperature dependencies. Further results for some layer structures are given elsewhere¹⁴ and work towards the simulation of film growth and direct laser writing is in progress.

In the next section we describe the numerical procedure and discuss its relations to the other alternatives available. The third section contains the results of the spot temperature and temperature distribution dependence on various parameters, and comparisons with other published data. Finally, the last section contains conclusions.

II. NUMERICAL APPROACH

The model describes the time evolution and the asymptotic stationary state of the temperature distribution in a semi-infinite homogeneous substrate irradiated with a laser beam. The elementary processes included so far are the incident beam reflection and penetration into the substrate, absorption with conversion to heat in the substrate, and the consequent heat diffusion. The explicit numerical simulation does not impose restrictions on the laser beam intensity distribution, temperature-dependent reflectivity or absorption. If essential, it is also possible to allow absorbed energy transport in some other form before transformation to heat.

A. Power absorption

To compare with published data, we have used the Gaussian intensity distribution for the incident laser beam, which is aligned perpendicularly to the substrate surface.

For the incident laser power $P_0 = \pi w^2 I_0$ the total absorbed intensity distribution at the surface ($r = \sqrt{x^2 + y^2}$, $z = 0$) then becomes

$$I(r, 0, T_s) = [1 - R(T_s)] I_0 e^{-r^2/w^2}, \quad (1)$$

where I_0 is the (maximum) intensity at the spot center, $R(T_s)$ is the reflectivity at the surface temperature $T_s(r) = T(r, 0)$ and w is the "1/e value" of the spot radius, defining the spot diameter $d_s = 2w$. The penetrating intensity is assumed to decay according to

$$I(r, z, T) = I(r, 0, T_s) e^{-\int_0^z \alpha(T) dz}, \quad (2)$$

where $\alpha(T)$ is the absorption coefficient and the temperature $T(r, z)$ depends on the space coordinates explicitly. To assure the energy conservation in the numerical procedure the domain considered is divided into volume elements $\Delta V = \Delta x \Delta y \Delta z$ around the grid points, where the absorbed power per unit volume is evaluated from the intensity decay as

$$p(r, z, T) = \Delta I(r, z, T) / \Delta z, \quad (3)$$

with ΔI evaluated from Eq. (2).

B. Solution of the heat equation

From the assumption that the heat flux is proportional to the temperature gradient and the continuity equation, the equation for the heat transfer is obtained,

$$\frac{\partial \epsilon}{\partial t} = \nabla \cdot (k \nabla T) + p. \quad (4)$$

Here, k is the heat conduction coefficient, ϵ is the heat (energy) per unit volume, and p is the source (or loss) of heat from Eq. (3). Substitution $d\epsilon = c\rho dT$ gives the conventional parabolic (diffusion) equation,

$$c\rho \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + p, \quad (5)$$

where c and ρ are the specific heat and mass density of the material, respectively.

Let us consider an orthogonal coordinate system and temperature-dependent heat conductivity $k(T)$. The finite difference for the x component of the heat conduction term $\nabla \cdot (k \nabla T)$ can be written using three consecutive grid points, labeled x_1 , x_2 , and x_3 . Then, at x_2 ,

$$\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) \Big|_{x_2} = \left(k_b \frac{T_3 - T_2}{x_3 - x_2} - k_a \frac{T_2 - T_1}{x_2 - x_1} \right) / \Delta x_2, \quad (6)$$

where Δx_2 is the size of the element around x_2 . In Eq. (6) we have introduced two values of the heat conduction coefficient, k_a and k_b . The term $k_a (T_2 - T_1) / (x_2 - x_1)$ is the heat flux from x_1 to x_2 , or between the volume elements around these points. Formula (6), if written at the grid point x_1 , contains the same flux term, where it is now essential to use the same value k_a of the heat conductivity. It simply assures that the heat flux out from the volume element around the grid point x_1 is equal to that into the adjacent volume element around the next grid point x_2 , taking care of the energy conservation. It should be noticed that first resolving $\nabla \cdot (k \nabla T) = \nabla k \cdot \nabla T + k \nabla^2 T$ leads to more complex discretization, and in particular, neglect of the term $\nabla k \cdot \nabla T$ means neglect of the energy conservation.

The heat flux conservation condition for the heat flow from x_1 to x_2 can be used to find an estimate for k_a in terms of k_1 and k_2 . It leads to the evaluation of arithmetic average of the heat resistances $1/k$ rather than the average of the heat conductances k , and results in the form

$$k_a = 2k_1 k_2 / (k_1 + k_2), \quad (7)$$

written for the point a , midway between x_1 and x_2 .¹⁵

The first-order difference seems to be accurate enough for the time derivative at the left-hand side of Eqs. (4) or (5). It has proved not to be crucial in description of the time evolution, and in particular, the stationary state is independent of the details of time discretization. Furthermore, in search of the stationary state only, we may consider the length of the time step as just a mixing or extrapolation factor between two sequential iteration steps.

C. Boundary conditions

Numerical methods involve boundary conditions (BC) at the boundaries of the explicitly treated domain. If the volume of interest has some symmetry, only a part of the system may need be considered and the properties of the whole volume are obtained through the symmetry operations of the system. In such a case the same symmetry operations define also natural BC for the faces between the reduced parts of the whole volume.

In the simulation of time evolution, the time dependence should be included in the BC, and in the case of complex layer structures, sophisticated considerations of the heat flow might be needed.¹⁶ Usually, the boundaries are set far enough into the region of the asymptotic behavior of all involved processes, unless the BC are meant to have some influence in the simulation by purpose.

The BC in our case may be defined by the known heat flux sufficiently far from the laser spot, "sufficiently far" meaning at the hemisphere of the size where the absorption region (spot) may be considered pointlike. For the stationary state, this results in the condition

$$\frac{\partial T}{\partial r} = - \frac{P}{2\pi k r^2}, \quad (8)$$

or

$$T = (A/r) + T_\infty, \quad (9)$$

where P is the total absorbed power, T_∞ is the asymptotic (environment) temperature, and A is computed during the calculation. We have adopted this condition in the form of a loss term at the boundary. Condition (9) does not fully take into account the time evolution at the boundaries, but provided that only the asymptotic stationary temperature distribution is of interest, the BC (9) is sufficient.

For the simulation of time evolution we have used BC

$$T = (B e^{-\lambda r} / r) + T_\infty, \quad (10)$$

where now two adjustable parameters B and λ appear. This form will be shown to be flexible enough to follow the time evolution at the boundaries of relatively small grids. BC (9) and (10) lead to the same stationary state, but BC (9) gives faster convergence. Thus, a procedure using (9) can be considered to be a fast iteration towards the stationary state rather than a simulation of time evolution.

The surface boundary conditions are derived from the zero heat flux through the surface and most conveniently accomplished by setting the heat conductivity to zero. This is independent of the grid point distribution, which may be defined basically in two ways at the surface. The surface boundary can be either at a grid point or between two adjacent grid points. Setting the surface boundary halfway between the grid points leads to a simple grid structure with equal volume elements around all grid points. With a coarse grid this requires an extrapolation of the surface temperature, which is directly obtained with the other choice where the grid point is located at the surface boundary. The latter choice on the other hand, leads to either a concept of a partially filled volume elements or can be included by a scheme with volume elements where the representative grid point is located far from the volume element centerpoint. Also, with nonequidistant grids the latter choice, as an advantage, allows the volume element faces to be located at the midway between two grid points, thereby giving higher accuracy or simplifying the use of relations like Eq. (7).

For the sake of testing, we have applied both of these two alternatives, and found them equal in results. In the following calculations we have adopted the latter scheme, which gives the surface temperatures directly.

III. CALCULATIONS AND RESULTS

We have carried out various tests of grid size, time evolution, and boundary conditions for the linear equation (temperature-independent parameters) and nonlinear equation (temperature-dependent parameters). The temperature distributions from the linear calculation can be compared to the exact analytical data and those from the nonlinear calculation can be compared to the experiments and analytical approximations. In the following, we therefore consider a Gaussian-shaped beam with the diameter $d_s = 5 \mu\text{m}$ defined by the $1/e$ value of the intensity, initial power $P_0 = 0.8 \text{ W}$ (or 0.5 W) and the initial Si substrate temperature $T_\infty = 300 \text{ K}$.

A. Linear case

In the linear equation we have first set $k = k(652 \text{ K}) = 0.5416 \text{ W/cm K}$, $c = 1 \text{ J/g K}$, and the transmission $1 - R = 0.6$ (leading to the absorbed power $P = 0.48 \text{ W}$), which are reasonably close to the physical parameters of silicon for the laser light with $\lambda = 514 \text{ nm}$ and the temperatures considered. The heat conductivity is justified to give the temperature rise of 1000 K at the spot from the analytical solution³ for the stationary state $T_{\text{max}} = P/2\sqrt{\pi kw} + T_\infty = 1300 \text{ K}$. The laser power is let to absorb and transform into the heat at the top surface layer, physically meaning very large (infinite) absorption coefficient α . We first consider the spot temperature (maximum temperature at the surface and spot center) as a parameter that describes the quality of the calculation.

To find the maximum step length for the numerical grid, evaluation of T_{max} was carried out using grid the size of $10 \mu\text{m}$ (outwards from the spot center to each direction), and the $1/r$ boundary condition in Eq. (9), until the convergence

criterion $0.2 \text{ K}/\mu\text{s}$ was achieved. We obtained the spot temperatures $T_{\text{max}} = 1243, 1276, \text{ and } 1293 \text{ K}$ with the step lengths $2, 1, \text{ and } 0.5 \mu\text{m}$, respectively. So, the step length $0.5 \mu\text{m}$, i.e., one-tenth of the spot diameter, seems to be small enough to be used for finding a reasonably accurate stationary spot temperature in the linear case.

A closer examination revealed the obvious fact that step size along the z axis (perpendicular to the surface) is more crucial due to the infinite absorption coefficient. It was found out also that larger step lengths can be used further away from the beam region without considerable loss of accuracy. Therefore, in order to save computer capacity in the following calculations we have employed a horizontal grid of 12 steps outwards from the spot, the first six steps being $0.5 \mu\text{m}$, the next five steps being $1 \mu\text{m}$ each and the last $2 \mu\text{m}$, ranging to $10 \mu\text{m}$ from the spot. The vertical grid consists of 14 steps starting with four $0.25\text{-}\mu\text{m}$ steps, four $0.5\text{-}\mu\text{m}$ steps, and four $1\text{-}\mu\text{m}$ steps and ranging to $10 \mu\text{m}$, as well. This grid gives $T_{\text{max}} = 1290 \text{ K}$ for the linear case. Much less computer time is consumed also by first using a coarse grid, which allows longer time steps, and then continuing with the final dense grid to the stationary state.

The time evolution of the spot temperature T_{spot} (towards T_{max} is shown in Fig. 1 for different boundary conditions and grid sizes. We see that simulation with the large grid ($50 \mu\text{m}$) gives relatively accurate shape of the exact time evolution of the spot temperature. The simulation with the grid of $10 \mu\text{m}$ does not differ very much from that, if the boundary condition (10) is used. But the use of a small grid ($10 \mu\text{m}$) and BC (9) speeds up the convergence to the stationary state beyond the correct time evolution, the rate depending on both the grid size and the step length. The convergence is achieved even in less than $20 \mu\text{s}$ of simulation

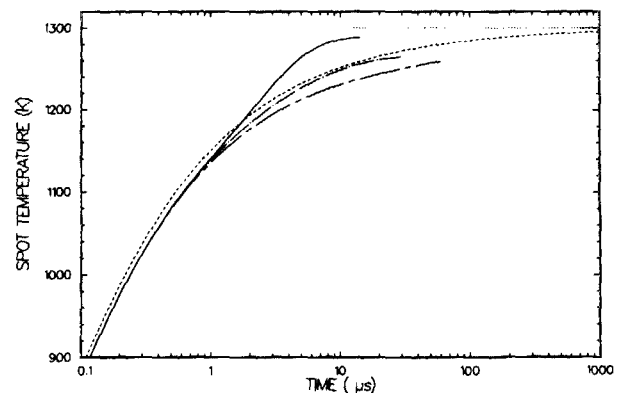


FIG. 1. The simulated time evolution of the spot temperature T_{spot} using the temperature-independent material parameters (linear case) and infinite absorption coefficient ($\alpha = \infty$) compared to the exact analytical solution (dashed curve). The dotted curve indicates the asymptotic stationary limit. The solid curve presents the "iteration" with BC (9) and $10\text{-}\mu\text{m}$ -grid, chain-dotted, and chain-dashed curves show the time evolution when BC (10) is applied with grid sizes 10 and $50 \mu\text{m}$, respectively. All calculations correspond to the spot diameter $5 \mu\text{m}$, incident power $P_0 = 0.8 \text{ W}$, and surface reflectivity $R = 0.4$, and the constant heat conductivity justified to that at 652 K in order to result in 1000 K rise from 300 K . All simulated time evolutions are cut off at the "convergence" limit $0.2 \text{ K}/\mu\text{s}$.

time (less than $6 \mu\text{s}$ for $P_0 = 0.5 \text{ W}$), while the real time evolution requires about $200\text{--}500 \mu\text{s}$ to achieve the same rise of spot temperature. Hence, we conclude that for the correct time evolution a large grid or time-dependent BC are required, while if only the stationary state is of interest, a small grid and the correct stationary state BC are more useful forcing the iteration (rather than simulation) to a rapid convergence.

B. Temperature-dependent parameters

The use of a finite but constant absorption coefficient α lowers the spot temperature due to the beam penetration into the surface. For the Ar^+ laser and silicon we have used the expression¹⁷

$$\alpha(T) = 6.28 \times 10^3 e^{T/430} \text{ cm}^{-1} \quad (11)$$

for the absorption coefficient, where T is written in kelvins (K).

The heat conductivity of silicon has been fitted to the experimental data^{18,19} as

$$k(T) = \begin{cases} 0.00717e^{-0.003719(T-1700)} + 0.210 & \text{if } T > 719.83, \\ 311.1/(T-77.8), & \text{otherwise,} \end{cases} \quad (12)$$

in units W/cm K . Implementation of $k(T)$ from Eq. (12) leads to higher or lower spot temperature compared to the use of the constant value above, depending on the laser power. The constant value $k = 0.5416 \text{ W/cm K}$ was justified to give 1000 K rise for the spot temperature at incident power $P_0 = 0.8 \text{ W}$.

The reflectivity of silicon is given by⁵

$$R(T) = 0.367 + 4.2 \times 10^{-5} T. \quad (13)$$

Its temperature dependence is weak and it does not affect T_{max} much for $P_0 = 0.8 \text{ W}$. The specific heat, fitted to the data in Ref. 20, in units J/g K , is

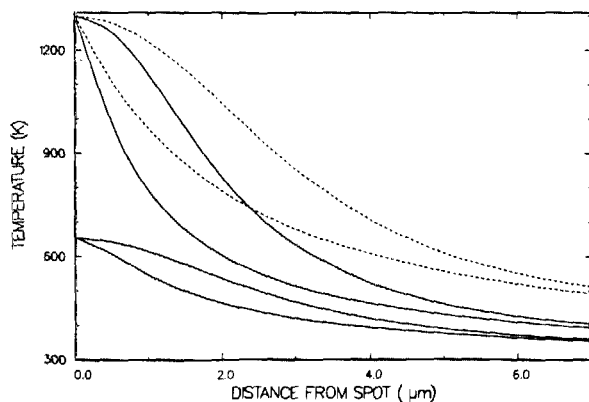


FIG. 2. The stationary surface and depth temperature profiles (the upper and the lower of the two curves, respectively) for the temperature-dependent (solid curves) and temperature-independent constant material parameters with $\alpha = \infty$ (dashed curves). The four uppermost curves correspond to the incident power $P_0 = 0.8 \text{ W}$ and the two lowest to $P_0 = 0.5 \text{ W}$, with $5\text{-}\mu\text{m}$ spot width. The temperature-independent heat conductivity (dashed curve) is justified, as explained in the text of Fig. 1, to match the spot temperature to that of the temperature-dependent case for 0.8 W (solid curve).

$$c(T) = \begin{cases} 0.8472 - 6.506 \times 10^{-6} (573 - T)^{1.77} & \text{if } T < 512.77, \\ 0.7555 + 0.0001609T, & \text{otherwise.} \end{cases} \quad (14)$$

It has an effect on the time evolution but does not affect to the stationary state. The mass density of silicon was taken as $\rho = 2.33 \text{ g/cm}^3$.

In Fig. 2 the temperature distributions from the linear and nonlinear calculations are compared, and in Fig. 3 the curves of constant temperature in the xz plane are shown. We see that the linear equation leads to a much too wide temperature distribution. Also scaling down the linear spot temperature from 1300 K (-300 K) by $0.5 \text{ W}/0.8 \text{ W}$ gives 925 K , which is much higher than the 650 K from the nonlinear calculation in Fig. 2. This shows the importance of the temperature dependence of the material properties. However, fortuitously good results can be obtained by suitably fitting the parameters for a certain power, beam width, or substrate temperature.

From Fig. 3 we can estimate that at the $10\text{-}\mu\text{m}$ distance from the spot the equitemperature surfaces are almost spherical, which explains the success of the use of such a small computation domain. It can be shown³ that the equitemperature surfaces for a temperature-independent heat conductivity case have the same shape with those in Fig. 3, they only correspond to different temperatures.

C. Laser power dependence

The numerically calculated spot temperature T_{max} dependence on the incident power P_0 is shown in Fig. 4. A comparison with the experimentally measured spot temperatures¹³ shows a good overall agreement.

The dashed curves give the theoretical limits³ in a sense that the upper and the lower curves correspond to the infinite and room-temperature absorption coefficients α , respectively. In practice, the value of α varies from 1.26×10^4 to $3.16 \times 10^5 \text{ cm}^{-1}$ for the temperatures from 300 to 1685 K (Si melting point). The temperature dependence of the heat conductivity is included through Kirchhoff transformation. It should be noted here that the linear model would imply

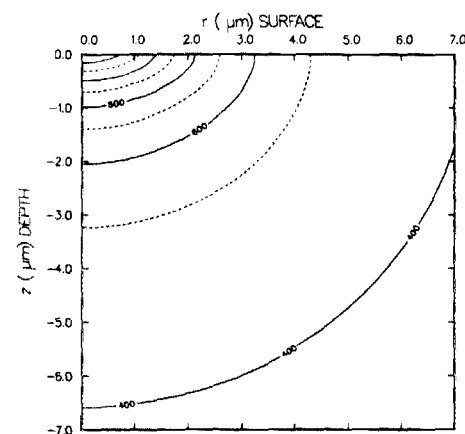


FIG. 3. The curves of constant temperature in the xz plane for the nonlinear case, incident power $P_0 = 0.8 \text{ W}$ and spot diameter $5 \mu\text{m}$. These curves, in a way, "connect" the two uppermost solid curves in Fig. 2.

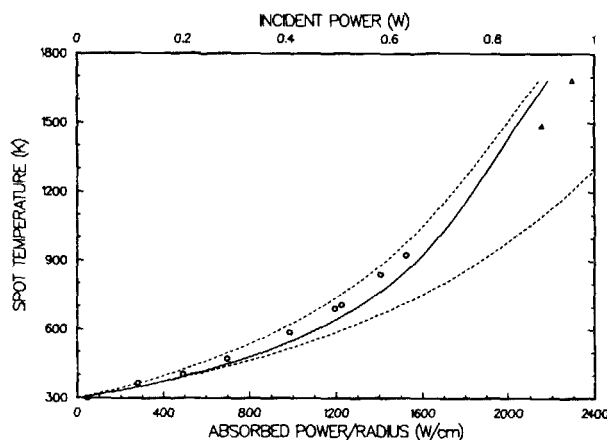


FIG. 4. The spot temperature as a function of laser power/spot radius. The full curve is our calculated result for which the approximate $[R = R(T)]$ incident powers P_0 are given at the upper horizontal axis corresponding to the $5\text{-}\mu\text{m}$ spot width. The open circles and triangles are experimental¹³ results for $\lambda = 514\text{-nm}$ wavelength and multiline light of Ar laser, respectively. The dashed curves are "theoretical" results with the surface reflectivity $R = 0.4$, absorption coefficients $\alpha = \alpha(300\text{ K})$ (lower curve) and $\alpha = \infty$ (upper curve), and Kirchhoff transformation for including the correct temperature dependence of the heat conductivity.

just a linear rise of the spot temperature versus absorbed power. Numerical integration was used to evaluate the effects from both the finite absorption coefficient and the temperature dependence of the heat conductivity on the "theoretical" curves in Fig. 4.

The simulated curve behaves reasonably in respect with the theoretical limits, first following the room-temperature curve and then approaching the upper limit at higher temperatures. On the other hand, there exist analytical results, which deviate remarkably from ours. A major part of the deviation can often be explained by the neglect of the finite $\alpha(T)$ in analytical approaches, although even in that case the resulting upper limit curve can be considered to be in a reasonable agreement with experiments, see Fig. 4. However, this may not be the case with more complex substrate structures.

IV. CONCLUSIONS

We have found numerical finite-difference simulations straightforward, and therefore also a transparent way of including all nonlinearities, i.e., temperature dependencies, in the solution of heat equation. Simulations are also very simple and flexible in changing and extending the used model. Time evolution of the three-dimensional temperature distributions can be followed explicitly, if pulsed lasers or time-dependent phenomena are of interest. In that case, however, the boundary conditions should be carefully chosen. On the other hand, boundary conditions can be used to speed up convergence to the stationary state.

In our experience, the largest limitations are presently found in the computer capacity, which often permit calculations with only a coarse numerical grid, at least in the preliminary approaches. On the other hand, with careful modeling and discretization of the equations rapid convergence in

the temperature distributions with respect to space and time grids can be achieved. In the present case this means the proper choice of boundary conditions and numerical parameters, and furthermore, taking care of the energy conservation in the discretization of equations.

These kind of simulations can be used as a completion of analytical models as well as an aid in experiments or process design of microelectronics. Temperature distribution is the basic quantity behind the dynamics of solid-state chemistry and surface reactions, and it must be accurately known in order to reliably obtain qualitative and quantitative predictions. Power dependence of the temperature distributions in the micrometer scale, which is in a central role in process design, can be reliably found as we have shown in this work. This may be a valuable tool, especially in process design involving complex substrate structures with layers or even components.

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