

NUMERICAL SIMULATION OF TEMPERATURE DISTRIBUTIONS IN LAYERED STRUCTURES DURING LASER PROCESSING

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A numerical simulation approach for the evaluation of temperature distribution in layer structured substrates during laser processing is introduced. The explicit finite-difference solution of the heat equation is used and the full non-linearity of the heat diffusion is taken into account by temperature dependent substrate parameters. The heat equations for layered structures are solved using both rectangular and cylindrical coordinate systems. The method is applied to CW Ar⁺ laser-induced temperature distributions in some commonly used layer structures in microelectronics, such as silicon on sapphire (SOS) and SiO₂ coated silicon. Results are compared with experiments.

1. Introduction

Laser processing of surfaces and interfaces has become a standard tool in a variety of applications, especially in microelectronics [1,2]. The applications, such as annealing, chemical vapour deposition, etching, cutting and joining, are mostly based on the conversion of laser energy to heat in the absorption process, even in the micrometer scale of layered structures. Therefore, the temperature distribution induced by a laser beam has a central role in planning and analysis of the processes. Furthermore, to avoid thermal damage, post-processing of circuits containing active components should be done with careful control of temperature distribution.

Most practical structures used in microelectronics consist of layers of different materials. Laser heating of layered structures has been investigated using analytical and numerical models [3–7], numerical simulation [8–11] and experimental methods [7,10]. Some of the theoretical studies are based on crude approximations, such as infinite absorption coefficient of the light and temperature-independent thermal and optical parameters. Fully non-linear treatments are very few.

Numerical simulation is a straightforward approach even for the most non-linear and complex systems with conductors, electronic components, etc., where analytical and other numerical approaches become too laborious or

unsolvable. A numerical simulation procedure is presented, which is simple and general, without the usual limitations of analytical approaches. It is based on the finite-difference solution of the heat conduction equation and composed of the elementary processes. It allows straightforward inclusion of temperature driven processes like deposition, etching, diffusion of dopants etc. Furthermore, the full temperature dependence of heat conductivity, absorption coefficient, surface reflectivity and heat capacity, that we have found to be essential, is easily included. The method is described elsewhere in detail [12].

In this study, the simulation procedure for calculation of CW Ar⁺ laser-induced temperature distributions in silicon-on-sapphire and in silicon dioxide coated silicon has been applied. Surface and depth profiles for temperature are presented, as well as isotherms and spot temperature plots against incident power. A comparison with the results for bare silicon is made, and the width and shape of surface temperature profiles is discussed due to their relevance for the spatial resolution of the temperature driven process such as deposition and etching.

2. Simulation procedure

The incident laser beam hits the substrate perpendicularly (in the z -direction) with the total power $P_0 = \pi w^2 I_0$, where I_0 is the intensity. For a Gaussian shaped radial intensity distribution ($r = \sqrt{x^2 + y^2}$) and surface temperature (T_s) dependent reflectivity (R) the penetrating intensity distribution reads as

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

which also defines the "1/e value" of the spot diameter $d_s = 2w$.

The intensity absorbed into the volume elements of the numerical grid is

$$\Delta I(r, z) = I(r, z) \{1 - \exp[-\alpha(T)\Delta z]\}, \quad (2)$$

where r , z , T and Δz are the coordinates, temperature and thickness, respectively, of the element considered. To assure conservation of the absorbed energy in the numerical process, the intensity decay $I(r, z + \Delta z) = I(r, z) - \Delta I(r, z)$ is related to the absorbed power density through $p = -\Delta I/\Delta z$.

The heat equation is numerically solved both in rectangular and cylindrical coordinate systems. In the former the equation reads as

$$c\rho \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + p \quad (3)$$

with the volume elements $\Delta V = \Delta x \Delta y \Delta z$ and in the latter as

$$c\rho \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(rk \frac{\partial T}{\partial r} \right) + \left[\frac{1}{r} \frac{\partial}{\partial \theta} \left(k \frac{\partial T}{\partial \theta} \right) \right] + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) + p \quad (4)$$

with the volume elements $\Delta V = \Delta r \Delta \theta \Delta z$. In the present work, only a standing laser beam and vertical structures in layered substrates, that retain the cylindrical symmetry of the heat conduction, are considered. Therefore, lateral heat flux exists only in the radial direction and consequently the angular dependent term (in square brackets) in eq. (4) vanishes. Hence, the cylindrical approach is reduced to two dimensions, reducing the numerical efforts considerably.

The derivatives in eqs. (3) and (4) are written using first order finite-difference, the right hand side of the equations are evaluated for each volume elements, and the consequent temperature rise is obtained from the left hand side. The iteration (or time evolution) is continued until the temperature rise in the spot is less than 0.2 K/ μ s. This gives temperatures that differ from the steady-state ones by less than 1 K.

The applied surface boundary condition (BC) is zero heat flux, which is accomplished by setting the heat conductivity to zero. The BC at the outermost grid points were chosen to be $T - T_\infty \sim 1/r$, a behaviour, which was previously found to increase to convergence [12] and is asymptotically exact for the homogeneous (non-layered) substrate. Although this BC is not rigorously correct for layer structures, it is close enough with relatively large numerical grids and it is very simple to use.

In the following the temperature dependent physical parameters used in calculations are listed. Temperature is given in K, heat conductivity in W $\text{cm}^{-1} \text{K}^{-1}$ and the absorption coefficient in cm^{-1} .

For the Ar⁺ laser ($\lambda = 514 \text{ nm}$) and silicon, expressions $\alpha(T) = 6.28 \times 10^3 \exp(T/430)$ for the absorption coefficient [13] and $R(T) = 0.367 + 4.29 \times 10^{-3}T$ for the surface reflectivity [14] are used. Absorption coefficients in silicon dioxide and sapphire are small enough to be neglected. The thermal conductivity of silicon has been fitted to the experimental data [15,16] as $k(T) = 311.1/(T - 77.8)$ if $T \leq 719.83$ and $k(T) = 0.00717 \exp[-0.003719(T - 1700)] + 0.210$ at higher temperatures. For silicon dioxide the expressions $k(T) = 0.0115 + 1.343 \times 10^{-5} (T - 300)$ if $T \leq 1000$ and $k(T) = 0.0209$ when $T > 1000$ have been obtained using the data given in ref. [17], and for sapphire the expression [5] $k(T) = 73.9/(T - 159)$ is adopted. The heat capacity has no effect on the steady-state temperature distributions, and therefore no other temperature dependences are implemented than that for silicon in our previous study [12].

The interference effects of the laser beam due to the layers [4,18] are ignored in the calculations, because they do not emerge to typical applications with relatively thick layers and high numerical aperture lenses. For thin layers,

however, where the interference might be considerable, it can be included with a little effort.

3. Silicon-on-sapphire

Silicon-on-sapphire layer structure (SOS) consists of a thin epitaxial layer of silicon on a single crystal sapphire (Al_2O_3) wafer. Heating effects of laser light in SOS have been studied recently using the Green function method [3,7]. In the latter study the surface temperature profiles have also been measured by Raman microprobe.

Here a $1\text{ }\mu\text{m}$ thick silicon layer on a semi-infinite sapphire irradiated with a Gaussian beam ($d_s = 5$ and $10\text{ }\mu\text{m}$) is considered. The steady state temperature distributions were calculated for several incident laser powers. Fig. 1 shows the surface temperature at the center of the beam (called spot, hereafter) as a function of the incident laser power. It should be noticed that about 40% of the incident power is reflected. By comparing the curves for 5 and $10\text{ }\mu\text{m}$

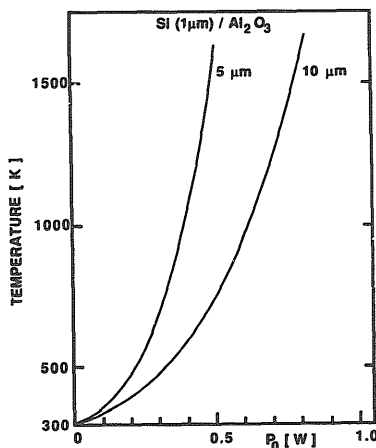


Fig. 1. The spot temperature for SOS irradiated by an Ar^+ laser (514 nm) as a function of incident laser power P_0 , for the beam widths 5 and $10\text{ }\mu\text{m}$. Note that the absorbed laser power $P = (1 - R)P_0$, where R is the surface reflection coefficient.

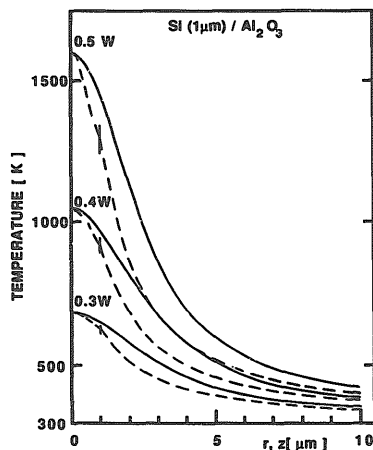


Fig. 2. Temperature profiles in SOS for $5\ \mu\text{m}$ laser beam and incident powers $P_0 = 0.3$ to $0.5\ \text{W}$. Surface profiles (—) and depth profiles (---). The silicon/sapphire interface is marked with a bar.

beams it can be seen that the spot temperature is not a function of P/w only, as it is in the case of non-layered material [19]. This is a consequence of the change in k and α at the interface, that is independent on w .

Fig. 2 shows the surface temperature profiles, which are found to be wider than the incident beam intensity distributions, and the corresponding depth profiles, which show a zero temperature gradient at the surface due to a finite absorption coefficient, and a “kink” at the interface due to the change in thermal conductivity.

The temperature distribution in a vertical rz -plane for a $0.5\ \text{W}$ and $5\ \mu\text{m}$ beam is shown in fig. 3. Because of the higher thermal conductivity of silicon, the horizontal temperature gradient is smaller in the silicon layer and the isotherms become almost vertical at larger distances. Figures like this can be used to estimate safety distances e.g. for active components in the post-processing and repairing of integrated circuits.

In our experiments with a $6.2\ \mu\text{m}$ TEM₀₀ beam the threshold power required to melt the surface of SOS ($1\ \mu\text{m}$ silicon on $430\ \mu\text{m}$ sapphire) was

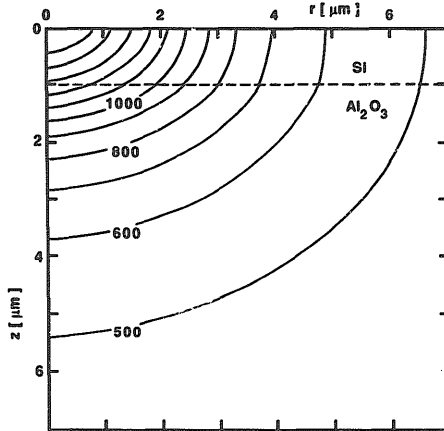


Fig. 3. The isotherms in SOS in a vertical plane cut through the laser beam. The beam width is 5 μm and incident power $P_0 = 0.5$ W. The broken line (— — —) denotes the silicon/sapphire interface.

0.55 W. This value is in a good agreement with the threshold value 0.59 W obtained by interpolation between the curves in fig. 1.

4. SiO_2 -covered silicon

Silicon dioxide glass is a common material used in microelectronics as an insulator or a passivation layer. Therefore, temperature distributions of SiO_2 covered silicon are needed when post-processing of integrated circuits is planned. Kotas et al. [10] have measured temperature on the surface of a thin (0.2 μm) oxide on silicon by a thin film thermocouple and also made calculations for temperatures.

A structure of a 2 μm thick SiO_2 (passivation) layer on silicon is considered. Now there are two regions of interest, the spot on the glass surface and another "spot" at the SiO_2/Si interface. It is expected that the temperature distribution in silicon covered by glass does not differ much from the uncovered silicon because of the high optical transmission and low thermal conductivity of glass. This behaviour for the interface spot temperature is

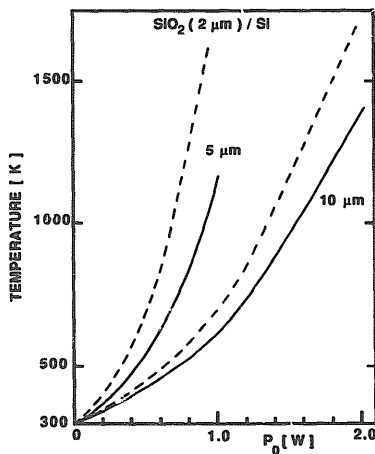


Fig. 4. The spot temperatures on SiO₂ (—) and on the SiO₂/Si interface (---) versus incident power P_0 for 5 and 10 μm beams.

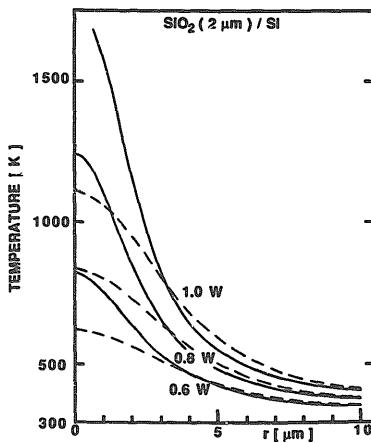


Fig. 5. The surface (—) and interface (---) temperature profiles in the SiO₂/Si layer structure for 5 μm laser beam and incident powers $P_0 = 0.6$ –1.0 W.

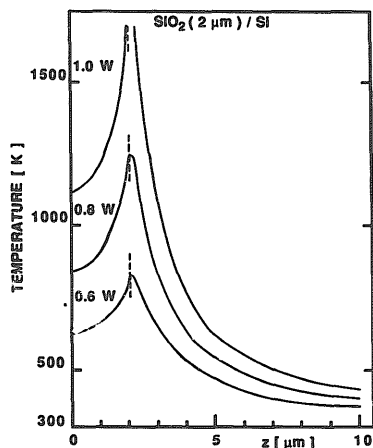


Fig. 6. Vertical temperature profiles along the laser beam axis in SiO_2/Si , for $5 \mu\text{m}$ beam and incident powers $P_0 = 0.6\text{--}1.0 \text{ W}$.

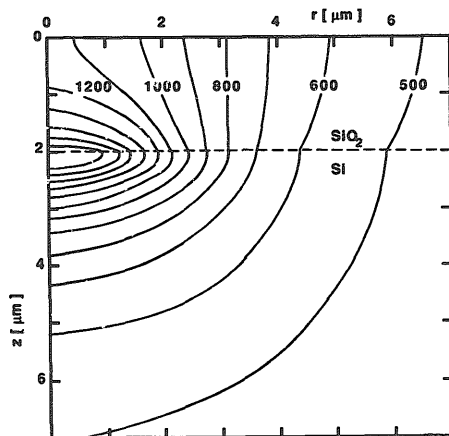


Fig. 7. The isotherms in SiO_2/Si in a vertical plane through the beam axis with the $5 \mu\text{m}$ laser beam and incident power $P_0 = 1.0 \text{ W}$. The SiO_2/Si interface is denoted by ---.

found in fig. 4. It is found that the interface spot temperature is relatively accurately a function of P/w only. But this does not hold for the much lower surface spot temperature. The temperature gradient in glass can also be seen to decrease with increasing beam width.

Fig. 5 shows the detailed surface and interface temperature profiles and the depth profiles are shown in fig. 6. The surface temperature, which plays a central role in pyrolytic laser-chemical processes, cannot be raised much over 1000 K without melting the silicon and glass at the interface. The melting may damage the glass and cause harmful effects in silicon. Finally, fig. 7 shows the detailed curves for constant temperature for the $5\text{ }\mu\text{m}$ beam and incident power of 1 W. At distances less than about $r = 3\text{ }\mu\text{m}$, heat flows from silicon to glass, but vice versa at larger distances.

5. Conclusions

The planning and use of pyrolytic laser processing are based on the laser beam induced temperature distributions in the substrate material. The surface

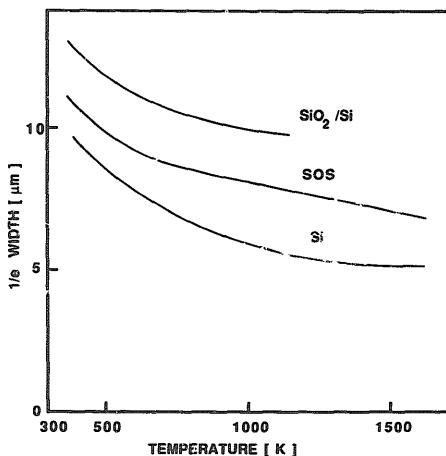


Fig. 8. The $1/e$ values of the temperature distribution widths on the SOS surface, on the surface of the SiO_2/Si structure and on the surface of bare Si, as a function of spot temperature. The $1/e$ width of the Gaussian incident beam is $5\text{ }\mu\text{m}$.

chemical processes like film growth and etching are driven by the surface temperature, but the whole temperature distribution is needed in detailed analysis of interface processes like joining and bulk processes like doping and annealing. Numerical simulation is, as shown above, a simple but reliable procedure in evaluation of temperature distributions, as needed for understanding and design of processes. Furthermore, the simplicity is retained even if non-linear temperature dependencies are fully included.

The spot temperature is the most important factor in laser processing. The control of spot temperature seems to be more subtle in layered structures than in e.g. bare silicon substrate [12]. Although, raising spot temperature on SOS requires less power, the thin silicon layer may be easily damaged. On the other hand the spot temperature at the glass surface cannot be raised very high without melting the silicon subsurface and damaging the whole structure.

For laser writing the surface temperature profiles give the basic information. Therefore, the widths of the temperature profiles are presented in fig. 8, which can be used to estimate spatial resolution in pyrolytic processes. It should be noticed that e.g. the growth rate is a sensitive function of surface temperature. If the deposition of silicon on SOS from silane (SiH_4) gas using a 1200 K spot temperature is considered, the use of Arrhenius' law and an activation energy of 51 kcal/mol results in a $1/e$ width of $1.4 \mu\text{m}$ for the decomposition rate profile which is considerably smaller than the widths of the corresponding temperature profile ($7.7 \mu\text{m}$) and intensity profile ($5 \mu\text{m}$).

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