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Experimental verification of temperature calculations in multilayers used for CO₂ laser recrystallization of silicon-on-insulator films

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Temperature profiles were calculated numerically for a three-layer stack of SiO₂-Si-SiO₂ on top of a monocrystalline Si substrate. The stack was locally heated by a CO₂ laser whereas the wafer background temperature was controlled by a heat chuck. The calculation method makes it possible to simulate temperatures as functions of laser power, spot radius, scan speed, substrate bias temperature, and layer thickness. These parameters play a major role in CO₂ laser recrystallization of polycrystalline silicon for making single crystalline silicon films on insulator films. It is shown that under conditions of maximum absorption experimental verification of the calculations is possible by measuring the recrystallized track width. A good agreement was found between the calculated and measured results.

I. INTRODUCTION

For the fabrication of silicon-on-insulator (SOI) materials by zone-melt recrystallization (ZMR) of polycrystalline silicon films on silicon dioxide, a knowledge of the temperature distribution in the materials is essential to optimize defect-free growth and to prevent degradation of devices already present in the substrate. To avoid excessive heating of device-containing wafers, small spots of lasers and electron beams are used for restricting the heat treatment in time and space on the wafer. Out of the two main candidates of cw lasers, Ar⁺ and CO₂, we have chosen to use the CO₂ laser for preparation of SOI films. Major advantages of a CO₂ laser over an Ar⁺ laser are its stability at high-output powers and the resulting reduced mechanical stress of the SOI films due to the weakening of surrounding insulating films¹ as SiO₂ is an absorbing medium for 10.6-μm radiation.

Temperature calculations have been published by several authors (see, e.g., Refs. 2–4), but there are practically no experimental verifications of the models and assumptions used. In the following we shall present a simplified model which is verified by measurements. A model which can be applied generally for calculating the temperature distribution in a practical stack of a capping, polycrystalline silicon, an insulator, and a bulk silicon wafer, should also include local thickness variations such as antireflective coating of the capping and seed holes in the insulator. However, such a model is rather complex and in the following we shall present a simplified model which can be numerically solved for calculating the temperature distribution in a set of three layers of uniform thickness on top of a well-defined substrate.

Absorption and reflection of laser energy are determined by the thickness of the layers and by the optical constants at high temperature. In general a high energy absorp-

tion and a very low reflection of the laser energy is required. In Sec. IV we shall describe how layer thickness can be optimized by applying temperature optical constants. In Sec. V we shall show that the calculated value of the optimum capping thickness agrees well with the experimentally found value for maximum absorption.

In addition we shall show that for the same optimized capping thickness, energy reflection is absent at temperatures just below the melting point. Under these conditions it can be assumed that all the energy emitted by the laser is used for heating the four-layer stack. Using this result, the calculated temperature distribution from Sec. II can be directly compared with the values found experimentally. Finally, it will be shown that a good agreement has been found.

II. MODEL FOR CALCULATING TEMPERATURE DISTRIBUTION

The model which is used consists of a structure of four uniform layers as given in Fig. 1. The thicknesses of the layers from top to bottom (*z* direction) are denoted by *d*₁, *d*₂, *d*₃, and *d*₄. It is assumed that the layers are not deformed during melting and recrystallization. The circular spot of the laser has an intensity profile which can be described by a Gaussian distribution

$$I(r) = (P/2\pi\sigma^2)e^{-r^2/2\sigma^2}, \quad (1)$$

in which *P* is the output power of the laser, *σ* the standard deviation, and *r* the radius. The heat equation describing the heat transport in each point *x*, *y*, and *z* > 0 in a medium which translates with the vector speed *v* is

$$\rho c \frac{\delta T}{\delta t} + \rho c \mathbf{v} \cdot \nabla T = \nabla \cdot (k(T) \cdot \nabla T), \quad (2)$$

FIG. 1. (a) Schematic of a three-layer structure on a silicon substrate and a Gaussian intensity profile of the CO_2 laser, and (b) top view of the moving spot.

in which k is the heat conduction coefficient, ρ the density, and c the specific heat. The temperature of the moving spot does not change with time, which means that only the stationary state has to be considered. The speed is only present in the x direction, and its component is u .

In this case Eq. (2) is reduced to

$$\nabla \cdot k(T) \nabla T = \rho c u \frac{\delta T}{\delta x}. \quad (3)$$

When the n th layer is considered, Eq. (3) gives

$$\nabla \cdot k_n(T_n) \nabla T_n = \rho_n c_n u \frac{\delta T_n}{\delta x}, \quad n = 1, \dots, 4. \quad (4)$$

The heat conduction of the SiO_2 layers can be taken constant for $1000 \text{ K} < T < 2100 \text{ K}$: (Ref. 5)

$$k_{1,3}(T_{1,3}) = 2.2 \text{ W m}^{-1} \text{ K}^{-1}.$$

In layers 2 and 4, the film of polycrystalline silicon and the monocrystalline substrate, the heat conduction is not constant with temperature. For the polycrystalline layer two states are distinguished, the molten and the solid state:

$$k_2(T_2) \begin{cases} k_2^{\text{melt}} = 64 \text{ W m}^{-1} \text{ K}^{-1} \text{ (Ref. 6)} \\ k_2^{\text{solid}} = A / (T_2 - B) \end{cases}. \quad (5)$$

The heat conduction in layer 4 can be described by

$$k_4(T_4) = A / (T_4 - B).$$

For $300 \text{ K} < T < 1685 \text{ K}$, $A = 2.99 \times 10^4 \text{ W m}^{-1}$, and $B = 99 \text{ K}$ (Ref. 2).

The following boundary conditions can be defined:

(i) At the interfaces between the layers temperature and heat flux are continuous. At $z = z_n$, $T_n = T_{n+1}$, and

$$k_n \frac{\delta T_n}{\delta z} = k_{n+1} \frac{\delta T_{n+1}}{\delta z}, \quad n = 1, 2, 3.$$

(ii) At the solid-liquid interface latent heat is released upon melting ($L = 1106 \text{ J/g}$).

(iii) At the solid-liquid interface the temperature is constant and equal to the melt temperature T_m : $T_2^l = T_2^s = T_m$.

(iv) At $z = z_0 = 0$ we assume that, $\delta T_1 / \delta z = 0$, i.e., the heat loss by radiation or convection in a direction normal to the surface of the wafer is negligible.

(v) At "infinity" the temperature T is equal to background temperature T_0 :

$$T \rightarrow T_0 \text{ as } r^2 + z^2 \rightarrow \infty$$

$$\text{with } r^2 = x^2 + y^2.$$

It is further assumed that the laser power is absorbed at the interface between the SiO_2 capping and the polysilicon layer (see Appendix A). The heat flux is described by

$$k_2(T_2) \frac{\delta T_2}{\delta z} - k_1(T_1) \frac{\delta T_1}{\delta z} = -\frac{P_A}{2\pi\sigma^2} e^{-r^2/2\sigma^2}, \quad (6)$$

for $z = z_1$ with P_A the absorbed part of the power P emitted by the laser. This equation replaces the assumption that at $z = z_1$ $k_1(\delta T_1 / \delta z) = k_2(\delta T_2 / \delta z)$ made under (i).

Equations and boundary conditions are made dimensionless. The dimensionless temperature θ is defined by the following expression: $T = T_0 + (T_m - T_0)\theta$. $\theta = 1$ means that $T = T_m$ and $\theta = 0$, $T = T_0$. In the same way x , y , and z are replaced by X , Y , and Z applying relations like $x = \sigma X$, etc.

The set of dimensionless differential equations obtained from Eq. (4) is then solved numerically by an iteration process which subsequently solves the temperature θ in each of the three layers and the substrate. This process is repeated until the solution converges to a limit value. (Details of the method can be found in Appendix B.)

The calculation method makes it possible to obtain temperature distributions for almost all sets of parameters (d_n , σ , P_A , u , T_0). To demonstrate the capability of the calculation method, two examples of practical results are given.

Figure 2 shows as an example a calculation of the temperature distribution in a silicon film of $0.5 \mu\text{m}$ on a $1.25 \mu\text{m}$ insulator. As can be seen, the isotherm $T = T_m$ ($\theta = 1$) nearly reaches the silicon substrate for a power of only 5.3 W and a σ of $23 \mu\text{m}$. The temperature in the middle of the central molten area of the $51 \mu\text{m}$ -wide cross section exceeds 2500 K ($\theta \geq 1.7$).

In Sec. VI calculated values of the width w will be compared with experimental ones assuming total absorption of the laser power emitted.

Figure 3 shows the influence of the standard deviation σ of the Gaussian spot on the maximum substrate temperature $T(0,0,z_3)$ and the maximum polysilicon temperature $T(0,0,z_1)$ for a given power P_A . The small σ window which

FIG. 2. A typical example of a dimensionless temperature distribution in a polycrystalline silicon film and a SiO_2 insulator for a Gaussian spot ($\sigma = 23 \mu\text{m}$, $P_A = 5.3 \text{ W}$, $u = 5 \text{ cm/s}$, and $T_0 = 450 \text{ K}$).

is available for melting and recrystallization requires good control of the beam shape. A wider window can be obtained for thicker thermal insulators and lower laser powers.

III. GENERAL REQUIREMENTS FOR THE THREE-LAYER STRUCTURE

A three-layer structure on top of a substrate as given in Fig. 1, which is subjected to a CO_2 laser treatment and which is to be used for making devices in two levels, has to satisfy the following conditions:

(i) The capping oxide on top is the main absorbing medium and energy coupler for the stack. The aim is to obtain complete absorption and no reflection at temperatures which lie slightly above the melting point of silicon.

(ii) The polysilicon layer has to be converted into a single crystalline film by the melt process. From the point of view of absorption a thick layer, e.g., $2.5 \mu\text{m}$, is preferred, but for device fabrication silicon film thickness should preferably range from 80 to 500 nm.

FIG. 3. Calculation of the maximum polysilicon temperature $T(0,0,z_1)$ and the maximum substrate temperature $T(0,0,z_3)$ as a function of σ of the Gaussian spot for two sets of values of d_{ox} and P_A . (a) $P_A = 5.3 \text{ W}$ and $d_{\text{ox}} = 1.25 \mu\text{m}$, (b) $P_A = 2.65 \text{ W}$ and $d_{\text{ox}} = 2.5 \mu\text{m}$.

(iii) The insulator, which lies directly on the silicon substrate, has to be thick enough to protect underlying devices against degradation during the melting process. Also, devices to be made later in the SOI layer can benefit from a thick insulator. However, from the point of view of wafer flatness, thin insulators causing less mechanical stress are better. An alternative structure of the insulator and its advantages has been described in Ref. 7.

(iv) The silicon substrate contains diffusions, gate dielectrics, polycrystalline silicon gates, and interconnect layers needed for devices. The substrate also functions as a heat sink during the ZMR process. Seeding of the SOI film for obtaining well-oriented silicon-on-insulator films occurs from the substrate through epitaxially filled holes.

It is difficult to meet all of the often conflicting requirements for the four layers. In the following we shall concentrate on the absorption of the CO_2 laser energy in the three-layer structure and see how the absorption can be made high for a stack of layers with practical thicknesses.

IV. HIGH-TEMPERATURE ENERGY ABSORPTION

A description of the process of energy absorption must include the effect of the complete stack of SiO_2 capping, poly Si, SiO_2 insulator, Si substrate, and the influence of the transition of phase changes. In order to melt the polysilicon layer, enough energy has to be concentrated on a small surface area. Due to the Gaussian distribution of the laser beam intensity in the focal plane a strong variation of temperature with position and time can be expected (see, e.g., Fig. 2). In the middle of the spot temperature may rise some hundreds of degrees above the melting point of silicon, whereas toward the outer edges a steep temperature gradient exists which finally approximates the background temperature outside the spot.

The main part of the absorption takes place at high temperatures in the central area of the spot. An useful description of the absorption process can therefore be obtained by using the electric field theory^{8,9} with refractive indices at high temperatures. Unfortunately measurements of n and k at high temperature are difficult, especially at a wavelength of $10.6 \mu\text{m}$.

The strong absorption peak of SiO_2 at $9 \mu\text{m}$ makes the n and k values at $10.6 \mu\text{m}$ lie in the steep flank of this peak as has been shown for instance by Philipp.¹⁰ The temperature dependence of the extinction, measured by McLachlan and Meijer,¹¹ appears to be small. We took as n and k values for the SiO_2 capping and insulator those of crystalline oxide and assumed that these values were also valid at high temperatures ($n = 2.06$ and $k = 0.025$).

For silicon layers a much higher variation of the optical constants with temperature has been observed. Free-carrier absorption increases strongly with temperature. We used n and k values as given in Fig. 4, which can be considered as an average of values reported by Van der Meulen and Hien at 633 nm ¹² and by Blomberg *et al.*¹³

Just below the melting temperature of silicon we estimate $n = 3.3$ and $k = 1.5$. Above the melting point the n and k values are changed to higher values, as has been demonstrated by Jellison¹⁴ for wavelengths ranging between 308

and 1152 nm. This increase in n and k values corresponds to a sharp increase in the reflection of the laser energy. This inevitably results in a fall in laser energy absorption and a stabilization around the melting temperature of the silicon.

Absorption, reflection, and transmission ratios are calculated as a function of temperature for different sets of layer thicknesses using the electric field theory. Optimization to high absorption and low reflection gave a specific set of layers:

SiO₂ capping: $d_1 = 1.1 \mu\text{m}$,
 polycrystalline Si: $d_2 = 2.5 \mu\text{m}$,
 SiO₂ insulator: $d_3 = 2.5 \mu\text{m}$.

Figure 5 shows how absorptance, reflectance, and transmittance of these layers vary with temperature. A high degree of absorption, low reflection, and transmission is found just below the melting point of the polysilicon layer. The multilayer structure has, however, some practical limitations from the point of view of mechanical stress and technological realization. Electric field theory calculations of the absorption, reflection, and transmission, in which each layer thickness has been varied, shows that the capping thickness is critical with a sharp maximum at about $1.1 \mu\text{m}$, but the polysilicon layer thickness can be reduced from 2.5 to $0.6 \mu\text{m}$ and the insulator thickness from 2.5 to $1.25 \mu\text{m}$ or lower. In this case the absorption is about 70%, the reflection $< 3\%$, and the rest, about 28%, is transmitted to the substrate where it will be absorbed by free carriers when the temperature is high enough (e.g., $300\text{--}500^\circ\text{C}$).

Complete absorption of the laser energy can therefore be expected for the following multilayer:

SiO₂ capping: $d_1 = 1.1 \mu\text{m}$,
 polysilicon film: $d_2 = 0.6 \mu\text{m}$,
 SiO₂ insulator: $d_3 = 1.3 \mu\text{m}$,
 and Si substrate ($300\text{--}500^\circ\text{C}$).

V. EXPERIMENTAL VERIFICATION OF THE INFLUENCE OF THE CAPPING LAYER THICKNESS ON THE ENERGY ABSORPTION OF A CO₂ LASER

The multilayer stack with an insulator of $1.3\text{-}\mu\text{m}$ thermal SiO₂ and a polysilicon layer of $0.7 \mu\text{m}$ was prepared by

FIG. 4. Optical constants n and k of silicon as a function of temperature.

FIG. 5. The calculated values of the absorptance A , the reflectance R_r , and the transmittance T_r of an optimized multilayer stack as a function of temperature.

conventional processing steps. The thickness of the capping layer on a wafer ranged from 0.2 to $2.1 \mu\text{m}$. It was made by a series of etching steps in which 16 areas, each with a width of 5 mm , were defined.

The intensity profile of the CO₂ laser beam had been measured in two orthogonal directions and checked for being Gaussian. The beam was focused by a parabolic mirror giving a standard deviation of the Gaussian spot in the focal plane of $38\text{--}40 \mu\text{m}$. The scan speed of the table was 5 cm/s , the scan direction was perpendicular to the etched stripes, and the pitch between two successive scans was $200 \mu\text{m}$. The wafer background temperature was 480°C . Three different powers were used.

The degree of absorption has been determined by measuring the width of the recrystallized track for each of the 16 areas of different thickness of the capping. The width of the tracks was measured microscopically after 20-s Wright etching¹⁵ of the polysilicon layer.

Figure 6 shows the width of the recrystallized tracks versus the thickness of the capping layer. For each of the three laser power values a distinct maximum was found at a thickness of about $1.0 \mu\text{m}$. A strong reduction of track width was found for capping thickness values below or above this value.

Figure 6 further shows that laser powers of 10 and 12 W can cause severe substrate damage due to high substrate temperatures which occur for this structure. When, on the other hand, the absorption was not high enough to cause melting, the laser track was not fully recrystallized. This result agrees well with the calculated value of $1.1 \mu\text{m}$ for the capping thickness as given in Sec. IV in which the high-temperature value of the optical constants n and k had been used.

VI. COMPARISON OF THE CALCULATED AND EXPERIMENTAL RESULTS

When the absorption of laser energy of an optimized stack is nearly 100%, it is possible to compare calculated results, in which the absorbed power P_A is used, with experimental results. The latter are related to the power P emitted

FIG. 6. Measured track width of recrystallized polycrystalline silicon as a function of the thickness of the capping layer for three different values of the CO_2 laser power P ($d_{\text{poly Si}} = 0.7 \mu\text{m}$, $d_{\text{insulation}} = 1.3 \mu\text{m}$, $T_0 = 480^\circ\text{C}$, $u = 5 \text{ cm s}^{-1}$, and $\sigma = 39 \mu\text{m} \pm 1$).

by the laser. In the following, three types of experiments are compared with the calculated results: the recrystallized track width w versus power P ; the width w versus the background temperature T_0 ; and the width w versus the standard deviation σ of the Gaussian spot.

A. The width w of the recrystallized track versus the emitted laser power P

The experiments were carried out on wafers with a multilayer structure as given in Fig. 7. The capping layer was $1.1 \mu\text{m}$, the polysilicon layer $0.5 \mu\text{m}$, and the total SiO_2 insulator thickness was $2.26 \mu\text{m}$. For reasons of stress reduction and additional verification of the crystalline state, the insulator of $2.26 \mu\text{m}$ was split up in two layers of 1.01 and $1.26 \mu\text{m}$ with another polysilicon layer of $0.5 \mu\text{m}$ in between. We

FIG. 7. Cross section of the multilayer structure used for the experimental verification of the calculated track width.

assumed that the model of heat conduction is not affected by this additional polysilicon film. The emitted laser power was measured with a bolometer and the Gaussian laser beam was checked for symmetry by measuring the intensity profile in two orthogonal directions. The width of the recrystallized track was measured microscopically after 20-s Wright etching of the recrystallized polysilicon layer.

The calculated width has been derived from the temperature distribution in the x - z plane (see also Fig. 2) by taking the distance between two isotherms where $T = T_m$. At low scan speeds ($v < 10 \text{ cm/s}$) the width measured in the x - z plane is equivalent to the width found in the y - z plane.

The results of the measurement and the calculation are given in Fig. 8. As can be seen the two results agree reasonably well, although the difference in shape increases at high power levels. A possible reason might be the observed deformation of the SiO_2 capping at high power. This deformation starts with a thinning of the capping in the middle of the track where the temperature is highest. At temperatures above the softening point SiO_2 layers become soft with viscosities which resemble a liquid film. As a result of this and of surface tension forces a transport occurs of relatively hot SiO_2 and liquid Si towards the edges of the track, leading to an additional widening of the track.

Another conclusion which can be drawn is that the absorbed power is nearly equal to the emitted power of the laser, which is in agreement with the high energy absorption which can be expected from the multilayer used (see Sec. IV).

B. The width w of the recrystallized track versus the background temperature T_0

Wafer structure and laser conditions are identical to those given in Sec. VI A. The background temperature was

FIG. 8. Width of the recrystallized Si track as a function of the absorbed power P_A (calculated) or of the total laser power P (measured).

measured in the middle of a test wafer on the heat chuck by means of a thermocouple.

Figure 9 shows that an increase of the substrate temperature from 550 to 700 K leads to a measured recrystallized track width which is practically identical to the calculated value.

C. The recrystallized track width w versus the standard deviation of the Gaussian beam

Wafer structure and laser conditions are the same as those given for Sec. VI A. The σ of the focused spot was derived from the measured beam profile and the optics used. Variations of σ were realized by defocusing. The focal plane was in that case above the surface of the wafer at some distance. Due to uncertainties in distance and beam profile, the σ values were estimated within $2\ \mu\text{m}$.

Figure 10 shows the recrystallized track width for some σ values. The experimental results are somewhat less profited than those found by calculation, but the general trend shows agreement.

VII. SUMMARY

Temperature distributions caused by heating with a Gaussian laser spot on three layers of uniform thickness can be calculated by solving the heat equations by a semianalytical method. The method of calculation can be applied to the process of zone-melt recrystallization of polysilicon to make silicon-on-insulator films. An extension of the calculation method to more practical structures, including antireflection layers and seed holes, is then necessary. We have shown that the thickness of the capping layer is essential for the absorption of laser energy. A calculated optimum for the absorption has been found for a capping layer thickness of $1.1\ \mu\text{m}$. Experiments confirmed that the maximum of the absorption lies close to this value at a capping thickness of $1.0\ \mu\text{m}$. A capping layer of $1.0\text{-}\mu\text{m}$ SiO_2 could be combined with practical thicknesses for the SOI film ($\approx 0.6\ \mu\text{m}$) and the insulator ($\approx 1.3\ \mu\text{m}$). For a background temperature of 300 to 500 °C complete absorption of the CO_2 laser energy occurs during recrystallization. It was possible to compare

FIG. 9. Width w of the recrystallized Si track as a function of the substrate bias temperature T_0 .

FIG. 10. Width w of the recrystallized track as a function of the standard deviation σ of the Gaussian beam as calculated (full line) and measured ($\circ$).

the calculated results directly to the measured ones using such an optimized structure. Good agreement was found for experiments in which the laser power, the substrate temperature, and the radius of the Gaussian spot were varied.

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APPENDIX A

As has been shown in Secs. IV and V, most of the energy is absorbed in the $1\text{-}\mu\text{m}$ -thick SiO_2 capping. It can be argued that this process can be modeled realistically by condition (6). The thermal conductivity of silicon dioxide is much smaller than that of silicon. Therefore, heat injected into the poorly conducting capping will flow towards the lower-lying regions by the shortest route, i.e., more or less in a one-dimensional fashion. Second, the ratio of the thickness of the capping and the width of the spot is much smaller than unity. These two effects cause the heat distribution through the interface to be almost exactly similar in shape and magnitude to the integrated heat input distribution in the capping. This phenomenon is quite similar to that of Ref. 16, where a two-layer system with a poorly conducting top layer was studied. In actual fact, our numerical calculations show that the capping itself does not have a strong influence on the temperature distribution. Only its heat-absorptive properties are of importance. Also, the absolute magnitude of the

second term on the left of Eq. (6) was found to be much smaller than that of the first.

APPENDIX B

In this appendix we shall describe the semianalytical method we used to solve the temperature problem. Many examples of temperature calculations in layered media that are technologically important can be found in the literature. When the thermal properties are constant in each of the separate layers, fully analytical solutions can be found (e.g., Refs. 16 and 17). In the case considered here the thermal properties are not constant, particularly owing to the presence of a molten zone. The problem is therefore basically nonlinear. However, a semianalytical approach is still possible.

The temperature is rendered dimensionless by means of the melting temperature T_m and the spatial variables by means of the laser spot width σ . As a result we obtain an equation of the kind

$$\nabla(K\nabla\theta) = \alpha(\delta\theta/\delta X), \quad (\text{A1})$$

in each of the layers considered in this problem (Fig. 1).

The dimensionless parameter α is given by

$$\alpha = \rho c u \sigma / k, \quad (\text{A2})$$

which can have different values in each of the four layers.

The dimensionless parameter K is equal to unity in the oxide layers, since we have assumed the oxide to have a thermal conductivity independent of the temperature.

In the silicon layers, K is a function of temperature which follows from Eq. (5):

$$K = \begin{cases} 1 & \text{for } \theta > 1 \\ \frac{A}{T_m k_{\text{melt}}} \frac{1}{\theta - B/T_m} & \text{for } \theta < 1 \end{cases}. \quad (\text{A3})$$

The values of the parameter α differ considerably in the various layers. This is due solely to the markedly different values of the thermal diffusivity

$$\kappa = k / \rho c, \quad (\text{A4})$$

in the various layers. For silicon the value of κ is of the order of $10^{-4} \text{ m}^2/\text{s}$. With a value of $u \sim 10^{-1} \text{ m/s}$ and $\sigma \sim 10^{-5} \text{ m}$ this yields $\alpha \sim 10^{-2}$. As a result, we may disregard the influence of the convective term in the silicon layers. Therefore

$$\nabla(K\nabla\theta) = 0, \quad (\text{A5})$$

in the silicon layers.

In the silicon-dioxide layers, on the other hand, κ has a value which is considerably smaller, namely $\sim 10^{-6} \text{ m}^2/\text{s}$. Therefore, α is not small in these layers and we are not allowed to leave out the term at the right-hand side of Eq. (A1).

As a result, in the silicon-dioxide layers we must consider the equation

$$\nabla^2\theta = \alpha(\delta\theta/\delta X). \quad (\text{A6})$$

The solution method we use is semi-analytical in the sense that we write down formal analytical solutions in each of the sublayers. These analytical solutions satisfy given temperature and heat flux conditions on the bounding interfaces. An iteration procedure is invoked to improve the interface tem-

peratures and heat fluxes until convergence to a final solution is attained.

To illustrate the method let us first describe the temperature calculation in the silicon-dioxide layers. The upper interface is denoted by $Z = Z_u$ and the lower by $Z = Z_l$. Let us assume that at a particular step within the iteration procedure a heat flux distribution is given on $Z = Z_u$ and a temperature on $Z = Z_l$:

$$\delta\theta/\delta z = g(X, Y) \quad \text{at } Z = Z_u, \quad (\text{A7})$$

$$\theta = h(X, Y) \quad \text{at } Z = Z_l. \quad (\text{A8})$$

Since the problem is linear, the solution can easily be given in terms of a series expansion of convolution integrals which involve the functions $g(X, Y)$ and $h(X, Y)$. The solution defines a heat flux distribution function on $Z = Z_l$, which we shall denote by $p(X, Y)$.

The layer below the silicon dioxide is a silicon layer. Writing $(Z_u)_{\text{silicon}} = (Z_l)_{\text{oxide}}$, we now have a temperature problem which involves Eq. (A5) and a boundary condition

$$\frac{\delta\theta}{\delta Z} = \frac{k_{\text{oxide}}}{k_{\text{silicon}}} p(X, Y), \quad (\text{A9})$$

on $Z = Z_u$. This is complemented by a temperature condition given by a previous iteration step:

$$\theta = q(X, Y) \quad \text{at } Z = Z_l. \quad (\text{A10})$$

By means of the well-known Kirchhoff transformation,

$$Q = \int_1^\theta K(\omega) d\omega, \quad (\text{A11})$$

we may transform the silicon problem into a linear one for Q which can be solved analytically.

Denoting the interfaces of Fig. 1 by I_{01} , I_{12} , I_{23} , I_{34} , and $I_{4\infty}$, respectively, we initialize the iteration procedure by taking $\theta = T_0/T_m$ on I_{23} , I_{34} , and $I_{4\infty}$. On the last interface the temperature will remain at T_0/T_m during the entire iteration process. Initially, the injected heat flux given by Eq. (1) is assumed to flow wholly into layer 2. This yields a temperature on I_{12} and a heat flux distribution on I_{23} . Next we solve the temperature problem in layer 3. This produces a new temperature on I_{23} and a heat flux distribution on I_{34} .

Now we solve the temperature problem in the silicon substrate, which is layer 4. This yields a new temperature distribution on I_{34} . The temperature problem in layer 1, the capping, is solved with the "no heat flux" condition on I_{01} and the newly calculated temperature on I_{12} . This yields a heat flux distribution in and out of layer 1 through interface I_{12} . We are now in a position to enter the next stage of the iteration process. The heat flux into layer 2 is obtained by subtracting the recently calculated heat flux into layer 1 from the injected heat flux defined by Eq. (1). This process is continued until convergence is reached.

During the entire iteration procedure we use under-relaxation. This is necessary to ensure convergence of the method, particularly when the thermal conductivities of the various materials differ markedly. If at a certain step during the iteration process a new temperature θ_{new} is predicted at a particular interface, we do not use this temperature for our next step, but rather

$$\theta = R\theta_{\text{new}} + (1 - R)\theta_{\text{old}}, \quad (\text{A12})$$

where θ_{old} is the temperature calculated at the same interface during the preceding iteration step. The same procedure is applied to the heat flux. The relaxation factor R was chosen between zero and unity. In each instance its value was obtained by numerical experimentation.

The analytical solutions we referred to earlier are given as very slowly converging series expansions. In their original state these series cannot be used in a practical iteration scheme, as tens of thousands of terms will have to be evaluated to obtain solutions which are only three figures accurate. This is why we apply a convergence accelerator first before the series are used in the actual iteration scheme. After the enhancement of convergence, only a hundred terms have to be calculated to achieve the same accuracy.

Dropping the convection term in layer 4 on the basis of the smallness of α [Eq. (A2)] is, strictly speaking, incorrect. The width of the temperature distribution on I_{34} is of the order of σ . The temperature drop below I_{34} occurs in a medium which is, practically speaking, infinitely thick. If layer 4 is stationary, which we have assumed by using Eq. (A5), the temperature is proportional to the inverse of the distance to the concentrated temperature profile on I_{34} . In a practical sense, the asymptotic conditions are reached at a distance of 10σ below I_{34} . Therefore, a realistic value of α for layer 4 will be at least ten times higher than that of Eq. (A2). Since the original α we calculated was of the order of 10^{-2} , it would seem that we can still safely use Eq. (A5) in layer 4. However, in this respect a problem arises when α becomes larger on account of larger substrate velocities. In such cases, as they stand, our calculations are valid in an approximate sense only.

Of course, we could also have solved this problem using finite differences or finite elements. It should be realized, however, that the problem is three-dimensional so that, in addition to a discretization in the lateral (x, y) directions, these methods also require a discretization in the z direction with a significant number of points between the interfaces. Our semianalytical method requires only a discretization in

the x and y directions on the interfaces. Therefore, with the same computer memory capabilities available, the present method allows a much finer spacing in the lateral directions, so that a more accurate solution can be expected. Moreover, whereas the fully numerical solution method requires the inversion of large sparse matrices, our semianalytical method makes use of a natural iteration scheme in which the temperature is calculated in each point consecutively. We think, therefore, that our semianalytical method is more efficient than one which is completely numerical.

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