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IMPLICIT MODIFIED ENTHALPY METHOD WITH APPLICATION TO THIN FILM MELTING

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ABSTRACT

During the thermal processing of thin films in which low intensity line heat sources are used, extended processing times are often required to reach steady state (~15 sec). In addition, the melting of the film may occur some time after processing has begun, and therefore there is no initial melting condition within the film. In such cases, computer simulations may become very time consuming, and the development of an efficient computational method which incorporates the initial formation of the melt during processing is necessary. A general technique was developed to accurately model two-dimensional heat conduction in a multilayer film structure with one-dimensional phase change in one of the thin films. These conditions frequently exist in thin film thermal processing when the thermal gradient through the thickness of the melting film can be considered negligible. The method involves an implicit formulation of the modified enthalpy method. The solid/liquid interface energy-balance equation is taken into account which allows the exact location of the interface to be tracked within a control volume. A comparison is made between the explicit and implicit modified methods to test efficiency and accuracy. The implicit method is then applied to the zone-melting recrystallization of a silicon thin film in a multilayer structure.

KEY WORDS Thin film melting Modified enthalpy method

INTRODUCTION

The need for single crystal silicon films in semiconductor applications has sparked much interest in the area of melting and re-solidification processes. Many of these processes are heat transfer dominated[1]. The quality of the recrystallized film is dependent on the temperature profile within the silicon during processing[2,3], and therefore careful control of the processing conditions is essential in obtaining desirable results. Owing to the small sizes of the structures involved (~1.0 μm), direct measurements are difficult to obtain and much effort has been directed towards costly trial-and-error process optimization. However, some researchers have turned to numerical techniques to obtain temperature profile predictions and to determine critical processing parameters.

A vast amount of work has been performed in the general area of change of phase problems. Several analytical solutions have been obtained for simple problems[4,5]. Owing to the complexity of the analysis, more involved problems required solution by numerical techniques. A comprehensive review of numerical-heat-transfer solidification processes has been published by Salcudean and Abdullah[6]. Özisik[5] has presented a review of both analytical and numerical solutions. The numerical techniques generally fall into one of two categories. The first category involves writing the conservation equations separately for the solid and liquid portions of the domain. Since the position of the solid/liquid interface must be tracked continuously,

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finite-difference approaches using a finite number of points can prove cumbersome. The second category involves rewriting the conservation equations in terms of temperature and enthalpy and are referred to as the enthalpy methods. Shamsundar and Sparrow[7] have presented a general implicit multi-dimensional finite difference formulation of the conventional enthalpy model. It was shown that the enthalpy and conventional forms of the conservation equations are equivalent. The location of the solid/liquid interface can be approximated from the enthalpy of the two-phase control volumes. Since the equation describing the energy-balance at the interface is eliminated from the analysis, temperature results are less accurate in the region surrounding the interface, especially when transition occurs at a discrete temperature. Non-physical temperature histories have been observed for materials with a single melt temperature[8,9], which can occur when the ratio of latent heat to change in enthalpy is high.

Several one-dimensional numerical techniques have been developed which incorporate the energy balance at the solid/liquid interface. Goodrich[10] described a Crank–Nicolson technique in which the one-dimensional conduction equation linked to the energy balance at the interface was solved by Gaussian elimination. An explicit enthalpy formulation was derived by Tacke[9]. By assuming linear temperature profiles between nodes, the heat content of the volume containing the interface is more accurately described. Voller[11] described an implicit method using a 'node-jumping' scheme. The interface is found at nodal positions by varying the time step. Good results were obtained, but steady state solutions cannot be calculated with the method, since the interface can only be found at fixed nodel positions.

An explicit two-dimensional modification of the enthalpy method, which incorporates the energy-balance equation, has been described by Rostrami *et al.*[12]. The method uses the enthalpy formulation to determine the enthalpy of the control volumes which may experience a change of phase. A control volume which is undergoing melting is not fixed at the melt temperature. The temperatures of the control volumes changing phase are found from the enthalpy–temperature relation. The location of the liquid pool may be found without knowing the location *a priori*. Since the exact location of the interface is known, the sudden change in thermal properties at the solid/liquid interface may be handled properly. Rostami and Grigoropoulos[13] have applied the technique to the modelling of laser processing of semiconductor films. Previous numerical work in thermal processing with a graphite-strip heater have used the conventional enthalpy method[14]. Im[15] has obtained temperature distributions assuming a planar interface from an analytical model. However, several aspects of the problem had to be simplified in order to obtain analytical solutions.

Radiant thermal processing of thin films with low intensity line sources, such as graphite strip or halogen lamp heaters, presents several complications which in combination make previous methods that track the solid/liquid interface not suitable: (i) thermal processing of the material requires extended processing times to reach steay state (~ 15 sec for graphite strip); (ii) the initial phase-change condition of the film is not known *a priori* since the phase change may occur after processing has commenced; (iii) one-dimensional phase change of the thin film is incorporated into the two-dimensional conduction equation in the film and substrate; and (iv) varying degrees of superheated solid and supercooled liquid may exist if the reflectivity of the melting material is higher in the liquid state than in the solid state[16].

In this paper, a fully implicit two-dimensional formulation of the modified enthalpy method with one-dimensional phase change is presented. The technique can be used to model any multilayered structure in which one of the thin films will experience a change of phase. In particular, the method can incorporate non-uniform heat absorption perpendicular to the direction of phase change in addition to the typical heat conduction through the interface. To demonstrate the method, the zone-melting recrystallization (ZMR) of a thin silicon film in a multilayered structure by graphite-strip heater is examined. Owing to the thinness of the films and the extended time required to reach steady state in certain types of thermal processing, the implicit formulation was developed to eliminate the time step restriction of the explicit method. A comparison of computational efficiency, temperature and melt width between the explicit and

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implicit modified enthalpy versions is presented. In cases where superheated solid and supercooled liquid exist at steady state, the standard discretization for the thermal gradients at the solid/liquid interface was found to cause a non-physical oscillating interface near the steady state solution. A modification in the calculation of the gradients was developed in order to alleviate this problem. Full steady state results are then shown using the implicit method with the modified thermal gradient calculation at the solid/liquid interface.

MODELLING OF THERMAL PROCESS

Thermal processing of thin film structures using ZMR processing involves local heating of the structure to crystallize a portion of the film material. Typically, a multilayer thin-film structure deposited on a thick substrate (wafer) ~ 6 cm in length is placed on a lower heater (susceptor) which heats the wafer close the melting temperature of the film. A line heat source located above the film structure locally heats the thin film further. Once a steady state melt pool has been established in the film, the heat source is scanned and the material is crystallized in the freezing wake. It may be noted that the heat absorption of the incident thermal radiation from the strip heater to the film changes abruptly at the solid/liquid interface due to the difference in reflectivity of solid and liquid silicon[14]. The process modelled is shown in *Figure 1*. The silicon substrate is 400 μm thick with capped silicon-on-insulator (SOI) film structure with film thicknesses $\sim 1.0\,\mu$m.

In these studies, the strip was considered stationary in the centre of the structure, which has been found to be accurate for low scanning speeds[17]. When the melt pool is being established, it grows at the same rate away from the centre of the wafer. Owing to this symmetry, only half the wafer was modelled and an uneven grid spacing was used to save computational time. A grid of 201 $\times$ 5 nodes was used in these calculations. The film structure was modelled as a single 1.0 μm silicon layer, which has been found to be a good approximation compared to a model incorporating the heat conduction within each film layer[14]. Therefore, the film and substrate have the same thermal properties in the solid phase. The grid spacing in the x direction is 20 μm under the strip where melting occurs and incrementally increases to 500 μm towards the edge

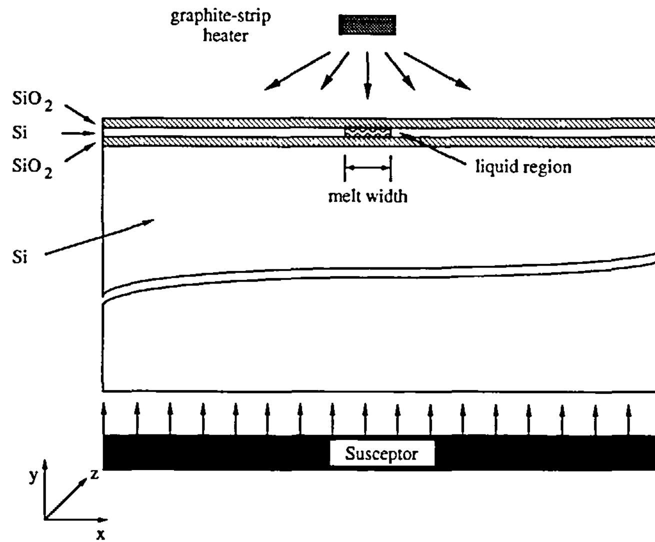

Figure 1 Schematic of ZMR thermal processing of a thin film structure

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of the wafer. In the y direction, one node is placed in the film layer and those remaining in the substrate. The heating source used is a thermally radiant graphite-strip heater with 3 mm × 1 mm cross-section located 2 mm above the film structure. Since the heat source is uniform in the z direction, conduction within the structure is assumed to occur in the x and y directions only. The two-dimensional transient heat conduction equation can be written as:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) + S \tag{1}$$

where ρ is the density, c is the specific heat, k is the thermal conductivity and S is the rate of heat generation per unit volume. Taking the melting point, T_m, as reference (i.e. the enthalpy is zero at the melting point temperature), the enthalpy in the solid and liquid phases, respectively, are defined as:

$$e_s = \int_{T_m}^{T} (\rho c)\,\mathrm{d}T \qquad \text{solid} \tag{2a}$$

$$e_l = \int_{T_m}^{T} (\rho c)\,\mathrm{d}T + L \qquad \text{liquid} \tag{2b}$$

where e is the enthalpy, and L is the latent heat of fusion per unit mass and the subscripts s and l represent the values on the solid and liquid sides of the interface, respectively. In general, the average enthalpy of a control volume can be expressed as[13]:

$$e = \rho c(T - T_m) + fL \tag{3}$$

where f is the volume fraction liquid phase (i.e. $f = 0.0$ for solid, $f = 1.0$ for liquid, and $0.0 < f < 1.0$ for a control volume containing both phases). The problem is split into two domains: the melting thin film and the solid substrate. In the film where melting may take place, (1) may be written in terms of enthalpy to give:

$$\frac{\partial e}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) + S \tag{4}$$

In the region where a change of phase will not occur (substrate), (1) is used.

When melting conditions exist within a control volume, part of the total energy contributes towards phase change, while that remaining raises the sensible energy. The conventional enthalpy method assumes that the temperature of a control volume is fixed when changing phase, and therefore all energy is directed towards melting the material. Physically, however, the average temperature of a finite volume varies from the melting point temperature once any melting has taken place. Since the melting film is thin, the thermal gradient through the film can be assumed negligible, and therefore melting occurs in one (x) dimension; however, two-dimensional heat conduction remains within the substrate and film structure. In the control volume changing phase, the distribution of the total energy may be found from the one-dimensional energy-balance conditions at the solid/liquid interface:

$$T_m = T_s = T_l \tag{5}$$

$$\rho L \frac{\partial X}{\partial t} = k_s \frac{\partial T_s}{\partial x} - k_l \frac{\partial T_l}{\partial x} \tag{6}$$

where $\partial X / \partial t$ is the velocity of the interface.

Owing to the symmetry of the domain, only half the wafer was modelled (see *Figure 2*) and the centre boundary condition became:

$$x = 0 \qquad \frac{\partial T}{\partial x} = 0 \tag{7}$$

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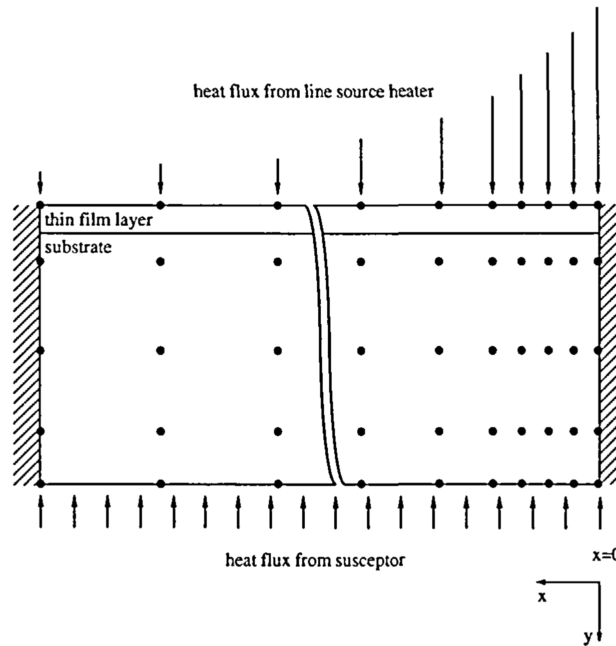

Figure 2 Schematic of boundary conditions, heat flux and relative nodal positioning for the computational domain

The edge of the wafer was assumed insulated and the boundary condition was:

$$x = D/2 \qquad \frac{\partial T}{\partial x} = 0 \tag{8}$$

where D is the length of the wafer.

In the y-direction, the radiative heat flux to and from the wafer structure is included into the source term at the top and bottom boundaries. Since the wafer is optically thick (transmissivity = 0), the heat flux in along the top of the structure can be approximated as[14]:

$$q(x) = F(x)_{1-2}(1 - R(x))\sigma T_h^4 - \varepsilon(x)_f \sigma T_f^4 \tag{9}$$

where $F(x)_{1-2}$ is the shape factor from the upper heater to a point on the wafer, σ is the Stefan–Boltzmann constant, T_h is the temperature of the line heat source, $R(x)$ and $\varepsilon(x)$ are the reflectivity and emissivity of a specific point on the wafer, respectively and T_f is the temperature at the specific point on the film. The shape factors were calculated with the Hottel cross-string method[18]. The heat flux was modelled as distributed heat sources in the film layer. Since the bottom of the structure was heated by a susceptor, a parallel plate radiative exchange was assumed between the susceptor and the bottom of the substrate[14].

Each control volume was assigned an emissivity and reflectivity value depending on the state of the control volume. When a control volume had not experienced any melting ($f = 0.0$), the solid values of reflectivity and emissivity were assigned to those volumes. Similarly, the liquid values were assigned to those volumes which had been totally melted ($f = 1.0$). For the control volume which contained the solid/liquid interface ($0.0 < f < 1.0$), average reflectivity and emissivity values were determined as a linear function of the volume fraction liquid for the control volume. In order to illustrate the new technique, the problem was simplified by neglecting the convective effects of the surrounding gas and assuming constant values for reflectivity and emissivity in the solid and liquid phases. For film thicknesses on the order of 1 μm, convective currents within the liquid silicon and variations in density are negligible.

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NUMERICAL METHOD

A control-volume formulation was used in the discretization of the transient two-dimensional heat conduction equations following the convention of Parankar[19] (see *Figure 3*). From equation (1), the temperature of a point may be expressed implicitly in terms of the neighbouring temperatures by:

$$T_p = (a_E T_E + a_W T_W + a_N T_N + a_S T_S + b)/a_p \tag{10}$$

The proper interface conductivities are determined in the usual fashion. Equation (10) is used to characterize the heat flow within the substrate. The heat flow within the film layer requires the enthalpy form of the heat conduction equation. Equation (4) is discretized somewhat differently and the coefficients must be modified. The initial step of discretizing (4) becomes:

$$\left(\frac{e_P - e_P^0}{\Delta t}\right)\Delta x \Delta y = a_E T_E + a_{W'} T_{W'} + a_N T_N + a_S T_S - T_P a'_P + S\Delta x \Delta y \tag{11}$$

where

$$a'_P = a_E + a_{W'} + a_N + a_S \tag{12}$$

By substituting (3) into (11), the conduction equation for the change of phase region becomes:

$$T_P = [\textstyle\sum a_{nb} T_{nb} + b' + a_P^{0\prime}(\rho c T_m - fL)]/(\rho c a_P^{0\prime} + a'_P) \tag{13}$$

where

$$a_P^{0\prime} = \frac{\Delta x \Delta y}{\Delta t} \tag{14}$$

$$b' = a_P^{0\prime} e_P^0 + S\Delta x \Delta y \tag{15}$$

$$\textstyle\sum a_{nb} T_{nb} = a_E T_E + a_W T_{W'} + a_N T_N + a_S T_S \tag{16}$$

When all temperatures are below the melting point, e_P^0 is found from:

$$e_P^0 = \rho c(T_P^0 - T_m) \tag{17}$$

and f for each control volume is set to 0.0.

The interface conductivities at the solid/liquid interface must be modified to include the sudden change of thermal conductivity at the interface. For example, the east interface conductivity, k_e, as shown in *Figure 4* may be expressed as:

$$k_e = \left(\frac{(\delta x)_{e-}}{k_P} + \frac{(\delta x)_{\text{int}-}}{k_{\text{int}-}} + \frac{(\delta x)_{\text{int}+}}{k_{\text{int}+}}\right)^{-1} (\delta x)_e \tag{18}$$

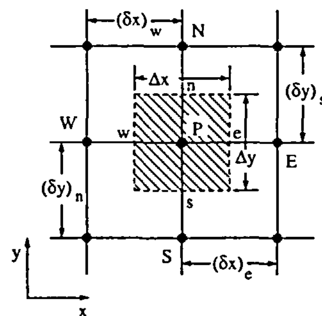

Figure 3 Schematic of control volume for interior node

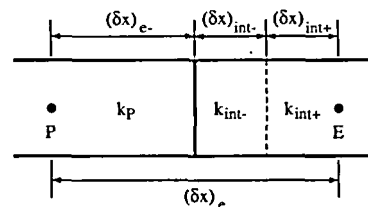

Figure 4 Schematic for calculation of interface conductivity at solid/liquid interface

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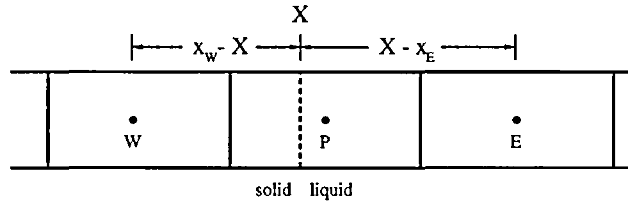

Figure 5 Schematic to calculate the distance from solid/liquid interface to neighbouring nodal temperature

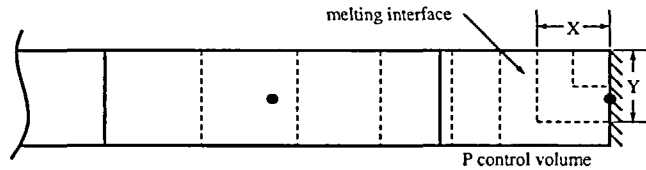

Figure 6 Progression of the melt pool in the thin film layer

It can be seen that (13) includes the volume fraction liquid for each control volume. If the correct values of f were known for each time step *a priori*, then the temperatures could be calculated directly from (10) and (13). However, since the interface location is dependent on the current temperatures, an iterative approach must be used. The interface energy-balance equation can be used as a check to determine whether the correct amount of energy has been contributed to phase change. The interface location, X, is the distance from the centre of the wafer (line of symmetry) to the melt front at a specific time. X can be found numerically from the discretized energy-balance equation:

$$\rho L \frac{X - X^0}{\Delta t} = k_s\left(\frac{T_W - T_m}{x_W - X}\right) - k_l\left(\frac{T_m - T_E}{X - x_E}\right) \tag{19}$$

where $x_W - X$ is the distance from the interface to node W and $X - x_E$ is the distance from the interface to node E as shown in *Figure 5*. When a control volume in the film first rises above the melt temperature, that volume is assumed to be changing phase. A quasi two-dimensional melt pool is initially assumed to form from the upper centre of the film with Y being equal to X (see *Figure 6*). Once Y has reached the bottom of the film, the interface is assumed to propagate vertically along the film in the x direction. When the interface is contained within the first control volume, the following finite difference approximation is used for the thermal gradient on the liquid side of the solid/liquid interface:

$$\frac{\partial T_l}{\partial x} = \frac{T_m - T_P}{X} \tag{20}$$

The interface location, X, is used to find the volume fraction liquid, f, for each control volume assuming a planar interface in the z direction.

In order to solve for both temperature and the solid/liquid interface location, (10), (13), and (19) must be satisfied simultaneously. The calculation of temperatures and interface location proceeds as follows:

(1) Before any melting has occurred, the temperatures of the domain are calculated using (10) in the substrate and (13) in the film with f equal to zero for all control volumes within the film.

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(2) Once a control volume in the film rises above the melt temperature, the melting of the film is assumed to have commenced.
(3) The limits between which the interface is to be searched are established in the first iteration as follows. The new temperatures are used in (19) to calculate the interface location, X, numerically. These temperatures were originally calculated assuming $X = 0$ (all $f = 0.0$), and it therefore was assumed that no energy was contributed to phase change. The interface location obtained with these temperature values would be the greatest possible distance the interface could travel within the time step. Since some of the energy must contribute to the latent heat, the interface location must be between the limits of zero and X.
(4) The established limits are bisected, and the bisected value is used as the next interface location guess, X_g.
(5) The interface location guess is converted to volume fraction liquid for each control volume.
(6) Equations (10) and (13) are solved for temperature using the new guessed values of f for each control volume.
(7) The new temperatures are used in (19) to check if the temperatures satisfy the equation. This calculated interface location will be called the interface check value, X_c. If the guessed value of interface location yields temperatures from (10) and (13) that, when inserted into (19), give the same value of X, both equations have been satisfied and the solution has been found for that time step.
(8) If X_c is greater than X_g, which was used to calculate the guessed f, then the interface location guess was too small and X_g is set as a lower limit. Similarly, if the checked interface location is less then that guessed, the guess was too large and X_g is set as an upper limit.
(9) Go to step (4) until convergence is met.
(10) In subsequent time steps, the initial limits are set during the first iteration as follows. The initial interface location guess is that found from the previous time step. If X_c is greater than X_g, then X_g is set as a lower limit and X_c is set as the upper limit. If, however, the checked interface location is less than that guessed, X_g is set as an upper limit and X_c is set as the lower limit.

The way the procedure works is further explained by *Figure 7*. As X increases, $\partial T_s/\partial x$ increases while $\partial T_l/\partial x$ decreases due to the change in solid/liquid interface location and the decrease in surrounding nodal temperatures. Any increase in the guessed value at a given time step will result in a lower check value. Therefore, the guessed and check values will move towards each other during successive iterations.

Since the speed of the solution is dependent on how close the initial guess for the interface location is to the final solution, there is an opportunity to increase the speed of the algorithm by providing a better guess. After the solution has been calculated for several time steps, the initial guess may be greatly improved by estimating the interface location for the next time step by using the velocity and acceleration of the melt front. Consider three previous locations of

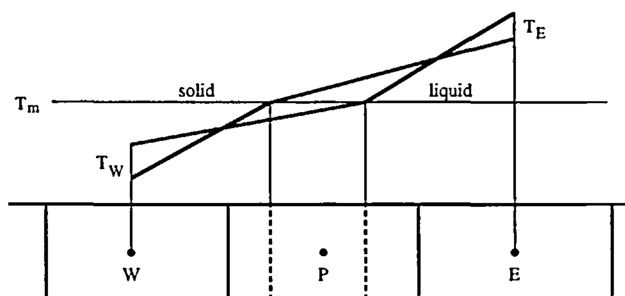

Figure 7 Effect of the position of interface on the thermal gradients at the solid/liquid interface

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the melt front and the fourth is to be estimated. If it is assumed that the velocity of the interface is constant during a time step, the velocity from 2 to 3 may be expressed as $(X_3 - X_2)/\Delta t$ and the velocity from 1 to 2 as $(X_2 - X_1)/\Delta t$. If the velocity remains constant during the two intervals, the fourth location can simply be expressed as $X_3 + \Delta t(X_3 - X_2)/\Delta t$. However, if the velocity changes during the two intervals, the acceleration of the front may be used to improve the guess by using:

$$X_4 = X_3 + \underbrace{\Delta t \left(\frac{X_3 - X_2}{\Delta t}\right)}_{\text{velocity term}} + \underbrace{\Delta t^2 \left(\frac{X_3 - 2X_2 + X_1}{\Delta t^2}\right)}_{\text{acceleration term}} \tag{21}$$

Using this technique, the interface location can be found in only a few iterations.

Using the conventional discretization for the thermal gradients as used in (19) can cause problems at steady state when superheated solid and supercooled liquid coexist. This can occur when the reflectivity of the material is greater in the liquid state. A problem can arise from the fact that the gradients do not remain continuous as the interface moves into a new control volume. From (6), the direction of the interface can be determined from the following conditions:

$$\frac{\partial X}{\partial t} > 0 \quad \text{if} \quad k_s \frac{\partial T_s}{\partial x} > k_l \frac{\partial T_l}{\partial x} \tag{22a}$$

$$\frac{\partial X}{\partial t} < 0 \quad \text{if} \quad k_s \frac{\partial T_s}{\partial x} < k_l \frac{\partial T_l}{\partial x} \tag{22b}$$

In some cases, the interface was found to move forward until the final steady state control volume was entered. Until this point, condition (22a) was satisfied. When the final control volume was entered, the gradients changed discontinuously in such a way that condition (22b) was satisfied and the interface would move in the reverse direction back into the previous control volume. At this point, the interface would oscillate between the two volumes and could not reach the steady state solution. A modification of the calculation of the thermal gradients at the solid/liquid interface was made so that the gradients would remain continuous as the interface entered a new control volume. To achieve this, a linear temperature profile was assumed between nodes as shown in *Figure 8*. Temperatures were then found at some fixed distance, Δl, on the solid, T_{sx}, and liquid, T_{lx}, sides of the interface. Assuming the interface temperature is T_m, the interface energy-balance equation takes the form:

$$\rho L \frac{X - X^0}{\Delta t} = k_s \left(\frac{T_{sx} - T_m}{\Delta l}\right) - k_l \left(\frac{T_m - T_{lx}}{\Delta l}\right) \tag{23}$$

The fixed distance, Δl, was set equal to δx to ensure reasonable resolution.

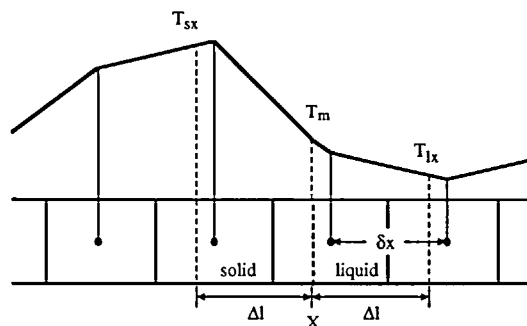

Figure 8 Calculation of thermal gradients using the modified thermal gradient method

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Table 1 Physical and optical properties used in the calculations

Silicon thermal conductivity (solid), $k_s = 0.2$ W/cm·°C
Silicon thermal conductivity (liquid), $k_l = 0.6$ W/cm·°C
Silicon density, $\rho = 2.3$ g/cm^3
Silicon specific heat, $c = 0.9268$ J/g·°C
Latent heat of fusion, $L = 1800.0$ J/g
Film reflectivity (solid), $R_s = 0.3$
Film reflectivity (liquid), $R_l = 0.7$
Film emissivity (solid), $\varepsilon_s = 0.6$
Film emissivity (solid), $\varepsilon_l = 0.2$

For the following calculations, the analysis of graphite-strip thermal processing was simplified in order to illustrate the method. The susceptor temperature was set at 1000.0°C and the melting temperature of silicon was considered to be 1412.0°C. The physical and optical properties used in the calculations are given in *Table 1*. All values were assumed constant to simplify the illustration of the method. Only the film structure was allowed to change phase, i.e. the substrate was allowed to superheat.

COMPARISON OF IMPLICIT AND EXPLICIT METHODS

The implicit and explicit formulations of the modified enthalpy methods were compared in terms of computational time and accuracy of results. A Convex C3200 (dual processor) was used in the calculations for each test case. A time step of 2.0×10^{-7} sec was used in the explicit method[12]. When the time step was cut in half, similar results were obtained, verifying the choice of time step. In the implicit method, a time step of 5.0×10^{-5} sec was used. Again, halving the time step produced nearly identical results. A tolerance of 1.0×10^{-5} was found to give desired accuracy. Graphite-strip thermal processing involves extended heating times (~ 15.0 sec) to reach steady state. Approximately one second of this time is required to reach the melt point with the remaining time (~ 14.0 sec) to melt the film material. Owing to the small time step necessary for the explicit method, a comparison of steady state solutions was not feasible; therefore comparisons were made for a portion of the total required time. Transient solutions of the melt width and centre film temperature (directly below the centre of the heat source) were obtained during 0.15 sec after melting had commenced. The beginning of melting is the period in which the greatest rate changes in temperature and melt width occur and therefore offer the most sensitive comparison of results between the two methods. At the end of the 0.15 sec period, the centre film temperature in the film obtained from the explicit method was 1414.424°C and the implicit method yielded a value of 1414.426°C, with the difference in absolute value varying not more than 2.26×10^{-3}°C during this period. Slight temperature oscillations were found to exist in the centre of the wafer when the interface was close to this region and disappeared as the interface progressed outward. However, these oscillations would presumably be less than those generated by the conventional enthalpy method because the temperature of a control volume changing phase is not fixed at the melt temperature. *Figure 9* shows the melt width as a function of time for each method. It can be seen that excellent agreement was obtained between the two methods. The explicit method required approximately 4.6 hours of CPU time compared to 0.8 hours needed for the implicit calculation, therefore decreasing computational time by of over 5.5 times.

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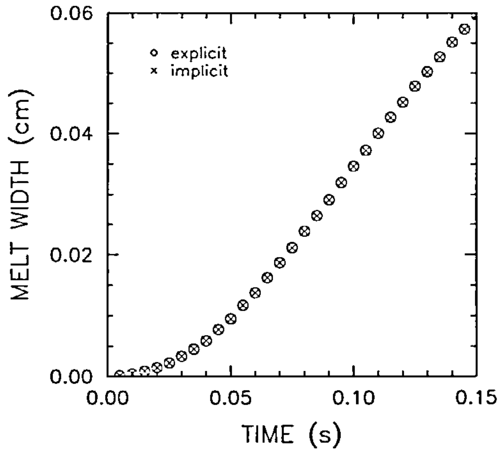

Figure 9 Comparison of melt width for implicit and explicit methods as a function of time

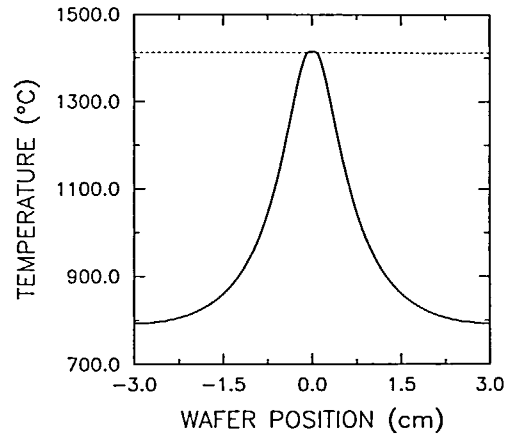

Figure 10 Steady state temperature profile using the implicit method (--- film melting point)

STEADY STATE RESULTS

Once the accuracy of the implicit method had been established, steady state solutions were obtained for full simulations using the implicit formulation with the modified thermal gradient calculation. The nodal grid spacing was reduced by a factor of two and no significant differences in results was found. Desired accuracy was obtained from a time step of 1.0×10^{-4} sec and a tolerance of 2.0×10^{-5}. The great advantage in computational efficiency of the implicit method may be realised when determining these steady state solutions. Using the explicit method, the amount of computer time used to calculate results for a certain time interval will remain constant for the entire simulation. The implicit method, however, will reduce the computational time significantly as the steady state solution is approached due to the fact that the number of iterations to solve for temperature per time step will decrease. Additionally, the algorithm can guess the next interface location with greater accuracy, therefore approaching the solution more efficiently. For the grid used in these calculations, the time step for the explicit method must be less than 4.26×10^{-6} sec. In comparing time to reach steady state, the implicit method would reduce computational time by an estimated 6 times if the largest possible time step allowed in the explicit method were used. However, if the individual film layers were modelled, the explicit time step restriction would be much more severe and the implicit method would be significantly faster. For example, the complete capped SOI film structure can be modelled with a control volume in each film instead of using a single bulk film. Assuming the properties of the oxide layers to be $k = 0.14$ W/cm·°C, $\rho = 1.2$ g/cm^3, and $c = 0.84$ J/g·°C, and each film layer 1.0 μm thick, the implicit method will run to steady state with acceptable accuracy using the same time step and tolerance as used in the above calculations. However, the explicit method will require a time step of at least 3.6×10^{-7} sec. The implicit method would decrease computational time by an estimated 46.2 times. If thinner films were modelled, even greater efficiency in computational time would result.

The steady state temperature distribution in the film is shown in *Figure 10*. The centre film temperature attained was 1415.375°C and drops to 793.459°C at the edge of the wafer. When the solid/liquid interface is observed more closely, it can be seen that a region of superheated solid exists in conjunction with a region of supercooled liquid as shown in *Figure 11*. These regions exist due to the fact that the reflectivity of the silicon film is greater in the liquid state.

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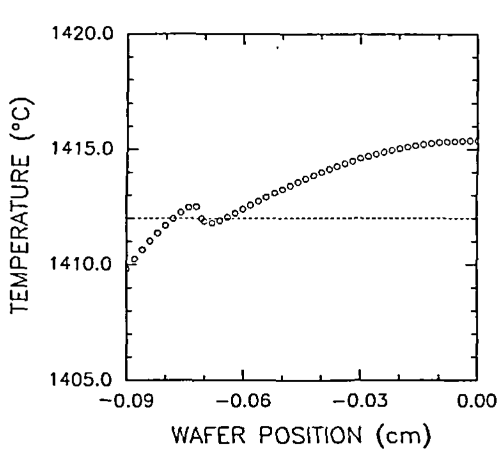

Figure 11 Temperature distribution at solid/liquid interface (--- film melting point)

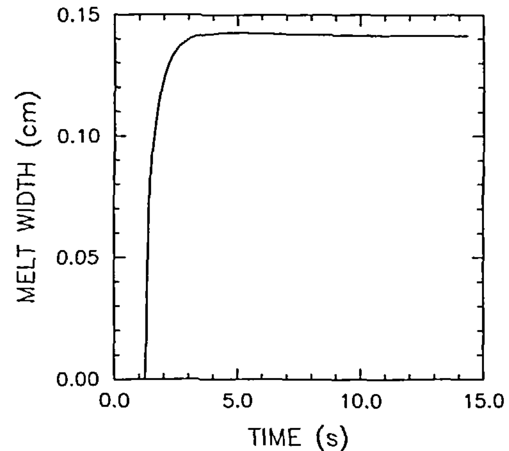

Figure 12 Melt width at the centre of the film as a function of time

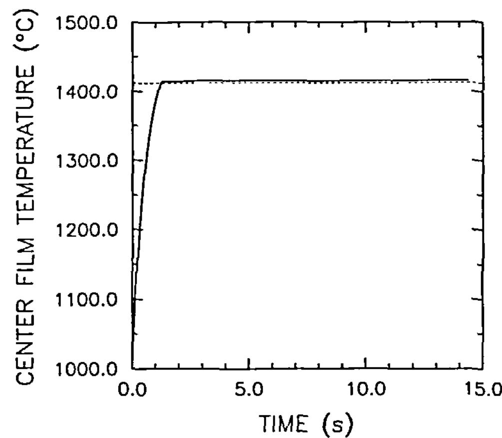

Figure 13 Centre film temperature as a function of time (--- film melting point)

The solid near the interface absorbs more heat than the adjacent liquid. In thermal processing, this may indicate an unstable interface[16].

Figure 12 shows the melt width as a function of time. The melt pool grows quickly at the start of melting and the size of the pool decreases slightly as it approaches the steady state location due to heat conduction down into the substrate. The steady state melt width attained was 0.1414 cm. The transient centre film temperature can be seen in *Figure 13*. The temperature rises quickly until the melting point is reached. At this time, the rate of temperature rise is decreased due to the decrease in energy absorption of the liquid film. Once the interface has travelled far from the centre of the wafer, the temperature decreases slightly because of the large decrease in energy absorption into the liquid pool. The temperature then rises again once the substrate has been heated sufficiently. Approximately 3.7 CPU hours were required to reach the steady state solution.

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CONCLUSION

A technique has been developed in which the one-dimensional energy-balance equation is coupled with the two-dimensional heat conduction equation. This is often the case in simulating the melting of a single thin film in a multilayer structure assuming that the thermal gradient through the thickness of the melting film is negligible. The modified enthaply method has been expressed in an implicit form. In some types of thermal processing, where extended processing times are necessary, the explicit method may take too long to obtain steady state solutions due to the restriction on the time step. The implicit formulation eliminates the stability criterion, therefore allowing larger time steps. Further, the method does not require an initial melting condition. The results of the implicit method were compared to those of the explicit method and excellent agreement was obtained. Computational efficiency was found to be far greater for the implicit method, especially when steady state results were desired. The implicit method was estimated to reduce computational time over 46.2 times when compared to the explicit method in reaching steady state temperature solutions in some models of graphite-strip thermal processing. The implicit method may be utilized to determine one-dimensional solutions which in turn may be used as approximate starting solutions for an explicit solution of two-dimensional problems. At steady state, regions of superheated solid and supercooled liquid were observed which were due to the difference in reflectivity of silicon between the solid and liquid states. In this situation, the conventional discretization of the thermal gradients at the interface was found to generate an oscillating interface near the steady state solution. The method of discretization was modified to prevent this oscillation.

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