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Application of forward five point central difference method in the temperature field model of laser processing silicon wafer

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Abstract. This paper develops an analysis of ultimate capacity of hot-rolled RHS and SHS, Traditional laser processing of silicon wafers usually uses phase transition method to remove materials, resulting in melting material resorting to overheated temperature and forming recast layer after cooling, which will affect the processing quality and material properties. This paper is Based on water jet assisted laser machining and the thought of energy balance, and apply prior to the central five point difference scheme to structure two dimensional transient temperature field model around cutting groove during the process of water jet assisted laser machining. At the same time, it will verify the applicability of the numerical model according to comparing the temperature field and the experimental results.

1. Introduction

Silicon is widely used in microelectronics, photovoltaic and high-density systems because of its excellent mechanical and electrical properties. With the pursuit of high performance and thin trend of electronic products, silicon material becomes thinner and thinner; As a result, their tensile strength, compressive strength are weaker and weaker, and they are very sensitive to mechanical external force. In order to rapidly and accurately cut these brittle materials, laser has been widely used because of its high photon energy and resolution for obtaining good cutting quality [1-2]. Conventional laser processing of silicon wafer uses multiple phase transition method to remove materials, and quality is acceptable in some low - level applications; However, there are excessive heat affected zones, large pollution and severe thermal deformation.

With the solution of mathematical physics problems, partial differential equations are applied in engineering practice, mechanisms produced by many phenomena are revealed and ,within the proper range ,make predictions about the subjects [3-5]. The experimental means can not effectively achieve the desired goal in some extreme conditions, such as ultra high temperature, minimal spatial scale and time scale. Sometimes the introduction of the experimental means itself can have a great impact on the subjects, for example, the famous uncertainty principle. At this point, numerical means can be divorced from the research entity itself, abstract the system model, and use mathematical model to explore the characteristics of the object, and carry out numerical experiments.

In this paper, it is based on the above reasons, and the temperature field model of nanosecond pulse laser processing of silicon wafer is constructed through the numerical methods. It requires a very high demand in temporal and spatial resolution on measuring equipment to extract transient temperature field in laser processing due to the use of nanosecond laser, and the processing area of work-piece in the micron scale. It can improve the effective number digital of numerical value to obtain high enough temporal and spatial resolution by the numerical method can solve the problems. Of course, it also can



use the non dimensional normalization to reduce the rounding error of data in the calculation process.

2. The processing conditions setting

In this paper, the size of the work-piece is x to $50\mu\text{m}$, y to $700\mu\text{m}$, and the length is 10ns . The width of x is divided into 26 nodes, and the length of Y is divided into 351 nodes, and the constant mesh spacing is $h=2\mu\text{m}$. x and y to the coordinates are:

$$\begin{aligned} x_i &= (i-1) \times h, i \in [1, 26] \\ y_j &= (j-1) \times h, j \in [1, 351] \end{aligned} \quad (1)$$

Two dimensional transient temperature model is made of double-layer structure. The first layer of two-dimensional node represents the node temperature stored in the previous time step, and the second layer two-dimensional node represents the node temperature under the current time step. When calculating the node temperature in the current time step, the current node temperature is stored in the current page of $26 \times 351 \times k$ to record the temperature distribution of the current time step; Then, the first layer node temperature region is replaced by the current node temperature of the second layer which is considered as the results of the previous time step, next empty the two layer node area value and the temperature distribution of the next time step is calculated by the first layer node, getting the whole time temperature changes of the work-piece through the cycle of calculation like mentioned above.

3. Model settings

3.1. Reference model

The laser uses a 1064nm solid-state laser with an output energy of 0.8mJ , and it is continuously adjustable. Work piece material is silicon with thickness of $700\mu\text{m}$, and the relevant material characteristics are shown in Table 1. The work-piece is placed on the worktable, and the spot diameter is $20\mu\text{m}$, and the water jet impact the softening region by 40 degree angle. Figure 2 is the energy density distribution of the laser spot. Laser light is loaded into the groove on the concave surface to conduct circulating heating in the process of material removal.

Table 1 Related properties parameters of silicon materials [6-7]

Characteristics	Numerical value
Density of silicon (kg/m^3)	$2.580 \times 10^3 - 0.171(T - T_M) - 1.61 \times 10^{-4}(T - T_M)^2; T > T_M$
Specific heat (J/kgK)	$2.432/\rho; T > T_M$
Heat conductivity (W/mK)	$9900/(T - 99); T > T_M$
Radiance	$0.66; T < T_M$ $0.27; T > T_M$
Absorption of silicon ($1/\text{m}$)	$2792.79; T < T_M$ $8.6 \times 10^7; T > T_M$
Melting point (K)	1687
Latent heat of vaporization (J)	8×10^7

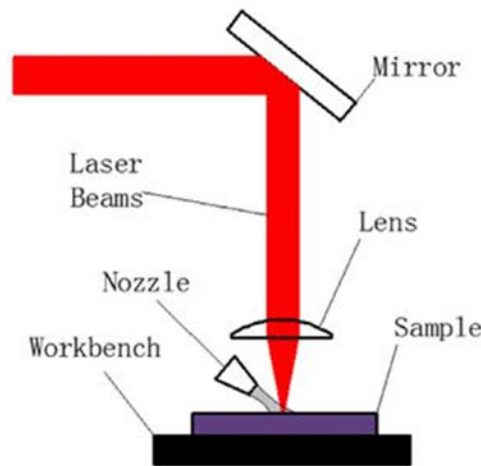


Fig. 1 Schematic diagram of water jet laser processing silicon wafer

The thermal phenomena in water jet assisted laser processing are convection, cooling and radiation. Figure 2 is the thermal analysis model which simulates the thermal effect of laser in the material using a framework for constructing a model with heat conduction nodes, in which the role of the black node is cooling while white node is heat conduction. The cooling effect of water flow exists in the machining process, and with the change of the groove, the cooling position changes with time. Convection considered as the boundary condition is a function of position and time. A 'dormant' convection cell is set in the material in order to avoid the complex motion of the convective boundary conditions. When the cutting is not in a region before the formation of the region, the convection units do not work in a 'sleep' state; when the cutting material is gradually deepened and removed, the removed parts which are filled with liquid exist the convection cooling effect, at this point, the convection units in the region are activated to produce cooling effect.

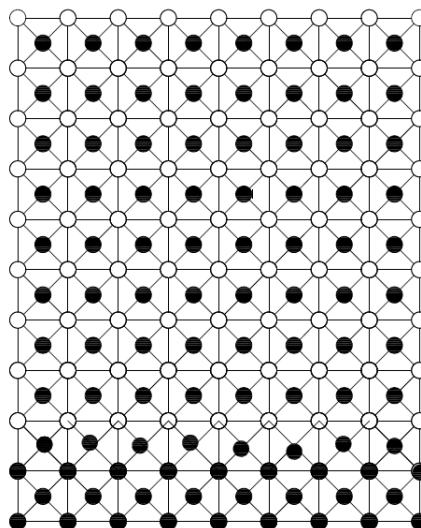


Fig. 2 Thermal analysis model of conduction cooling

With the removal of material, the loading position of laser irradiation in the groove is changeable and the laser is always loaded on the new concave surface. Formula 2 indicates the output power of

the selected solid state laser, where E_L is the output energy of laser; R_F is the reflectivity of material to laser; A_b is the laser absorption coefficient of silicon wafer; τ is the pulse width; d_L is the focal point of laser. The relevant parameters of the light source are shown in Table 2.

$$q(x, y, t) = \frac{E_L(1 - R_F)A_b e^{(-A_b y_i)} \frac{-4(x_i)^2}{d_L^2}}{\tau \rho A_L} e^{-\frac{4(x_i)^2}{d_L^2}}, t \leq \tau \quad (2)$$

Formula 3 shows the temperature distribution of laser loading; C_p is the specific heat of the material; K is the thermal conductivity of the material; ρ is the density of the material; T is the temperature of the material; The relevant parameters are shown in Table 2.

$$\frac{C_p \partial T(x, y, t)}{\partial t} = \frac{k}{\rho} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + q(x, y, t) \quad (3)$$

Table 2 Related parameters of laser heat source and water jet

Heat source parameter	Numerical value
Laser wave length (nm)	1064
Output energy (mJ)	0.3
Impulse frequency (kHz)	20
Pulse width (ns)	50
Water gage (Mpa)	20
Angle of shock(deg)	40
Focal diameter (um)	20

Water flow cooling work-piece during processing, cooling area except work-piece surface. When the material is removed to form a groove, the water flow gets into the groove to cool the cutting groove. With the processing carrying out, the shape of the groove is changed, and the cooling region is also changed along with the time of cutting. Convection as a cooling boundary condition is athletic. Formula 3 shows the cooling effect of water flow, where h is the cooling coefficient with its value ranging from 500 to 10000W/m² K.

$$k \frac{\partial T}{\partial n} = -h(T - T_s) \quad (4)$$

$$\tau_s = 4 \times 10^6 + 7.296 \times 10^9 e^{(-5.929 \times 10^{-3} T)} \quad (5)$$

$$\int C_p dT + L_m \geq H_s \leq \int C_p dT + L_m + L_v \quad (6)$$

$$\tau_w = p_w \sqrt{\frac{\cos^4 \theta_w}{4} + \sin^2 \theta_w \cos^2 \theta_w} \quad (7)$$

Formula 5 and 6 are considered as the principle of the material removal at different temperature; τ_w is the shear force of flow impact; τ_s is the shear stress of silicon material under different temperature; p_w is the impact force of water flow; θ_w is impact angle of water flow; H_s is the enthalpy value of the material; L_m is the latent heat of melt silicon and L_v is the latent heat of vaporization; $\tau_s < \tau_w$ is considered as the criterion for materials in water jet assisted laser processing and formula 7 is used in

material removal criteria in traditional laser processing.

3.2. model construction method

Taking silicon wafer as the research object, the temperature field model of the process is built firstly. The two-dimensional work-piece is dispersed into 26×351 lattice, space node spacing $2\mu\text{m}$. The convection coefficient matrix dimension 26×351 is prestored for convection coefficient of each lattice which is waiting to be activated. The temperature matrix size is $26 \times 351 \times k$, and k represents the time step, and the temperature distribution of the n time nodes can be stored. The sizes of the density matrix, the specific heat matrix, the thermal conductivity matrix, the absorption coefficient matrix, the reflectivity matrix, the thermal diffusion matrix, the heat source matrix are all 26×351 .

The error of the heat transfer model is the difference between the approximate solution of the differential equation and the exact solution of the partial differential equation. There are two sources leading error: The first one is the truncation error generated by each step, which is due to the approximate derivative, which depends on the distribution of the initial temperature, the treatment of the boundary conditions, the selection of the difference scheme and the selection of the Fourier number; Another error is a rounding error which is resulted by the precision of effective numbers retained and is inherent in the calculation. The stability of difference schemes of the heat transfer model is whether the calculation error with calculation with the calculation of unripe growth will go beyond the allowable range or not. And it is whether the results of data are sensitive to initial conditions and data error and rounding error of boundary conditions or not. The initial and boundary conditions are data measured which is unavoidable error in many cases, and there are also numerical rounding error in calculation. These errors can be amplified in the calculation, resulting in the instability of the solution, and the calculation will deviate from the real results. The Fourier number is less than $1/4$ in order to maintain the stability and take time for 5ns .

The processing of central lattice apply the forward five point difference scheme.

$$T_{i,j}^{k+1} = foui_{i,j}^k \times (T_{i+1,j}^k + T_{i-1,j}^k + T_{i,j+1}^k + T_{i,j-1}^k) + (1 - 4 \times foui_{i,j}^k) \times T_{i,j}^k + \text{deltat}_{i,j}^k / (\text{denss}_{i,j}^k \times \text{cp}_{i,j}^k) \times \text{phy}_{i,j}^k \quad (8)$$

$$foui = \alpha \times \text{deltat} / (h_i)^2 \quad (9)$$

Among them, phy is the heat source; $foui$ is the Fourier number of heat transfer; α is the heat transfer coefficient, $\text{deltat} = 5\text{ns}$. The boundary temperature around the boundary condition is the ambient temperature 300K , and the initial condition is the initial temperature of the whole region.

4. Application of the forward five point central difference method

4.1. Five point difference scheme for boundary point data processing

Energy balance method is used to deal with boundary node data, $IP + OP + S = E$. Where IP represents the energy flowing into the edge node; OP represents the energy of the outgoing side node; S is the heat source energy of the node; E represents an increase in energy within a single time step. As $S=0$ said pyrogen reaction. Taking the right node as an example, five points of temperature $t0, t1, t2, t3, t4$ respectively represents the central node, the next node, the left node, the upper node, the right node, so:

$$IP + OP + S = E$$

$$IP1 = (T1 - T0) \times \text{lammda} \times dx / (2 \times dy)$$

$$IP1 = (T2 - T0) \times \text{lammda} \times dy / (2 \times dx)$$

$$OP1 = (T0 - T3) \times \text{lammda} \times dx / (2 \times dy)$$

$$OP2 = h \times (T0 - Tf) \times dx \times dy / 2$$

$$E = \rho \times C / dtelta \times (T0^{k+1} - T0^k)$$

Tidy up:

$$T_{26,j}^{k+1} = \text{foui}_{26,j}^k \times (2 \times T_{25,j}^k + T_{26,j+1}^k + T_{25,j-1}^k) + (1 - 4 \times \text{foui}_{26,j}^k - 2 \times \text{foui}_{26,j}^k \times \text{biot}_{26,j}^k) \times T_{26,j}^k \\ + 2 \times \text{foui}_{26,j}^k \times \text{biot}_{26,j}^k \times Tf + \text{deltat} / (\text{dens}_{26,j}^k \times \text{cp}_{26,j}^k) \times \text{phy}_{26,j}^k$$

$$\text{biot} = h \times h_i / k$$

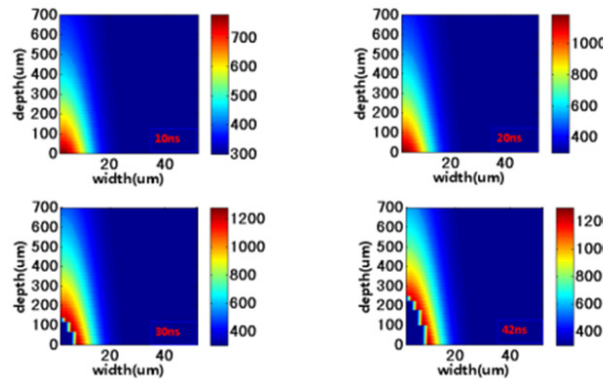
Where biot is the Biot number of the heat transfer theory.

4.2. Five point difference scheme for corner point data processing

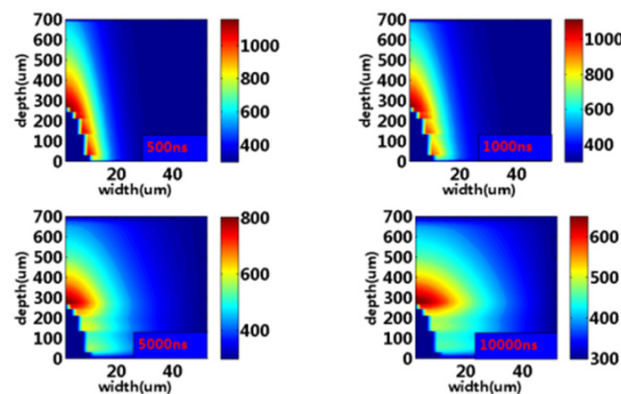
Similar data are processed at the corners using the same method as the boundary. The increase of convection surface at the corner results in conductivity reducing, and the calculation of the region in the X and Y direction is changed to half of the grid .

$$T_{1,1}^{k+1} = \text{foui}_{1,1}^k \times (2 \times T_{1,2}^k + 2 \times T_{2,1}^k) + (1 - 4 \times \text{foui}_{1,1}^k - 4 \times \text{foui}_{1,1}^k \times \text{biot}_{1,1}^k) \times T_{1,1}^k \\ + 4 \times \text{biot}_{1,1}^k \times Tf + \text{phy}_{1,1}^k \times \text{deltat}_{1,1}^k / (\text{dens}_{1,1}^k \times \text{cp}_{1,1}^k)$$

First calculate the temperature of grid point ,then calculate the temperature of the boundary node according to the energy balance, where the boundary nodes are divided into corners and edges which are processed respectively. Storage the temperature discrete data of each time step, then draw cloud pictures shown in Figure 3.



(a)The temperature distribution in the process of water jet assisted laser machining



(b) Temperature distribution of normal laser cutting groove
Fig. 3 temperature distribution of grooving in laser machining

5. Conclusion

Under the extreme conditions, the response or sensitivity of experimental instruments to laser processing can not meet the requirement. At this point, numerical means can be divorced from the research entity itself, abstract the system model, and use mathematical model to explore the characteristics of the object, and carry out numerical experiments. Based on the idea of energy balance, a two-dimensional transient temperature field model around a notch in a water jet assisted laser machining process is constructed by applying the forward central five difference scheme. At the same time, the temperature field is calculated by the numerical calculation, and the experimental results are compared to verify the applicability of the numerical model.

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