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Estimating thermal transport in deep X-ray lithography with an inversion method

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ABSTRACT This study proposes a general methodology for estimating the depth profile of the heat source of the thermal transport system during deep X-ray lithography. The exposure process in a lithography system is considered as an inverse heat conduction problem with an unknown heat source. The conjugate gradient method is used to solve the inverse problem. Numerical results confirm that the method proposed herein can accurately estimate the heat source even involving the inevitable measurement errors. Furthermore, this methodology can also be applied to estimate the local distribution of temperatures when using scanning thermal microscopy (SThM) to microthermally machine materials and will contribute to increase the quality of microthermally machined products. In addition, a thermomechanical data-storage system, which utilizes a resistively heated atomic-force-microscopy (AFM) cantilever tip to read and write data bits, can also adopt this inverse methodology to control the temperature of a polymer substrate.

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1 Introduction

Deep X-ray lithography, using synchrotron radiation to irradiate a photoresist deposited on a substrate through a mask, is an important technique in the fabrication of very small or high aspect ratio micro- and nanostructures [1–3]. This technology is capable of manufacturing complex microstructures with accurate dimensions. Polymethylmethacrylate (PMMA) is commonly used as photoresist and silicon as substrate.

During the exposure of the photoresist with radiation, high energy photons are absorbed in a mask, photoresist and substrate. This can lead to a temperature rise in all the components of the lithographic system and result in distortion and subsequent microstructure deformation. Recently, the thermal behavior of the system during operation has been studied [4–8]. Dai and Nassar [6], for example, analyzed the temperature distribution in X-ray irradiated resists with three-dimensional heat equations using a hybrid finite element and the generalized Marchuk splitting scheme. Cudin et al. [7] studied the variation of temperature and deformation in masks during deep X-ray lithography using a finite element method. Recently, Yang and Pitchumani [8] presented for the case of cylindrical symmetry an analytical solution for the temperature profiles in a resist irradiated with an X-ray beam. To accurately describe the thermal behavior of materials in a lithographic system, we must determine the heat generation in the layers, which depends on the material properties of the system, operating conditions and decays as a function of distance from the irradiated surface. To simplify the analysis, it is often assumed that the heat source is an exponential function of the penetrating depth [6, 8]. The heat source in the heat transfer problem of the lithographic system is difficult to measure directly, but it will affect the temperature distribution in the system.

In this paper, the heat transport problem during the deep X-ray lithography, including the unknown heat source, is treated as an inverse heat transfer problem. The inversion problem must be dealt with as an iteration algorithm. Many methods of solving the inverse problem have been developed, for instance, the sequential estimation method [9], the conjugated gradient method [10] and the Levenberg–Marquardt method [11]. In this paper the conjugated gradient method is used to estimate the heat source. The advantage of the conjugated gradient method is that an iterative regularization is implicitly built into the computational procedure. The method can quickly approach the target function, is very powerful and has been used frequently [12–15] to solve the function estimation problem.

2 Analysis

Consider the heat transfer problem of the deep X-ray irradiation process in a three-dimensional rectangular geometry, including a photoresist and a substrate, as shown in Fig. 1. The X-ray beam illuminates the resist coated substrate through a mask and penetrates the surface of the photoresist and into the substrate. X-ray induced heating of the two-layer sample decreases with depth and is affected by a cooling gas between mask and photoresist. The problem of heating during X-ray lithography of materials is, therefore, complicated. Generally, the heat source decays with penetrating depth is difficult to measure directly, and it influences the temperature

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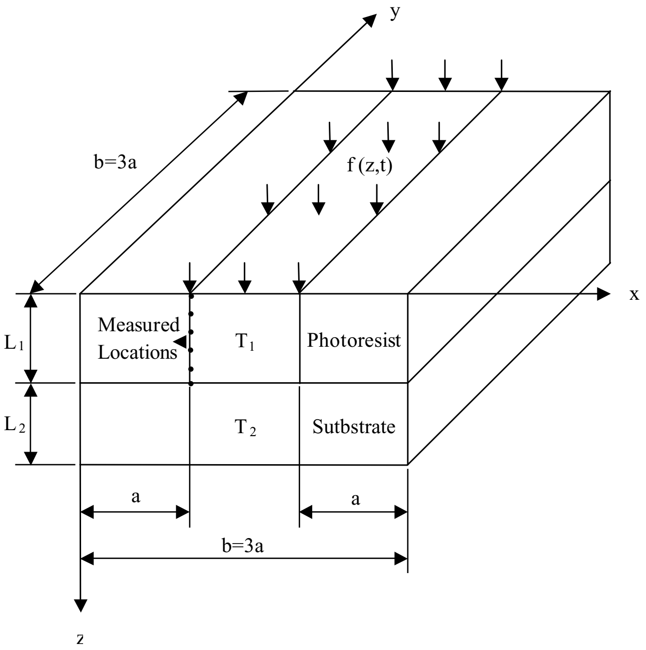

FIGURE 1 Schematic diagram of three-dimensional configuration of photoresist and substrate

fields within the exposed materials. The temperature distribution during X-ray lithography can be derived as a solution to the heat conduction problem for the photoresist and the substrate regions and, when the heat source is unknown, can be treated as a so-called "inverse heat conduction problem." In this paper, the conjugate gradient method is used to deal with the inverse problem. This method includes the following problems: the direct problem, the sensitivity problem and the adjoint problem, which are discussed as follows:

2.1 *Direct problem*

The three-dimensional heat conduction equations and the corresponding boundary and initial conditions for the deep X-ray lithography are [16]

$$k_1\left(\frac{\partial^2 T_1}{\partial x^2}+\frac{\partial^2 T_1}{\partial y^2}+\frac{\partial^2 T_1}{\partial z^2}\right)+g(x,y,z,t)=\rho_1 c_1\frac{\partial T_1}{\partial t}, \tag{1a}$$

$$k_2\left(\frac{\partial^2 T_2}{\partial x^2}+\frac{\partial^2 T_2}{\partial y^2}+\frac{\partial^2 T_2}{\partial z^2}\right)+g(x,y,z,t)=\rho_2 c_2\frac{\partial T_2}{\partial t}, \tag{1b}$$

$$T_1(x,y,L_1,t)=T_2(x,y,L_1,t), \tag{1c}$$

$$k_1\frac{\partial T_1(x,y,L_1,t)}{\partial z}=k_2\frac{\partial T_2(x,y,L_1,t)}{\partial z}, \tag{1d}$$

$$T_2(x,y,L,t)=T_\infty, \tag{1e}$$

$$k_{\mathrm{i}}\frac{\partial T_{\mathrm{i}}}{\partial n}=h(T_{\mathrm{i}}-T_\infty), \quad i=1,2, \tag{1f}$$

$$T_{\mathrm{i}}(x,y,z,0)=T_\infty, \quad i=1,2, \tag{1g}$$

where the subscripts 1 and 2 represent the photoresist and the substrate, respectively. $T(x,y,z,t)$ is the temperature distribution in the materials and T_∞ is the surrounding temperature. L is the total thickness of the photoresist with thickness L_1 and the substrate with thickness L_2, that is, $L=L_1+L_2$; k, ρ, and c are thermal conductivity, density, and specific heat, respectively. h is the convective heat transfer coefficient. Equations (1c) and (1d) express the boundary conditions at the interface between the photoresist and the substrate, which are assumed to be continuity of temperature and heat flux, respectively. Equation (1e) represents the boundary condition at the bottom surface of the substrate, which is kept at the temperature of the surroundings, and the other surfaces of the system are assumed to be convection boundary conditions due to air flow and described by Eq. (1f). $g(x,y,z,t)$ is a source term due to the irradiation and assumed to be a function of time and penetrating depth and written as

$$g(x,y,z,t)=f(z,t), \quad a\le x\le 2a, \quad 0\le y\le b. \tag{2a}$$

The regions for heat transfer and heat generation in the lithographic system are expressed as Ω and Ω_{g}, respectively. Ω consists of Ω_1 for the photoresist and Ω_2 for the substrate. Equation (2a) can be rewritten as

$$g(\Omega,t)=f(z,t)\delta(\Omega-\Omega_{\mathrm{g}}), \tag{2b}$$

where δ is the Dirac delta function.

2.2 *Sensitivity problem*

The solution of the direct problem with the unknown heat source $f(z,t)$ is now regarded as a problem of optimum control, which has the control function $f(z,t)$ and is intended to minimize the functional $J(f)$ defined by:

$$J[f(z,t)]=\int_0^{t_{\mathrm{f}}}\sum_{\mathrm{m}=1}^{\mathrm{M}}[T_1(a,0,z_{\mathrm{m}},t)-Y_1(a,0,z_{\mathrm{m}},t)]^2\mathrm{d}t, \tag{3}$$

where $T_1(a,0,z_{\mathrm{m}},t)$ is the estimated temperature on a specific position $x=a$, $y=0$, and along the z axis, $m=1$ to M, where M denotes the number of temperature measurements, and $Y_1(a,0,z_{\mathrm{m}},t)$ is the measured temperature at the same location and time as $T_1(a,0,z_{\mathrm{m}},t)$. t_{f} is the final time of the measurement.

To derive the sensitivity problem, it is assumed that when $f(z,t)$ undergoes a variation $\Delta f(z,t)$, the temperatures, T_1 and T_2, change by a corresponding amount ΔT_1 and ΔT_2. By replacing f with $f+\Delta f$, T_1 with $T_1+\Delta T_1$ and ΔT_2 with $T_2+\Delta T_2$ in the direct problem and subtracting it from its original problem expressed by Eq. (1). The sensitivity problem is defined as follows:

$$k_1\left(\frac{\partial^2 \Delta T_1}{\partial x^2}+\frac{\partial^2 \Delta T_1}{\partial y^2}+\frac{\partial^2 \Delta T_1}{\partial z^2}\right)+\Delta f(z,t)\delta(\Omega_1-\Omega_{\mathrm{g}})=\rho_1 c_1\frac{\partial \Delta T_1}{\partial t}, \tag{4a}$$

$$k_2\left(\frac{\partial^2 \Delta T_2}{\partial x^2}+\frac{\partial^2 \Delta T_2}{\partial y^2}+\frac{\partial^2 \Delta T_2}{\partial z^2}\right)+\Delta f(z,t)\delta(\Omega_2-\Omega_{\mathrm{g}})=\rho_2 c_2\frac{\partial \Delta T_2}{\partial t}, \tag{4b}$$

$$\Delta T_1(x,y,L_1,t)=\Delta T_2(x,y,L_1,t), \tag{4c}$$

$$k_1\frac{\partial\Delta T_1(x,y,L_1,t)}{\partial z}=k_2\frac{\partial\Delta T_2(x,y,L_1,t)}{\partial z}, \tag{4d}$$

$$\Delta T_2(x,y,L,t)=0, \tag{4e}$$

$$k_{\mathrm{i}}\frac{\partial\Delta T_{\mathrm{i}}}{\partial n}=h\Delta T_{\mathrm{i}},\quad i=1,2, \tag{4f}$$

$$\Delta T_{\mathrm{i}}(\Omega_{\mathrm{i}},0)=0,\quad i=1,2. \tag{4g}$$

2.3 *Adjoint problem and gradient equation*

To derive the adjoint problem, Eq. (1) is multiplied by the Lagrange multipliers, $\lambda_1(x,y,z,t)$ and, $\lambda_2(x,y,z,t)$, and the resulting expressions are integrated over time. Then the result is added to the right-hand side of Eq. (2) and the following form is obtained:

$$\begin{aligned}
&J[f(z,t)]\\
&=\int_0^{t_{\mathrm{f}}}\int_{\Omega_1}[T_1(\Omega_1,t)\\
&\quad -Y_1(\Omega_1,t)]^2\delta(x-a)\delta y\delta(z-z_{\mathrm{m}})\,\mathrm{d}\Omega_1\mathrm{d}t\\
&\quad +\int_0^{t_{\mathrm{f}}}\int_{\Omega_1}^{\lambda_1}(\Omega_1,t)\Bigg[k_1\left(\frac{\partial^2T_1}{\partial x^2}+\frac{\partial^2T_1}{\partial y^2}+\frac{\partial^2T_1}{\partial z^2}\right)\\
&\quad +f(z,t)\delta(\Omega_1-\Omega_{\mathrm{g}})-\rho_1c_1\frac{\partial T_1}{\partial t}\Bigg]\mathrm{d}\Omega_1\mathrm{d}t\\
&\quad +\int_0^{t_{\mathrm{f}}}\int_{\Omega_2}^{\lambda_2}(\Omega_2,t)\Bigg[k_2\left(\frac{\partial^2T_2}{\partial x^2}+\frac{\partial^2T_2}{\partial y^2}+\frac{\partial^2T_2}{\partial z^2}\right)\\
&\quad +f(z,t)\delta(\Omega_2-\Omega_{\mathrm{g}})-\rho_2c_2\frac{\partial T_2}{\partial t}\Bigg]\mathrm{d}\Omega_2\mathrm{d}t.
\end{aligned} \tag{5}$$

The variation of ΔJ is obtained by perturbing T_1 with ΔT_1 and T_2 with ΔT_2 in Eq. (4) and then by subtracting it from Eq. (5), the following is obtained:

$$\begin{aligned}
\Delta J=&\int_0^{t_{\mathrm{f}}}\int_{\Omega_1}^{2}(T_1-Y_1)\Delta T_1\delta(x-a)\delta y\delta(z-z_{\mathrm{m}})\,\mathrm{d}\Omega_1\mathrm{d}t\\
&+\int_0^{t_{\mathrm{f}}}\int_{\Omega_1}^{\lambda_1}(\Omega_1,t)\left[k_1\left(\frac{\partial^2\Delta T_1}{\partial x^2}+\frac{\partial^2\Delta T_1}{\partial y^2}+\frac{\partial^2\Delta T_1}{\partial z^2}\right)\right.\\
&\left.+\ \Delta f(z,t)\delta(\Omega_1-\Omega_{\mathrm{g}})-\rho_1c_1\frac{\partial\Delta T_1}{\partial t}\right]\mathrm{d}\Omega_1\mathrm{d}t\\
&+\int_0^{t_{\mathrm{f}}}\int_{\Omega_2}^{\lambda_2}(\Omega_2,t)\left[k_2\left(\frac{\partial^2\Delta T_2}{\partial x^2}+\frac{\partial^2\Delta T_2}{\partial y^2}+\frac{\partial^2\Delta T_2}{\partial z^2}\right)\right.\\
&\left.+\ \Delta f(z,t)(\Omega_2-\Omega_{\mathrm{g}})-\rho_2c_2\frac{\partial\Delta T_2}{\partial t}\right]\mathrm{d}\Omega_2\mathrm{d}t.
\end{aligned} \tag{6}$$

The second and third terms in the above equation is integrated by parts; the boundary and initial conditions of the sensitivity problem are utilized and then ΔJ is set to zero. After some manipulation, the adjoint problem is defined as follows:

$$k_1\left(\frac{\partial^2\lambda_1}{\partial x^2}+\frac{\partial^2\lambda_1}{\partial y^2}+\frac{\partial^2\lambda_1}{\partial z^2}\right)+\rho_1c_1\frac{\partial\lambda_1}{\partial t}=0, \tag{7a}$$

$$k_2\left(\frac{\partial^2\lambda_2}{\partial x^2}+\frac{\partial^2\lambda_2}{\partial y^2}+\frac{\partial^2\lambda_2}{\partial z^2}\right)+\rho_2c_2\frac{\partial\lambda_2}{\partial t}=0, \tag{7b}$$

$$\lambda_1(x,y,L_1,t)=\lambda_2(x,y,L_1,t), \tag{7c}$$

$$k_1\frac{\partial\lambda_1(x,y,L_1,t)}{\partial z}=k_2\frac{\partial\lambda_2(x,y,L_1,t)}{\partial z}, \tag{7d}$$

$$\lambda_2(x,y,L,t)=0, \tag{7e}$$

$$k_1\frac{\partial\lambda_1}{\partial n}=h\lambda_1+2\left(T_1-Y_1\right)\delta\left(x-a\right)\delta y\delta\left(z-z_{\mathrm{m}}\right), \tag{7f}$$

$$k_2\frac{\partial\lambda_2}{\partial n}=h\lambda_2, \tag{7g}$$

$$\lambda_{\mathrm{i}}(\Omega_{\mathrm{i}},t_{\mathrm{f}})=0,\quad i=1,2. \tag{7h}$$

Finally, the integral term is left as:

$$\Delta J=\int_0^{t_{\mathrm{f}}}\int_{\Omega_{\mathrm{g}}}(\lambda_1+\lambda_2)\Delta f(z,t)\,\mathrm{d}\Omega_{\mathrm{g}}\mathrm{d}t. \tag{8}$$

From a previously published analysis [10], the following is derived:

$$\Delta J=\int_0^{t_{\mathrm{f}}}\int_{\Omega_{\mathrm{g}}}J'\,[f(z,t)]\Delta f(z,t)\,\mathrm{d}\Omega_{\mathrm{g}}\mathrm{d}t, \tag{9}$$

where J' s the gradient of the functional J.

A comparison of Eqs. (8) with (9) leads to the following gradient equation:

$$J'=\lambda_1(\Omega_{\mathrm{g}},t)+\lambda_2(\Omega_{\mathrm{g}},t). \tag{10}$$

2.4 *Conjugate gradient method for minimization*

Assuming the functions of $T_{\mathrm{i}}(\Omega_{\mathrm{i}},t)$, $\Delta T_{\mathrm{i}}(\Omega_{\mathrm{i}},t)$, $\lambda_{\mathrm{i}}(\Omega_{\mathrm{i}},t)$, $i=1,2$ and J' are available at the Kth iteration, the iterative process for estimating the unknown function $f(z,t)$ by the conjugate gradient method is performed. The function $f(z,t)$ can be evaluated at the $(K+1)$th step by:

$$f^{\mathrm{K}+1}=f^{\mathrm{K}}-\beta^{\mathrm{K}}P^{\mathrm{K}},\quad K=0,1,2,\ldots, \tag{11}$$

where β^{K} is the step size of the search and P^{K} is the direction of the descent given by:

$$P^{\mathrm{K}}=J'^{\mathrm{K}}+\gamma^{\mathrm{K}}P^{\mathrm{K}-1},\quad K=1,2,3,\ldots, \tag{12}$$

where γ^{K} is the conjugate coefficient and determined from:

$$\gamma^{\mathrm{K}}=\frac{\int_0^{t_{\mathrm{f}}}\int_{\Omega_{\mathrm{g}}}(J'^{\mathrm{K}})^2\,\mathrm{d}\Omega_{\mathrm{g}}\mathrm{d}t}{\int_0^{t_{\mathrm{f}}}\int_{\Omega_{\mathrm{g}}}(J'^{\mathrm{K}-1})^2\,\mathrm{d}\Omega_{\mathrm{g}}\mathrm{d}t},\quad \text{with }\gamma^0=0. \tag{13}$$

The function $J[f(z,t)]$ at iteration $K+1$ is obtained by rewriting Eq. (3) as:

$$J(f^{\mathrm{K}+1})=\int_0^{t_{\mathrm{f}}}\sum_{\mathrm{m}=1}^{\mathrm{M}}[T_1(f^{\mathrm{K}}-\beta^{\mathrm{K}}P^{\mathrm{K}})-T_1^*]^2\mathrm{d}t. \tag{14}$$

Expanding Eq. (14) into a Taylor series yields:

$$J(f^{\mathrm{K}+1})=\int_0^{t_{\mathrm{f}}}\sum_{\mathrm{m}=1}^{\mathrm{M}}[T_1(f^{\mathrm{K}})-\beta^{\mathrm{K}}\Delta T_1(f^{\mathrm{K}})-T_1^*]^2\mathrm{d}t. \tag{15}$$

The sensitivity function $\Delta T_1(f^{\mathrm{K}})$ and $\Delta T_2(f^{\mathrm{K}})$ are taken as the solution of Eq. (4) at the measured time by setting $\Delta f = P^{\mathrm{K}}$. The search step size β^{K} can be determined by minimizing the function given by Eq. (15) with respect to β. After rearrangement, the following expression is obtained:

$$\beta^{\mathrm{K}} = \frac{\int_0^{t_{\mathrm{f}}} \sum_{\mathrm{m}=1}^{\mathrm{M}} \Delta T_1(P^{\mathrm{K}})[T_1(f^{\mathrm{K}}) - T_1^*]\,\mathrm{d}t}{\int_0^{t_{\mathrm{f}}} \sum_{\mathrm{m}=1}^{\mathrm{M}} \Delta T_1^2(P^{\mathrm{K}})\,\mathrm{d}t}. \tag{16}$$

2.5 Stopping criterion

For an ideal case without any measurement errors, the checked condition for the minimization of the criterion is:

$$J(F^{\mathrm{K}+1}) \le \varepsilon, \tag{17}$$

where ε is a small specified number. However, the observed displacement data contains measurement errors. The iteration is necessary for yielding a minimization of the function based on Eq. (3). The discrepancy principle is used to stop the iteration process [10]. The principle indicates that the discrepancy between the computed temperature and the measured temperature is approximately equal to the standard deviation of the measurement σ, that is, $T_1 - Y_1 \approx \sigma$, σ is assumed to be a constant. Substituting σ into Eq. (3), the stopping criterion can be expressed as

$$\varepsilon = M\sigma^2 t_{\mathrm{f}}. \tag{18}$$

Equation (17) with ε determined from Eq. (19) is used to stop the iteration.

3 Results and discussion

3.1 Computation procedure

The computational procedures for estimating the heat source by inverse methodology are summarized as follow:

Step 1. Assume the value for $f^{\mathrm{K}}(z,t)$ and suppose that $f^{\mathrm{K}}(z,t)$ is available at iteration K.
Step 2. Solve the direct problem of Eq. (1) to obtain $T_1(\Omega_1,t)$ and $T_2(\Omega_2,t)$.
Step 3. Check the stopping criterion given by Eq. (17) and continue the iteration if not satisfied.
Step 4. Solve the adjoint problem described by Eq. (7) to obtain $\lambda_1(\Omega_1,t)$ and $\lambda_2(\Omega_2,t)$.
Step 5. Compute the gradient in the functional from Eq. (10).
Step 6. Compute the conjugation coefficient from Eq. (13) and then the direction of descent from Eq. (12).
Step 7. Set $\Delta f = P^{\mathrm{K}}$ and then solve the sensitivity problem given by Eq. (4).
Step 8. Compute the step size of the search β^{K} from Eq. (16).
Step 9. Compute the new estimations for $f^{\mathrm{K}+1}$ from Eq. (11) and go back to Step 1.

3.2 Error analysis

Error analysis is important in assessing the accuracy of the result obtained using the inverse methodology. The relative error between the exact and estimated value of the heat source can be computed by

$$\varepsilon_{\mathrm{e}} = \left\{ \int_0^{t_{\mathrm{f}}} \int_{\Omega_{\mathrm{g}}} [f^*(z,t) - f(z,t)]^2\,\mathrm{d}\Omega_{\mathrm{g}}\mathrm{d}t \Bigg/ \int_0^{t_{\mathrm{f}}} \int_{\Omega_{\mathrm{g}}} \mathrm{f}^{*2}(z,t)\,\mathrm{d}\Omega_{\mathrm{g}}\mathrm{d}t \right\}^{1/2}, \tag{19}$$

where $f^*(z,t)$ is the exact heat source. The measurement of the temperature in the photoresist region is necessary for estimating the heat source. If a computer simulation is used, the temperatures involve random measurement errors and random noise is added to the error free simulated data to generate the measured temperatures and they are

$$T_1(\Omega_1,t) = \bar{T}_1(\Omega_1,t) + \eta\sigma, \tag{20}$$

$$T_2(\Omega_2,t) = \bar{T}_2(\Omega_2,t) + \eta\sigma, \tag{21}$$

where $\bar{T}_1(\Omega_1,t)$ and $\bar{T}_2(\Omega_2,t)$ denote the temperatures of the direct problem with the exact heat source and η is a random variable within the range of –2.576 to 2.576 for 99% confidence bounds and σ is the standard deviation of the measurement.

3.3 Application of inverse methodology

In this paper a methodology is proposed to estimate the heat source of the thermal diffusion problem during X-ray lithography. This methodology can also be applied to other problems, which involve heat generation like microthermal machining by scanning thermal microscopy (SThM) and thermomechanical data storage by atomic force microscopy (AFM). SThM is capable of investigating thermal physical properties [17, 18] and nanomachining [19]. During nanomachining, the tip of the SThM thermal probe has a resistive heater and is used as a tool for microthermal machining the materials. The heat transfer problem in the material includes internal heat generation, which causes a rise in temperature throughout the heated region, and is taken advantage of microthermal machining. It is necessary to control the heat generation carefully to keep the temperature of the small region that is being machined slightly higher than the melting temperature of the workpiece without melting a larger area of the workpiece. It is difficult to measure and control the heat source during processing. By understanding the dynamic processes, the quality of microthermal machining can, however, be influenced. The methodology in the paper presented can be used to calculate the heat generation and obtain the distribution of the temperature of a workpiece. Similarly, when a resistively heated AFM cantilever tip is used for a thermomechanical data-storage system, the tip scans over a polymer substrate to read and write data bits. Heat generated in substrate leads to a temperature rise and subsequently results in a thermoplastic deformation of that particular location of the substrate [20, 21]. To increase storage density and recording

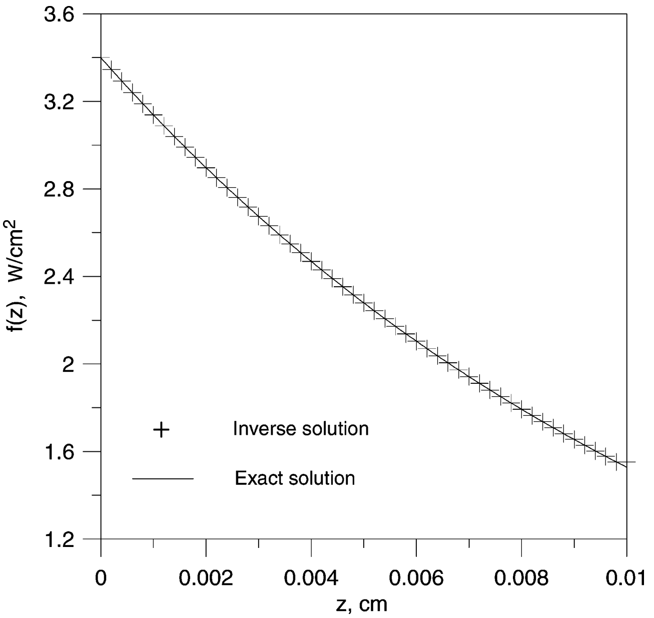

FIGURE 2 Estimated heat source at an initial guess of $f^0 = 10^{-2}$ and at the tenth iteration with $\sigma = 0.0$

data rate, we should accurately control the heat source produced in the substrate. This inverse methodology can be used to estimate the heat generation and may be useful for an AFM-base ultrahigh-density data storage system.

3.4 *Numerical results*

To demonstrate the accuracy of the present method, the exact heat source is assumed to be a function of an exponential depth, and it is

$$f(z) = 3.4 \cdot \exp(-0.8z)\ W/\mathrm{cm}^2 \tag{22}$$

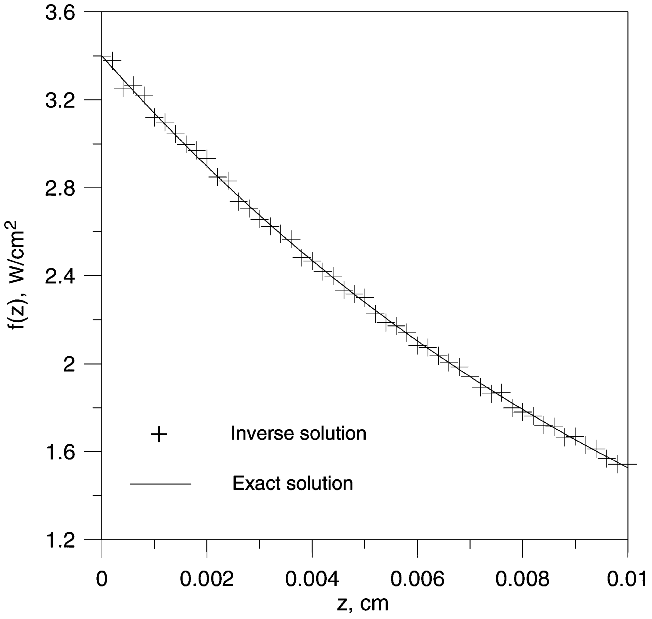

FIGURE 3 Estimated heat source at an initial guess of $f^0 = 1.0$ and at the tenth iteration with $\sigma = 0.005$

Figure 2 depicts the estimated heat source with the initial guess $f^0 = 10^{-2}$ at the tenth iteration without measurement error (i.e., $\sigma = 0.0$). It can be seen that the estimation of heat source $f(z)$ is almost identical to the exact value. After the 10 th iteration, the estimated heat source at initial guess value $f^0 = 1.0$ with $\sigma = 0.005$ is shown in Fig. 3. The standard deviation of measurement error is taken as $\sigma = 0.005$, which corresponds to the measurement error of 1.3%. As expected, the discrepancy between the inverse and the exact solution increased with increasing the measurement error. However, from the figure it can be seen that the solution obtained by the inverse method with the large measurement error is in agreement with the exact solution. It shows that the method presented here is excellent for the use of estimating the heat source.

4 Conclusion

A methodology for estimating the heat source of the photoresist-substrate system due to irradiation during X-ray lithographic processing is presented. The determination of the heat source is treated as an inverse heat conduction problem. The conjugate gradient method is applied to treat the inverse problem using the available temperature measurements. Numerical results show that the method can accurately estimate the heat source even for problems with error of temperature measurement. The proposed method can also be applied during microthermal machining to determine the heat source and the temperature distribution of the workpiece when using scanning thermal microscopy (SThM). In addition, this inverse methodology can also be used to estimate the heat generation in a thermomechanical data storage system with an atomic force microscope (AFM). It may contribute to increase storage density in an AFM-base ultrahigh-density data storage system.

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