

Mesh-Free Modeling and Control of Thermal/Diffusion Fields Created by Nano-Sources

Marios Alaeddine¹, Teiichi Ando², and Charalabos C. Doumanidis³

¹Marios Alaeddine, Children's Hospital, Harvard Medical School, 300 Longwood Avenue, Boston, MA 02115 USA
e-mail: marios.alaeddine@childrens.harvard.edu

²Teiichi Ando, Advanced Materials Laboratory, Northeastern University, 360 Huntington Avenue, Boston, MA 02115
e-mail: tando@coe.neu.edu

³Charalabos C. Doumanidis, University of Cyprus, 75 Kallipoleos Ave, 1678 Nicosia, Cyprus e-mail: cdoumani@ucy.ac.cy

Abstract— This paper presents an analytical model of the temperature and concentration dynamic distributions generated in a substrate material from exothermic material transformations of reactive thin film nano-sources. The computationally parallel and mesh-less model is based on a system of lumped energy and mass balances, currently existing kinetic growth theories, and Green's function analysis. An analytical Green-Galerkin method is presented which allows to control the 3-D temperature field that is generated inside the substrate volume through external surface heating by nano-sources. A dual technique allows observation and modeling of the internal thermal distribution in the substrate through surface temperature measurements only.

I. INTRODUCTION

Since the early days of mankind, thermal processing of materials has played a pivotal role in the advancement of human civilization. Today, thermal processing is still found to be at the heart of the modern manufacturing industry, playing a primary role in surface engineering, microelectronics, chemical/biomedical technologies etc. Despite the numerous scientific and engineering accomplishments in macro- and microscale thermal processing, however, the ongoing technological advancements in nanoscale science and engineering, as well as the constantly growing demand for miniaturization of engineering components and devices have presented unprecedented challenges to the currently existing thermal manufacturing technologies and theory.

In terms of in-process control of micro-/ nano-scale thermal / diffusion phenomena in such processes, recent progress has been recently achieved in research of heat nano-sources [1, 2]. Such reactive multi-material thin film arrangements can be designed and fabricated to release the desired amounts of heat and/or material from the surface to the 3-D volume of a thick (micro- or macro-scale) substrate, in a spatially and temporally concentrated fashion. Such nano-scale singular, impulsive energy and mass sources represent ideal actuators in terms of space and time resolution, controllability and flexibility. Previous modeling research addressed nickel aluminide coatings of micrometer thickness processed on a robotic plasma arc laboratory station, through in-process infrared thermal sensing and off-line metallographic analysis [3]-[4]. A numerical observer strategy was developed to address the problem of thermal observability in infinite-dimensional heat conduction systems [5]-[6]. It was based on Galerkin optimization of an energy index employing Green's functions. Green's

functions have been used extensively in macro- and micro-scale modeling and are currently attracting much attention for use in nanoscale applications (non-equilibrium Green's functions, [7], [8]). The method was utilized to solve various one-dimensional problems of increasing complexity where temperature measurements were performed existed strictly at the endpoints [6]. Furthermore, two-dimensional problems were also studied where sensing was carried out solely on the boundaries [5]. In both the one and two-dimensional cases, the Green-Galerkin method was able to estimate the space- and time-dependent temperature evolution along the length and surface respectively. This proved the validity of the method and suggested its value for modeling of the temperature distribution generated within a 3-D substrate form heat sources on its 2-D surface. Successful modeling and in-process regulation of the energy generation from such nano-sources is of primary importance in several industrial applications, such as rapid thermal processing of semiconductor wafers, micro-electro-mechanical systems packaging etc.

To this end, this paper presents an analytical model of the temperature and concentration dynamic distributions generated in a thick substrate material from the exothermic material transformations of nano-thick reactive thin films (such as nickel and aluminum) deposited on the external surface of the substrate. The model, which is computationally parallel and mesh-less (i.e., decoupled with the capability to be solved numerically by multiple processors in real time) is based on a system of lumped energy and mass balances, currently existing kinetic growth theories, and Green's function analysis. The previously developed Green-Galerkin method is further studied and utilized to address the dual question of distributed parameter thermal control.

II. DISTRIBUTED PARAMETER THERMAL CONTROL

In thermal control, a specified dynamic thermal distribution $T_d(P;t)$ is desired in the volume of substrate points P as a function of time t (Fig. 1). This should be accomplished by application of external dynamic heat influx distribution $Q_s(R;t)$ from sources located on surface points R at times t . Heat transfer is assumed by linear conduction in the volume, while linear heat loss effects by convection and linearized radiation can be considered on the part surface. Since arbitrary specification of T_d does not necessarily satisfy Fourier's heat conduction equation inside the substrate, three questions arise regarding thermal control:

- Does such a distribution $Q_S(R; t)$, which can create a thermal field $T(P, t)$ such that $T(P; t) \approx T_d(P; t)$ exist? (Controllability question)
- Assuming its existence, how can this surface heat input function $Q_S(R; t)$ be obtained? (Control-input question)
- What desired distributions $T_d(P; t)$ can be obtained exactly by all feasible heat input distributions $Q_S(R; t)$? (Controllable subspace question)

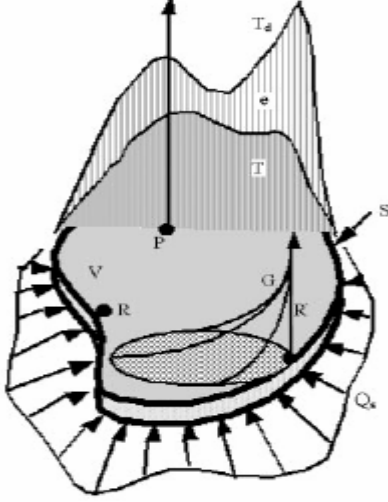


Fig. 1. Control volume in the scenario of thermal control.

III. A GREEN-GALERKIN THERMAL CONTROLLABILITY METHOD

The Galerkin optimization method, which was utilized to solve the dual problem of thermal observation [5]-[6], will also be employed here to address the problem of thermal control. This method deals with obtaining approximate solutions to problems that are highly complex to solve for exact solutions. This is achieved by assuming a solution composed of functions that satisfy all the specified boundary conditions. The assumed solution varies along the surface and within the volume via interpolation functions. However, since this solution is just an approximation, it will not satisfy exactly the governing equations. As a result, there exists an error, labeled the *residual*. Hence, the method optimizes the volume and surface residuals, by making them minimal at all points of the solution domain. This can be stated as:

$$\int_V I_V * R_V dV + \int_S I_S * R_S dS = 0 \quad (1)$$

where I_V and I_S denote the interpolation function within the volume and along the surface respectively, R_V the volume residual, and R_S the residual along the surface.

This method is employed to define a heat input distribution $Q_S(R; t)$ from sources on the substrate surface, that will generate an internal temperature field $T(P; t)$, that approaches the specified $T_d(P; t)$ as closely as possible. This is performed by setting the volume residual to be the fictitious volumetric heat input required internally in the substrate, to produce the exact desired dynamic temperature field. This can be stated as:

$$R_V(P; t) = \rho c \frac{\partial T_d}{\partial t}(P; t) - \nabla(K \nabla T_d(P; t)) + h(T_d(R; t) - T_\infty) \quad (2)$$

where R_V denotes the volume residual, ρ the density, c the specific heat capacity and K the thermal conductivity of the material, h the convection coefficient, and T_∞ the ambient temperature of the surroundings. For Neumann boundary conditions, the boundary residual is expressed as the difference between the heat flux exchanged by conduction—between the volume of the solid and the surface point where heating exists—and the heat flow that is actually applied, that is

$$R_S(R; t) = K \frac{\partial T_d}{\partial n}(R; t) - Q_S(R; t) \quad (3)$$

where R_S denotes the surface residual and n is the outward normal from this boundary. Employing the Galerkin methodology, namely equation (1), to minimize the volume and surface residuals as defined, it can then be stated that for every test point R' chosen on the substrate surface and time τ ,

$$\int_0^\infty \left[\int_V \int_S G(P, R'; \tau - t) * R_V(P; t) dV + \int_V \int_S G(R, R'; \tau - t) * R_S(R'; t) dS \right] d\tau = 0 \quad (4)$$

where both the volume and surface interpolation functions I_V and I_S have been set to the Green's function $G(P/R, R', \tau - t)$. The Green's function describes the conduction of heat within the volume or over the surface of a substrate with chosen geometry and boundary conditions [9]. This G signifies the temperature developed at point P/R and time τ , due to an impulsive unit heat input (1J) at location R' and time t . Since the unit heat source is singular both in space and time (i.e. an infinitely concentrated and impulsive Dirac function), it is particularly appropriate in modeling the effects of a discrete nano-source to a substrate continuum. At the same time, G denotes the interpolation function necessary for the Galerkin optimization.

Substituting the residuals of equations (2) and (3) into equation (4), what is obtained is

$$\int_t^\infty \int_S G(R, R'; \tau - t) * Q_S(R'; t) dS dt = \int_t^\infty \left[\int_V G(P, R'; \tau - t) * Q_V(P; t) dV + \int_S G(R, R'; \tau - t) * K \frac{\partial T_d(R'; t)}{\partial n} dS \right] d\tau \quad (5)$$

where the right-hand side of equation (5) can be calculated and represented as $C(R; t)$:

$$\int_t^\infty \int_S G(R, R'; \tau - t) * Q_S(R'; t) dS dt = C(R; t) \quad (6)$$

i.e. $G(R; t) \otimes Q_S(R'; t) = C(R; t)$

Therefore the required dynamic surface heat input distribution $Q_S(R';t)$ from the nano-sources can be determined by deconvolution of equation (6).

A simple explicit technique for deconvolving Eq. 6 backwards in time is described in [5]. This involves discretizing the volume into N elements and then selecting N nodal points within the volume with coordinates R_i , for $i = 1$ to N . In addition, equation (6) requires N number of nodal test points over the surface of the substrate with coordinates R'_i , also for $i = 1$ to N . Varying progressively the control period from 0 to ψ in N steps of duration Δt , generates a linear $N \times N$ system, thus allowing to write equation (6) in matrix form as

$$[C] = [G] * [Q_S] \quad (7)$$

where Q_S is a column vector ($N \times 1$ matrix) composed of all the unknown values of the required heat input field at the N selected nodal points on the surface with coordinates R'_i . More specifically,

$$[Q_S] = \begin{bmatrix} Q_S(R'_1; t) \\ \vdots \\ Q_S(R'_N; t) \end{bmatrix} \quad (8)$$

Rearranging the terms in equation (7), it can be finally said that

$$[Q_S] = [G]^{-1} * [C] \quad (9)$$

thus solving for the unknown nano-source heat input values at all chosen locations R'_i over the substrate surface.

IV. DISTRIBUTED PARAMETER THERMAL MODELING

A dual approach to the previous controllability analysis leads to a model of the observability problem: In this case, an initial temperature distribution in the substrate $T(P;0)$ must be identified by dynamic measurements of the temperature field $T_S(R;t)$ on the substrate surface only, under known heating conditions (usually assumed $Q_S(R;t) = 0$ without loss of generality). Temperature measurements on the surface can be carried out e.g. by nano-sensors such as thin-film thermocouples or infrared micro-pyrometry. The relevant observation questions arise:

- Is it possible to identify the initial temperature distribution $T(P;0)$ that exists within the volume of a solid, strictly by measurements of the surface temperature field $T_S(R;t)$ over an observation period $0 \leq t \leq \psi$? (Observability Question)
- Assuming the above statement possible, how can this initial temperature distribution $T(P;0)$ be obtained? (Open-Loop Observation)
- What initial temperature distributions $T(P;0)$ can be successfully observed by surface temperature measurements $T_S(R;t)$ alone? (Observability Subspace)

Following a similar Green-Galerkin formulation, one arrives at a similar convolution expression over the volume V of the substrate:

$$\begin{aligned} H(P';t) &= D(P';t) \otimes T(P;0) \quad \text{where} \\ H(P';t) &= \int_0^\psi \int_S G(R, P', \tau - t) * h(T_S(R;t) - T_\infty) dS d\tau \quad \text{and} \\ D(P';t) &= \int_0^\psi \int_S G(R, P', \tau - t) * K \rho c \frac{\partial G(R, P'; t - 0)}{\partial n} dS d\tau \end{aligned} \quad (10)$$

which can also be solved by deconvolution in a similar manner to equations (7), (8), (9):

$$[T] = [D]^{-1} * [H] \quad \text{where} \quad [T] = \begin{bmatrix} T(P_1;0) \\ \dots\dots\dots \\ T(P_N;0) \end{bmatrix} \quad (11)$$

providing the initial internal temperatures $T(P_i;0)$ at a number of discrete points P_i in the substrate, $i = 1 \dots N$.

V. ALGORITHM IMPLEMENTATION TO THE ONE-DIMENSIONAL PROBLEM

To model a heat conduction problem it is first necessary to determine the applicable Green's function. This is dependent on the solid geometry and boundary conditions. In the particular case, the model chosen is a finite wire of length $0 \leq x \leq L$ (Fig. 2). A temperature distribution, $T(x;0)$, exists along the length of the wire at an initial time $t = 0$. Temperature measurements are available at one endpoint, namely $x = 0$, thus providing $T_S(0;t)$ for all times within the observation period $0 \leq t \leq \psi$; the other endpoint is assumed insulated and inaccessible to measurements. Of note, the model uses the assumption of homogeneous, isotropic, time invariant properties and no phase transformations.

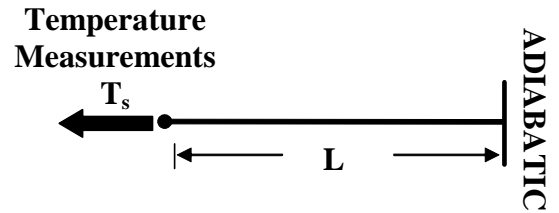


Fig. 2. One-dimensional observability model.

The Green's function expressing the evolution of temperature on the model of the latter figure is provided by Beck et al. [10] and is found to be:

$$\begin{aligned} G(x, x', \tau - t) &= \frac{1}{\sqrt{4\pi\alpha(\tau - t)}} \left\{ \exp\left[-\frac{(x - x')^2}{4\alpha(\tau - t)}\right] \right. \\ &+ \exp\left[-\frac{(x + x')^2}{4\alpha(\tau - t)}\right] + \exp\left[-\frac{(2L - x - x')^2}{4\alpha(\tau - t)}\right] \left. \right\} \\ &- \frac{h}{K} \exp\left[\frac{h(x + x')}{K} + \frac{h^2\alpha(\tau - t)}{K^2}\right] \end{aligned}$$

$$\times \operatorname{erfc} \left\{ \frac{x+x'}{\sqrt{4\alpha(\tau-t)}} + \frac{h}{K} \sqrt{\alpha(\tau-t)} \right\} \quad (12)$$

where x' and t , are the location and time of application of a heat input respectively. Furthermore, α denotes the thermal diffusivity of the material, defined as $\alpha = K/(\rho c)$ in units of (m^2/s).

The model used to study the one-dimensional problem consists of a steel bar with length $L = 0.05$ (m) and cross-sectional area $A = 0.0001$ (m^2). The properties of the steel material chosen are $\rho = 7830$ (kg/m^3), $c = 434$ ($\text{J}/(\text{kg}\cdot\text{K})$) and $K = 64$ ($\text{W}/\text{m}\cdot\text{K}$). In addition, the numerical value assigned to the convection coefficient h is 10 ($\text{W}/(\text{m}^2\cdot\text{K})$).

The numerical implementation of the Green-Galerkin observability method involves the following two steps:

1. The length of the wire shown in Fig. 2 is discretized into $N = 5$ elements of which five nodal points P_i are selected for thermal observation. The coordinate values of these selected points are:

$$\begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_5 \end{bmatrix} = \begin{bmatrix} 0.01 \\ 0.02 \\ 0.03 \\ 0.04 \\ 0.05 \end{bmatrix} \quad (13)$$

where all the dimensions are in meters (m).

2. Next, five test points P'_i need to be selected. These are also employed in the Green-Galerkin observability method (see equations (10), (11)). The coordinate values of these randomly selected test points are:

$$\begin{bmatrix} P'_1 \\ P'_2 \\ P'_3 \\ P'_4 \\ P'_5 \end{bmatrix} = \begin{bmatrix} 0.005 \\ 0.015 \\ 0.025 \\ 0.035 \\ 0.045 \end{bmatrix} \quad (14)$$

again in units of meters (m).

Finally, various simulations are conducted to investigate the ability of the proposed method to observe/reconstruct the temperature field, which existed at the initial time of observation, by boundary temperature measurements alone. In all cases, the influence of the time step Δt , which is employed in the numerical procedure proposed for deconvolving equation (11), is also investigated.

The simulation conducted involves having an initial temperature field along the length of the wire of Fig. 2, consisting of a single peak at $x = L/5$ (Fig. 3). The time step chosen for the numerical implementation of the Green-Galerkin observability method is $\Delta t = 10$ seconds. Hence, to generate a linear 5×5 system requires the observation period to be of duration $\psi = 50$ seconds. The evolution of the initial temperature field along the wire is also seen at times $t = \Delta t, 2 \Delta t, \dots, \psi$ seconds (Fig. 3).

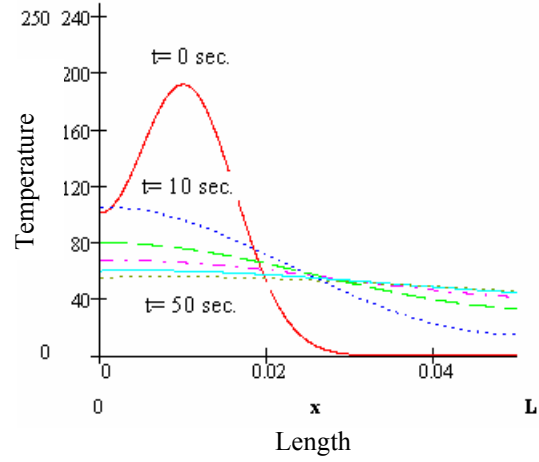


Fig. 3. Evolution of the initial temperature field during the observation period at various times t (time step = 10 seconds).

TABLE 1. TEMPERATURE MEASUREMENTS AT BOUNDARY $x = 0$.

Time t (sec.)	10	20	30	40	50
$T_s(0;t)$ (deg.)	105.7	79.9	67.4	60.2	55.5

From the temperature curves of Fig. 3, five temperature measurements are taken at the boundary at $x = 0$ (see table 1). Employing these measurements into the proposed observability method generates the temperature distribution shown in Fig. 4. The latter figure indicates that the Green-Galerkin method is able to reconstruct (dashed line) the actual temperature field (solid line) that initially existed along the length of the wire strictly by temperature measurements on the boundary. To study the effect of the time step, Fig. 4 also shows the temperature profile $T(x;0)$ computed with a time step $\Delta t = 5$ seconds. Again the resulting temperature distribution generated by the Green-Galerkin method (shown also in Fig. 4) indicates that the technique is successful in observing the temperature distribution that was chosen to exist at time $t = 0$ along the length of the wire, with little improvement in the quality of estimation.

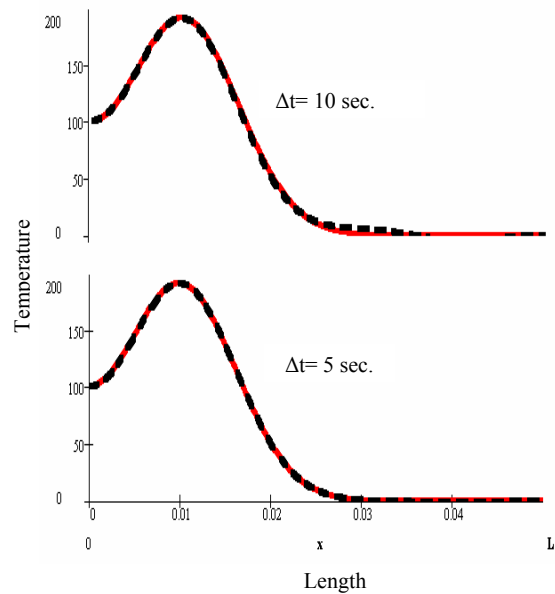


Fig. 4. Actual versus observed temperature field.

VI. CONCLUSION

In conclusion, this paper developed an analytical modeling and control approach to the dynamic thermal distribution in a substrate continuum heated on its surface by discrete nano-sources. The singular nature of such sources in both spatial and time scales (i.e. their highly concentrated and impulsive character) led to representation of their thermal effects by Green's functions. A Galerkin optimization method was also adopted to yield a mesh-less formulation to the controllability and observability problem, that is well suited for in-process parallel computation. This inverse conduction control problem yields the required external heat influx distribution required from the nano-sources to achieve a specified internal temperature field in the substrate. Its dual observation problem provides estimates of the volume thermal distribution by temperature measurements on the surface only, e.g. through thin-film thermocouples. The numerical technique for linear deconvolution was applied to the one-dimensional problem. Further work is in progress for real-time use of such controllers and observers based on the Green-Galerkin approach, and the experimental validation of their performance with nano-sources and sensors in the laboratory.

VII. REFERENCES

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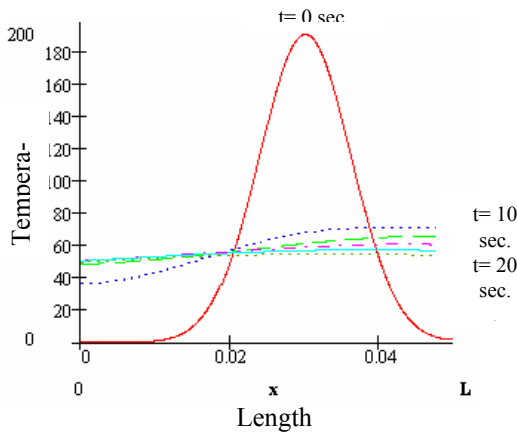


Fig. 5. Evolution of the initial temperature field during the observation period at various times t (time step = 10 seconds).

TABLE 2. TEMPERATURE MEASUREMENTS AT BOUNDARY $x=0$.

Time t (sec.)	10	20	30	40	50
$T_s(0;t)$ (deg.)	36.7	48.6	50.7	50.6	49.7

The next temperature profile chosen to test the proposed technique consists of a single peak at $x = 3L/5$ (see Fig. 5). The time step that is first selected for the numerical processing is $\Delta t = 10$ seconds. The five temperature measurements obtained at the boundary at $x = 0$ by analytically modeling the initial temperature field (Fig. 5) are provided in table 2.

Figure 6 depicts the observed temperature distribution (dashed line) that is obtained when employing the Green-Galerkin method. A time step of five seconds is also used to test the effect of Δt on the numerical processing.

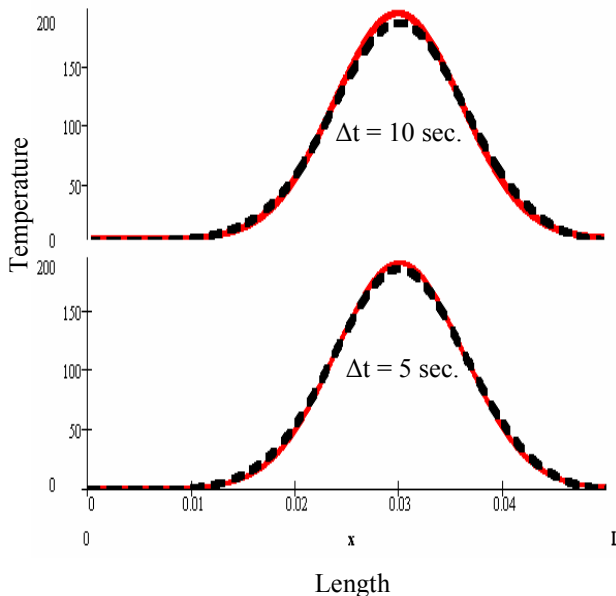


Fig. 6. Actual versus observed temperature field.