Applied Surface Science 258 (2012) 7266–7273

Contents lists available at SciVerse ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Numerical simulation of the unsteady non-linear heat transfer problems. Application on nanosecond laser annealing of Si

G.C. Bourantas [a], D.P. Korfiatis [b], V.C. Loukopoulos [b,*], K.-A.Th. Thoma [b]

[a] Institute of Chemical Engineering and High Temperature Chemical Processes Foundation for Research and Technology, P.O. Box 1414, GR-26504, Patras, Greece
[b] Department of Physics, University of Patras, Patras, 26500, Rion, Greece

ARTICLE INFO

Article history:
Received 18 January 2012
Accepted 14 March 2012
Available online 5 April 2012

Keywords:
Nanosecond laser
Unsteady non-linear heat transfer problems
Meshfree point collocation method

ABSTRACT

The aim of the present work is the numerical simulation of the unsteady non-linear heat transfer problems. A nanosecond Gaussian in time and space pulse is considered as the heat source acting on a Si substrate. Four different scenarios are considered in order to examine the influence of the laser parameters on the Si surface temperature, namely variation of the fluence of the laser beam, the radius of the laser beam at the Si surface, the duration of the pulse and finally the number of laser pulses. A meshfree point collocation method (MPC) has been employed for the solution of the problem. More precisely, the moving least squares (MLS) approximation is incorporated for the construction of the shape functions, in conjunction with the general framework of the point collocation method. The accuracy and stability of the proposed scheme are demonstrated through three representative benchmark problems in 1D, 2D and 3D. Numerical results are found to be in very good agreement with analytical, numerical and experimental results presented in the literature.

1. Introduction

Laser-material interaction has been intensively studied over the past few decades. The complexity of processes involved makes work on this topic a challenge for scientists. Related applications predominately in areas of edge technologies like micromachining [1,2], laser deposition [3], nanoparticle fabricating [4] and so on, require firm understanding of the physical processes involved. The calculation of the relevant parameters such as fluence thresholds, and temperature distribution in the material as a function of time are of great importance for applications and a combination of both experimental and computational work is needed to achieve this goal. As the fundamental process in the laser-material interaction is heat transfer from the laser to the material, a large number of analytical and numerical models found in the literature focus on this process aiming towards a fuller understanding of both thermal and non-thermal procedures involved [5] and the prediction of the outcome of this interaction.

Solving heat transfer problems analytically, except for a few simplified cases, can present difficulties, due to the complexity of the equations involved. In most instances, this leads to the formulation of a model needed to be treated numerically. Traditional numerical techniques, such as finite differences (FDM) [6,7], finite volume methods (FVM) [8], finite element methods (FEM) [9], and boundary element methods (BEM) [10], have been effectively and routinely applied. In spite of their great success, traditional numerical methods still have some elementary drawbacks that impair their computational efficiency and even limit their applicability in more practical problems, particularly in three-dimensions. The main reasons of deficiency are related to the use of low order piecewise polynomial approximations, and the necessity to create a mesh in the application domain and its boundary. As a result, the numerical solution depends strongly on the mesh properties. More precisely, the FVM and FEM have been the dominant numerical schemes applied to a variety of practical engineering and physical problems, since they have the advantage of being applicable at irregular geometries. Despite the fact that mesh generation can be fully automated in two dimensions, this can be a troublesome procedure at three dimensions, usually demanding substantial human intervention. Thus, in the majority of heat transfer problems, mesh generation is a far more time consuming and expensive task than the solution of the partial differential equations (PDEs) themselves.

Consequently, the development and application of new numerical methods can prove to be a major contribution in the field. Recently, in the general area of computational mechanics there is a growing interest in developing so called meshless methods or particle methods as alternatives to traditional grid-based methods. The key idea of these methods is to provide numerical solutions on a set of arbitrarily distributed points without using any mesh to connect them. Meshfree (or meshless) methods, are a class of

* Corresponding author.
E-mail address: vxloukop@physics.upatras.gr (V.C. Loukopoulos).

0169-4332/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.apsusc.2012.03.071

numerical techniques that rely on interpolation/approximation on (non-ordered in general) spatial point distributions and offer the possibility of reducing significantly the effort devoted to form the numerical model. Meshless techniques overcome the aforementioned difficulties associated with meshing by eliminating the mesh altogether. Interpolation/approximation is performed in terms of nodal points distributed at the analysis domain using functions that provide compact support. A weighted residual technique is used to generate the discrete set of equations corresponding to the governing partial differential equations. Several meshfree methods have been proposed since the prototype of the meshfree methods, the smoothed particle hydrodynamics (SPH) was introduced [11,12].

The proposed numerical scheme in this paper is employed in nanosecond laser annealing of silicon, by far the most common material in semiconductor industry with a large number of innovative applications based on laser treatment of it. A three-dimensional transient conductive model is solved by using an in-house meshless point collocation code. The article is organized as follows: in Section 2, a brief description of the MLS approximations and of the corresponding MLS shape functions is given. In Section 3, the description of the discretization steps of the diffusion equation, which models the physical problem, is presented. Numerics take place in Section 4, where three benchmark problems are solved. All cases are extensively validated through direct comparison with either the analytical solutions, or other established computational techniques, such as FEM or EFG, and the efficiency of the proposed meshless technique is demonstrated. Following, in Section 5, a case study for the heat transfer characteristics in a silicon sample under intense nanosecond laser irradiation takes place. Conclusions are summarized in Section 6.

2. Moving least squares shape functions

Among the available meshless approximation/interpolation schemes, the MLS method [13] is widely used, due to its completeness and robustness [11,12]. Its kernel is a direct approximation of the field variables on a local scheme and is easily extended to n-dimensional problems. A brief summary of the MLS approximation schemes follows for 2D, with an extension to 3D.

Within the MLS context, the approximation $T^h(\boldsymbol{x})$ of the unknown field function $T(\boldsymbol{x})$ is expressed as

$$T^h(\boldsymbol{x}) = \sum_{i=1}^{m} p_i(\boldsymbol{x})\alpha_i(\boldsymbol{x}) = \boldsymbol{p^T}(\boldsymbol{x})\boldsymbol{a}(\boldsymbol{x}) \tag{1}$$

where $\boldsymbol{p^T}(\boldsymbol{x})$ is a polynomial based on space coordinates, m is the total number of the terms in the basis and $\boldsymbol{a}(\boldsymbol{x})$ is the vector of coefficients. Herein, a second order ($m = 6$) polynomial basis for 2D problems has been used (($m = 10$) polynomial basis for 3D problems). There exists a unique local approximation associated with each point in the domain. In order to determine the form of $\boldsymbol{a}(\boldsymbol{x})$, a weighted discrete error norm is constructed and minimized. Additionally, in the present paper a Gaussian weight function is used [12,14], yet the support domain does not have a standard point density value. Instead, a constant number of nodes are used for the approximation of the field function.

Finally, the approximation function takes the form

$$T^h(\boldsymbol{x}) = \underbrace{\boldsymbol{p}^T(\boldsymbol{x})\boldsymbol{A}^{-1}(\boldsymbol{x})\boldsymbol{B}(\boldsymbol{x})}_{\boldsymbol{\varphi}(\boldsymbol{x})}\boldsymbol{T}_s \tag{2}$$

here the spatial dependence has been lumped into one row matrix, $\boldsymbol{\varphi}(\boldsymbol{x})$ and, therefore, the approximation takes the form of a product of a matrix of shape functions with a vector of nodal data, while matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ are defined in [12]. Derivatives of the shape functions [15] may be calculated by applying the product rule to

$$\boldsymbol{\varphi} = \boldsymbol{p}^T\boldsymbol{A}^{-1}\boldsymbol{B}. \tag{3}$$

3. Governing equations and solution procedure

3.1. Governing equations

In the present study a general form of energy equation for three-dimensional heat transfer in anisotropic materials with temperature and spatial dependent material properties is given as:

$$\rho(\boldsymbol{x}, T)c(\boldsymbol{x}, T)\frac{\partial T}{\partial t} = \nabla(k(\boldsymbol{x}, T)\nabla T) + Q(\boldsymbol{x}, t) \tag{4}$$

with the following initial and boundary conditions:

$$T(\boldsymbol{x}, 0) = T_i \quad \text{on} \quad V \tag{5}$$

$$T(\boldsymbol{x}, t) = T_{S_D} \quad \boldsymbol{x} \in \partial\Omega^D \tag{6}$$

$$T(\boldsymbol{x}, t) = h(T - T_\infty) \quad \boldsymbol{x} \in \partial\Omega^N \tag{7}$$

where $\partial\Omega^D$ and $\partial\Omega^N$ are the Dirichlet and the Neumann boundaries of the spatial boundary $\partial\Omega$ and, $\partial\Omega = \partial\Omega^D \cup \partial\Omega^N$, $\partial\Omega^D \cap \partial\Omega^N = \varnothing$.

Meshless Point Collocation method for the governing equations

The Meshless Point Collocation method is a meshless "strong-form" description one. The "strong-form" description of the governing equations and boundary conditions is used and discretized by collocation techniques. The aforementioned formulation has the following attractive advantages. The formulation is truly meshless and the implementing procedure is straightforward, while the algorithms and the implementation can be kept simple, particularly when handling problems with Dirichlet boundary conditions [12]. Under these conditions, strong-form methods are highly efficient computationally, even with polynomial approximation functions, and the solution can be systematically obtained with increased accuracy, compared to FEM, FDM, or other computational methods. In general, MFree strong-form methods may still suffer from some local stability and accuracy issues, depending on the problem [12]. However, these local restrictions are now systematically avoided with the utilization of Type-I nodal distribution and proper local point cloud refinement procedures, in accordance with [14–17], even for natural or mixed type boundary conditions.

In this section we present the collocation scheme using the MLS approximation to spatially discretize the unsteady homogeneous diffusion equation. We also present a θ-weighted time-stepping scheme for temporal discretization. As mentioned above, the governing equation of the unsteady problem is considered:

$$\begin{gathered}\rho(\boldsymbol{x}, T)c(\boldsymbol{x}, T)\frac{\partial}{\partial t}T(\boldsymbol{x}, t) - \boldsymbol{L}T(\boldsymbol{x}, t) = Q(\boldsymbol{x}, t) \quad \forall x \in \Omega \subset R^d, \quad t > 0, \\ \boldsymbol{G}T(\boldsymbol{x}, t) = g(\boldsymbol{x}, t), \quad \forall x \in \Omega \subset R^d, \quad t > 0,\end{gathered} \tag{8}$$

where $\boldsymbol{L}$, the "diffusion" operator, is defined as $\boldsymbol{L} = \nabla(k(\boldsymbol{x}, *)\nabla *)$ and $\boldsymbol{G}$ is the boundary operator, which can be Dirichlet, Neumann or a mixed operator. The above set of equations has to be implemented with an initial condition of the form

$$T(\boldsymbol{x}, t) = T_0(\boldsymbol{x}), \quad t = 0 \tag{9}$$

where $g(\boldsymbol{x}, t)$ and $T_0(\boldsymbol{x})$ are known functions.

The MLS approximation leads to:

$$T(\boldsymbol{x}, t) = \sum_{i=1}^{N} \varphi_i(\boldsymbol{x})T_i(t) \tag{10}$$

The nodes of the domain Ω are ordered as distributed nodes of Type-I, situated within the interior and at the boundary $\partial\Omega$. n_d is set