

# A finite difference method for studying thermal deformation in a 3D thin film exposed to ultrashort pulsed lasers

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## Abstract

Ultrashort pulsed lasers have been attracting worldwide interest in science and engineering communities. Studying the thermal deformation induced by ultrashort pulsed lasers is important for preventing thermal damage. This article presents a new numerical method for studying thermal deformation in a 3D thin film exposed to ultrashort pulsed lasers. The method is obtained based on the parabolic two-step model and implicit finite difference schemes on a staggered mesh. It accounts for the coupling effect between lattice temperature and strain rate, as well as for the hot electron-blast effect in momentum transfer. In particular, a fourth-order compact scheme is developed for evaluating those stress derivatives in the dynamic equations of motion. The method allows us to avoid non-physical oscillations in the solution. Its performance is demonstrated by a numerical example.

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## 1. Introduction

Ultrafast lasers with pulse durations of the order of sub-picoseconds to femtoseconds possess exclusive capabilities in limiting the undesirable spread of the thermal process zone in the heated sample [1]. The application of ultrashort-pulsed lasers includes structural monitoring of thin metal films [2,3], laser micromachining and patterning [4], structural tailoring of microfilms [5], and laser synthesis and processing in thin-film deposition [6]. Recent applications of ultrashort-pulsed lasers have been in different disciplines such as physics, chemistry, biology, medicine, and optical technology [7–10]. The non-contact nature of femtosecond lasers has made them an ideal candidate for precise thermal processing of functional nanophase materials [1].

Success of high-energy ultrashort-pulsed lasers in real applications relies on three factors [1]: (1) well characterized pulse width, intensity and experimental techniques; (2) reliable microscale heat transfer models; and (3) pre-

vention of thermal damage. Up to date, a number of models that focus on heat transfer in the context of ultrashort-pulsed lasers have been developed [11–23]. However, only a few mathematical models for studying thermal deformation induced by ultrashort pulsed lasers have been developed [1,24–26]. Tzou and his colleagues [1] presented a one-dimensional model in a double-layered thin film. The model was solved using a differential-difference approach. Chen and his colleagues [24] considered a two-dimensional axisymmetric cylindrical thin film and proposed an explicit finite difference method by adding an artificial viscosity term to eliminate numerical oscillations. Recently, we have developed a new method for studying thermal deformation in 2D thin films exposed to ultrashort pulsed lasers [27–29]. The method is obtained based on the parabolic two-step heat transport equations and implicit finite difference schemes on a staggered mesh. It accounts for the coupling effect between lattice temperature and strain rate, as well as for the hot electron-blast effect in momentum transfer. Numerical results show that there are no numerical oscillations in the solution. Unfortunately, when applied to a 3D thin film case, the non-physical oscillations in the stress ( $\sigma_z$ ) appear in the solution. This is probably

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## Nomenclature

$C_{e0}$	electron heat capacity	$z_s$	optical penetration depth
$C_l$	lattice heat capacity	$r_s$	spatial profile parameter of laser
$G$	electron–lattice coupling factor	$\alpha_T$	thermal expansion coefficient
$J$	laser fluence	$\Delta t, \Delta x, \Delta y, \Delta z$	time increment and spatial step sizes, respectively
$K$	bulk modulus	$\Delta_{-t}, \delta_x$	finite difference operators
$K_e$	thermal conductivity	$\varepsilon_x, \varepsilon_y, \varepsilon_z$	normal strains in the $x$ , $y$ and $z$ directions, respectively
$R$	surface reflectivity	$A$	electron-blast coefficient
$T_e$	electron temperature	$\gamma_{xy}, \gamma_{xz}, \gamma_{yz}$	shear strain
$T_l$	lattice temperature	$\lambda$	Lame's coefficient
$t, t_n$	time	$\mu$	Lame's coefficient
$t_p$	laser pulse duration	$\rho$	density
$u, v, w$	displacements in the $x$ , $y$ and $z$ directions, respectively	$\sigma_x, \sigma_y, \sigma_z$	normal stresses in the $x$ , $y$ and $z$ directions, respectively
$u^n(i, j, k)$	numerical solution of $u(x_i, y_j, z_k, t_n)$	$\sigma_{xy}, \sigma_{xz}, \sigma_{yz}$	shear stresses in the $x$ , $y$ and $z$ directions, respectively
$v_1, v_2, v_3$	velocity components in the $x$ , $y$ and $z$ directions, respectively		
$x, y, z$	Cartesian coordinates		

because we used a relatively coarse grid in the computation. However, a finer mesh increased dramatically the computation cost. In this article, we extend our research to a 3D thin film case by developing a fourth-order compact finite difference scheme for solving the dynamic equations of motion. Result shows that the non-physical oscillations disappear.

## 2. Mathematical model

Consider a three-dimensional thin film in Cartesian coordinates, which is exposed to ultrashort pulsed lasers, as shown in Fig. 1. The governing equations for studying thermal deformation in the thin film can be expressed as follows:

(1) *Dynamic equations of motion* [1,24,27,30].

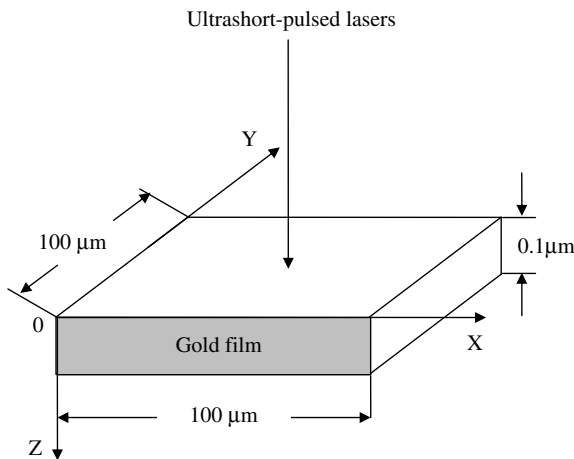


Fig. 1. A 3D thin film with the dimension of  $100 \mu\text{m} \times 100 \mu\text{m} \times 0.1 \mu\text{m}$ , irradiated by ultrashort-pulsed lasers.

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma_x}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} + 2AT_e \frac{\partial T_e}{\partial x}, \quad (1)$$

$$\rho \frac{\partial^2 v}{\partial t^2} = \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + 2AT_e \frac{\partial T_e}{\partial y}, \quad (2)$$

$$\rho \frac{\partial^2 w}{\partial t^2} = \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_z}{\partial z} + 2AT_e \frac{\partial T_e}{\partial z}, \quad (3)$$

$$\sigma_x = \lambda(\varepsilon_x + \varepsilon_y + \varepsilon_z) + 2\mu\varepsilon_x - (3\lambda + 2\mu)\alpha_T(T_l - T_0), \quad (4a)$$

$$\sigma_y = \lambda(\varepsilon_x + \varepsilon_y + \varepsilon_z) + 2\mu\varepsilon_y - (3\lambda + 2\mu)\alpha_T(T_l - T_0), \quad (4b)$$

$$\sigma_z = \lambda(\varepsilon_x + \varepsilon_y + \varepsilon_z) + 2\mu\varepsilon_z - (3\lambda + 2\mu)\alpha_T(T_l - T_0), \quad (4c)$$

$$\sigma_{xy} = \mu\gamma_{xy}, \quad \sigma_{xz} = \mu\gamma_{xz}, \quad \sigma_{yz} = \mu\gamma_{yz}, \quad (4d)$$

$$\varepsilon_x = \frac{\partial u}{\partial x}, \quad \varepsilon_y = \frac{\partial v}{\partial y}, \quad \varepsilon_z = \frac{\partial w}{\partial z}, \quad (4e)$$

$$\gamma_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}, \quad \gamma_{xz} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}, \quad \gamma_{yz} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}. \quad (4f)$$

Here,  $u, v, w$  are the displacements in the  $x, y, z$  directions, respectively;  $\varepsilon_x, \varepsilon_y$  and  $\varepsilon_z$  are the normal strains in the  $x, y$  and  $z$  directions, respectively;  $\gamma_{xy}$  is the shear strain in the  $xy$  direction,  $\gamma_{xz}$  is the shear strain in the  $xz$  direction,  $\gamma_{yz}$  is the shear strain in the  $yz$  direction;  $\sigma_x, \sigma_y$  and  $\sigma_z$  are the normal stresses in the  $x, y$  and  $z$  directions, respectively;  $\sigma_{xy}$  is the shear stress in the  $xy$  direction,  $\sigma_{xz}$  is the shear stress in the  $xz$  direction,  $\sigma_{yz}$  is the shear stress in the  $yz$  direction;  $T_e$  and  $T_l$  are electron and lattice temperatures, respectively;  $T_0$  is the initial temperature;  $\rho$  is density;  $A$  is electron-blast coefficient;  $\lambda = K - \frac{2}{3}\mu$  [31] and  $\mu$  are Lamé's coefficients; and  $\alpha_T$  is the thermal expansion coefficient.

(2) *Energy equations* [1,24,27,32].

$$C_e(T_e) \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial x} \left( k_e(T_e, T_1) \frac{\partial T_e}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_e(T_e, T_1) \frac{\partial T_e}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_e(T_e, T_1) \frac{\partial T_e}{\partial z} \right) - G(T_e - T_1) + Q, \quad (5)$$

$$C_1 \frac{\partial T_1}{\partial t} = G(T_e - T_1) - (3\lambda + 2\mu)\alpha_T T_0 \frac{\partial}{\partial t} (\varepsilon_x + \varepsilon_y + \varepsilon_z), \quad (6)$$

where the heat source is given by

$$Q(x, y, z, t) = 0.94J \frac{1-R}{t_p z_s} \exp \left[ -\frac{z}{z_s} - \frac{(x-x_0)^2 + (y-y_0)^2}{r_s^2} - 2.77 \left( \frac{t-2t_p}{t_p} \right)^2 \right]. \quad (7)$$

Here,  $C_e(T_e) = C_{e0}(\frac{T_e}{T_0})$  is the electron heat capacity,  $k_e(T_e, T_1) = k_0(\frac{T_e}{T_1})$  is the thermal conductivity,  $G$  is the electron-lattice coupling factor,  $C_1$  is the lattice heat capacities, respectively;  $Q$  is energy absorption rate;  $J$  is laser fluence;  $R$  is surface reflectivity;  $t_p$  is laser pulse duration;  $z_s$  is optical penetration depth;  $r_s$  is spatial profile parameter. Eqs. (5) and (6) are often referred to as parabolic two-step heat transport equations.

The boundary conditions are assumed to be stress free and thermally insulated:

$$\sigma_x = 0, \quad \sigma_{xy} = 0, \quad \sigma_{xz} = 0, \quad \text{at } x = 0, L_x, \quad (8a)$$

$$\sigma_y = 0, \quad \sigma_{xy} = 0, \quad \sigma_{yz} = 0, \quad \text{at } y = 0, L_y, \quad (8b)$$

$$\sigma_z = 0, \quad \sigma_{xz} = 0, \quad \sigma_{yz} = 0, \quad \text{at } z = 0, L_z, \quad (8c)$$

$$\frac{\partial T_e}{\partial \vec{n}} = 0, \quad \frac{\partial T_1}{\partial \vec{n}} = 0, \quad (9)$$

where  $\vec{n}$  is the unit outward normal vector on the boundary. It should be pointed out that insulated boundaries are imposed due to the assumption that there are no heat losses from the film surfaces in the short time response.

The initial conditions are assumed to be

$$T_e = T_1 = T_0, \quad u = v = w = 0, \\ u_t = v_t = w_t = 0, \quad \text{at } t = 0. \quad (10)$$

### 3. Finite difference method

Using a similar argument as that in [27–29], we introduce three velocity components  $v_1, v_2$  and  $v_3$  into the model and re-write the dynamic equations of motion, Eqs. (1)–(4), as follows:

$$v_1 = \frac{\partial u}{\partial t}, \quad v_2 = \frac{\partial v}{\partial t}, \quad v_3 = \frac{\partial w}{\partial t}, \quad (11)$$

$$\rho \frac{\partial v_1}{\partial t} = \frac{\partial \sigma_x}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} + 2AT_e \frac{\partial T_e}{\partial x}, \quad (12)$$

$$\rho \frac{\partial v_2}{\partial t} = \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + 2AT_e \frac{\partial T_e}{\partial y}, \quad (13)$$

$$\rho \frac{\partial v_3}{\partial t} = \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_z}{\partial z} + 2AT_e \frac{\partial T_e}{\partial z}, \quad (14)$$

$$\frac{\partial \varepsilon_x}{\partial t} = \frac{\partial v_1}{\partial x}, \quad \frac{\partial \varepsilon_y}{\partial t} = \frac{\partial v_2}{\partial y}, \quad \frac{\partial \varepsilon_z}{\partial t} = \frac{\partial v_3}{\partial z}, \quad (15a)$$

$$\frac{\partial \gamma_{xy}}{\partial t} = \frac{\partial v_1}{\partial y} + \frac{\partial v_2}{\partial x}, \quad \frac{\partial \gamma_{xz}}{\partial t} = \frac{\partial v_1}{\partial z} + \frac{\partial v_3}{\partial x}, \\ \frac{\partial \gamma_{yz}}{\partial t} = \frac{\partial v_2}{\partial z} + \frac{\partial v_3}{\partial y}. \quad (15b)$$

To develop a finite difference scheme, we first construct a staggered grid as shown in Fig. 2, where  $v_1$  is placed at  $(x_{i+\frac{1}{2}}, y_j, z_k)$ ,  $v_2$  is placed at  $(x_i, y_{j+\frac{1}{2}}, z_k)$ ,  $v_3$  is placed at  $(x_i, y_j, z_{k+\frac{1}{2}})$ ,  $\gamma_{xy}$  and  $\sigma_{xy}$  are placed at  $(x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}, z_k)$ ,  $\gamma_{xz}$  and  $\sigma_{xz}$  are placed at  $(x_{i+\frac{1}{2}}, y_j, z_{k+\frac{1}{2}})$ ,  $\gamma_{yz}$  and  $\sigma_{yz}$  are placed at  $(x_i, y_{j+\frac{1}{2}}, z_{k+\frac{1}{2}})$ , while  $\varepsilon_x, \varepsilon_y, \varepsilon_z, \sigma_x, \sigma_y, \sigma_z, T_e$  and  $T_1$  are at  $(x_i, y_j, z_k)$ . Here,  $i, j$  and  $k$  are indices with  $1 \leq i \leq N_x + 1$ ,  $1 \leq j \leq N_y + 1$  and  $1 \leq k \leq N_z + 1$ . We denote  $v_1^n(i + \frac{1}{2}, j, k), v_2^n(i, j + \frac{1}{2}, k)$  and  $v_3^n(i, j, k + \frac{1}{2})$  as numerical approximations of  $v_1((i + \frac{1}{2})\Delta x, j\Delta y, k\Delta z, n\Delta t)$ ,  $v_2(i\Delta x, (j + \frac{1}{2})\Delta y, k\Delta z, n\Delta t)$  and  $v_3(i\Delta x, j\Delta y, (k + \frac{1}{2})\Delta z, n\Delta t)$ , respectively, where  $\Delta t, \Delta x, \Delta y$  and  $\Delta z$  are time increment and spatial step sizes, respectively. Similar notations are used for other variables. Furthermore, we introduce the finite difference operators,  $\Delta_t$  and  $\delta_x$ , as follows:

$$\Delta_t u_i^n = u_i^n - u_i^{n-1}, \quad \delta_x u_i^n = u_{i+\frac{1}{2}}^n - u_{i-\frac{1}{2}}^n.$$

It should be pointed out that the staggered-grid method is often employed in computational fluid dynamics to prevent the solution from oscillations [33]. For example, if  $v_1$  and  $\varepsilon_x$  in Eq. (15a) are placed at a same location, employing a central finite difference scheme may produce a velocity component  $v_1$ , a wave solution, implying oscillation.

To avoid non-physical oscillations in the solution, we develop a fourth-order compact finite difference scheme for stress derivatives  $\frac{\partial \sigma_x}{\partial x}, \frac{\partial \sigma_{xy}}{\partial y}, \frac{\partial \sigma_{xz}}{\partial z}$ , etc. in Eqs. (12)–(15). To this end, we let

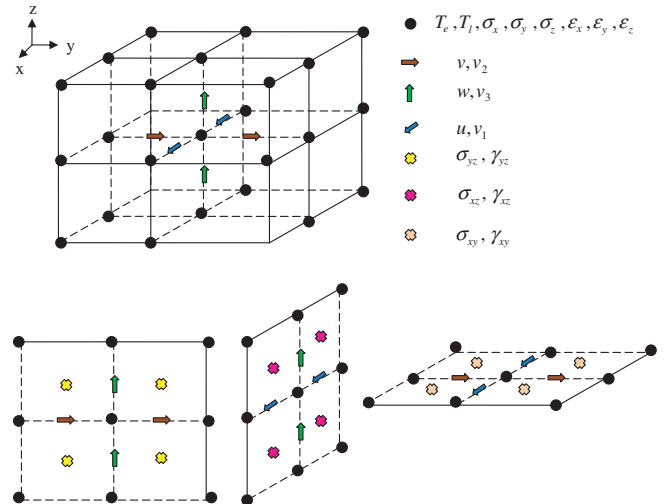


Fig. 2. A 3D staggered mesh and locations of variables.

$$a \frac{\partial \sigma_x(i-1)}{\partial x} + b \frac{\partial \sigma_x(i)}{\partial x} + a \frac{\partial \sigma_x(i+1)}{\partial x} = \frac{\sigma_x(i+\frac{1}{2}) - \sigma_x(i-\frac{1}{2})}{\Delta x}, \quad 2 + \frac{1}{2} \leq i \leq N_x - \frac{1}{2}, \quad (16)$$

where  $a$  and  $b$  are unknown constants. Here, we omit indices  $j, k$ , and  $n$  for simplicity. Using the Taylor series expansion, we obtain

$$\sigma_x(i+\frac{1}{2}) = \sigma_x(i) + \frac{\Delta x}{2} \frac{\partial \sigma_x(i)}{\partial x} + \frac{\Delta x^2}{2!2^2} \frac{\partial^2 \sigma_x(i)}{\partial x^2} + \frac{\Delta x^3}{3!2^3} \frac{\partial^3 \sigma_x(i)}{\partial x^3} + \frac{\Delta x^4}{4!2^4} \frac{\partial^4 \sigma_x(i)}{\partial x^4} + O(\Delta x^5), \quad (17a)$$

$$\sigma_x(i-\frac{1}{2}) = \sigma_x(i) - \frac{\Delta x}{2} \frac{\partial \sigma_x(i)}{\partial x} + \frac{\Delta x^2}{2!2^2} \frac{\partial^2 \sigma_x(i)}{\partial x^2} - \frac{\Delta x^3}{3!2^3} \frac{\partial^3 \sigma_x(i)}{\partial x^3} + \frac{\Delta x^4}{4!2^4} \frac{\partial^4 \sigma_x(i)}{\partial x^4} + O(\Delta x^5), \quad (17b)$$

$$\frac{\partial \sigma_x(i+1)}{\partial x} = \frac{\partial \sigma_x(i)}{\partial x} + \Delta x \frac{\partial^2 \sigma_x(i)}{\partial x^2} + \frac{\Delta x^2}{2} \frac{\partial^3 \sigma_x(i)}{\partial x^3} + \frac{\Delta x^3}{3!} \frac{\partial^4 \sigma_x(i)}{\partial x^4} + O(\Delta x^4), \quad (17c)$$

$$\frac{\partial \sigma_x(i-1)}{\partial x} = \frac{\partial \sigma_x(i)}{\partial x} - \Delta x \frac{\partial^2 \sigma_x(i)}{\partial x^2} + \frac{\Delta x^2}{2} \frac{\partial^3 \sigma_x(i)}{\partial x^3} - \frac{\Delta x^3}{3!} \frac{\partial^4 \sigma_x(i)}{\partial x^4} + O(\Delta x^4). \quad (17d)$$

Substituting the above equations into Eq. (16) and comparing the corresponding terms, we obtain

$$2a + b = 1, \quad a = \frac{1}{24}, \quad b = \frac{11}{12}, \quad (18)$$

with truncation error of  $O(\Delta x^4)$ . It should be pointed out that the dissipative term  $\frac{\partial^3 \sigma_x(i)}{\partial x^3}$  has been eliminated from the truncation error. Hence,  $\frac{\partial \sigma_x}{\partial x}$  can be obtained by solving the following tridiagonal system

$$\frac{1}{24} \frac{\partial \sigma_x(i-1)}{\partial x} + \frac{11}{12} \frac{\partial \sigma_x(i)}{\partial x} + \frac{1}{24} \frac{\partial \sigma_x(i+1)}{\partial x} = \frac{\sigma_x(i+\frac{1}{2}) - \sigma_x(i-\frac{1}{2})}{\Delta x}, \quad 2 + \frac{1}{2} \leq i \leq N_x - \frac{1}{2}, \quad (19)$$

Table 1  
Thermophysical properties

Properties	Unit	Value
$\rho$	kg/m <sup>3</sup>	19,300
$A$	J m <sup>-3</sup> K <sup>-2</sup>	70
$K$	Pa	$217 \times 10^9$
$\mu$	Pa	$27 \times 10^9$
$\alpha_T$	K <sup>-1</sup>	$14.2 \times 10^{-6}$
$C_{e0}$	J/(m <sup>3</sup> K)	$2.1 \times 10^4$
$C_l$	J/(m <sup>3</sup> K)	$2.5 \times 10^6$
$G$	W/(m <sup>3</sup> K)	$2.6 \times 10^{16}$
$K_e$	W/(m K)	315
$R$		0.93
$t_p$	s	$0.1 \times 10^{-12}$
$z_s$	m	$15.3 \times 10^{-9}$
$r_s$	m	$1.0 \times 10^{-6}$
$J$	J/m <sup>2</sup>	500,2000

where

$$\frac{\partial \sigma_x(\frac{3}{2})}{\partial x} = \frac{\sigma_x(2) - \sigma_x(1)}{\Delta x}, \quad \frac{\partial \sigma_x(N_x + \frac{1}{2})}{\partial x} = \frac{\sigma_x(N_x + 1) - \sigma_x(N_x)}{\Delta x}. \quad (20)$$

Using a similar argument, we can evaluate other stress derivatives in Eqs. (12)–(14). Hence, the implicit finite difference schemes for solving Eqs. (12)–(14) can be written as follows:

$$\begin{aligned} \rho \frac{1}{\Delta t} \Delta_{-i} v_1^{n+1}(i+\frac{1}{2}, j, k) &= \frac{\partial \sigma_x^{n+1}(i+\frac{1}{2}, j, k)}{\partial x} + \frac{\partial \sigma_{xy}^{n+1}(i+\frac{1}{2}, j, k)}{\partial y} \\ &+ \frac{\partial \sigma_{xz}^{n+1}(i+\frac{1}{2}, j, k)}{\partial z} + A \frac{1}{\Delta x} \delta_x (T_c^2)^{n+1}(i+\frac{1}{2}, j, k), \end{aligned} \quad (21)$$

$$\begin{aligned} \rho \frac{1}{\Delta t} \Delta_{-i} v_2^{n+1}(i, j+\frac{1}{2}, k) &= \frac{\partial \sigma_y^{n+1}(i, j+\frac{1}{2}, k)}{\partial y} + \frac{\partial \sigma_{xy}^{n+1}(i, j+\frac{1}{2}, k)}{\partial x} \\ &+ \frac{\partial \sigma_{yz}^{n+1}(i, j+\frac{1}{2}, k)}{\partial z} + A \frac{1}{\Delta y} \delta_y (T_c^2)^{n+1}(i, j+\frac{1}{2}, k), \end{aligned} \quad (22)$$

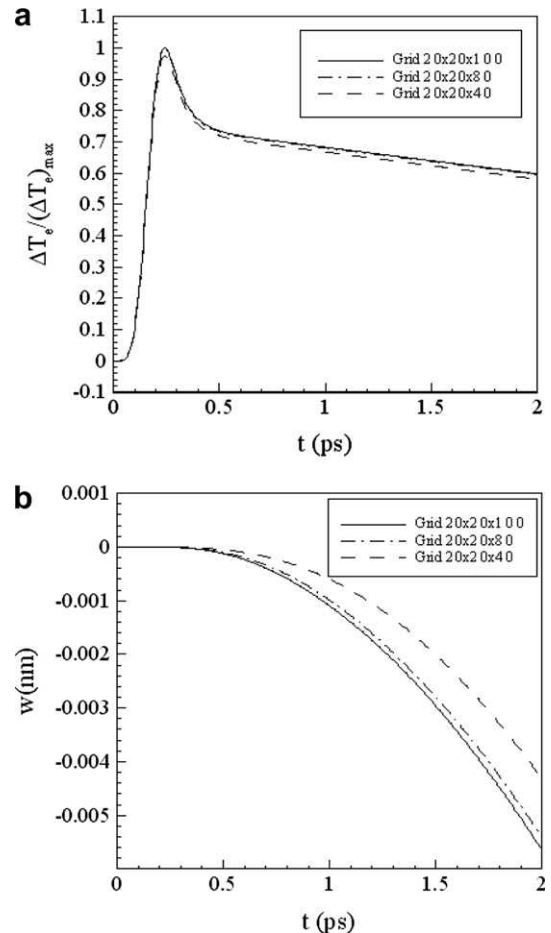


Fig. 3. Change in electron temperature and displacement ( $w$ ) at the center of top surface versus time for various grids ( $20 \times 20 \times 40$ ,  $20 \times 20 \times 80$ ,  $20 \times 20 \times 100$ ) and laser fluence  $J$  of 500 J/m<sup>2</sup>.

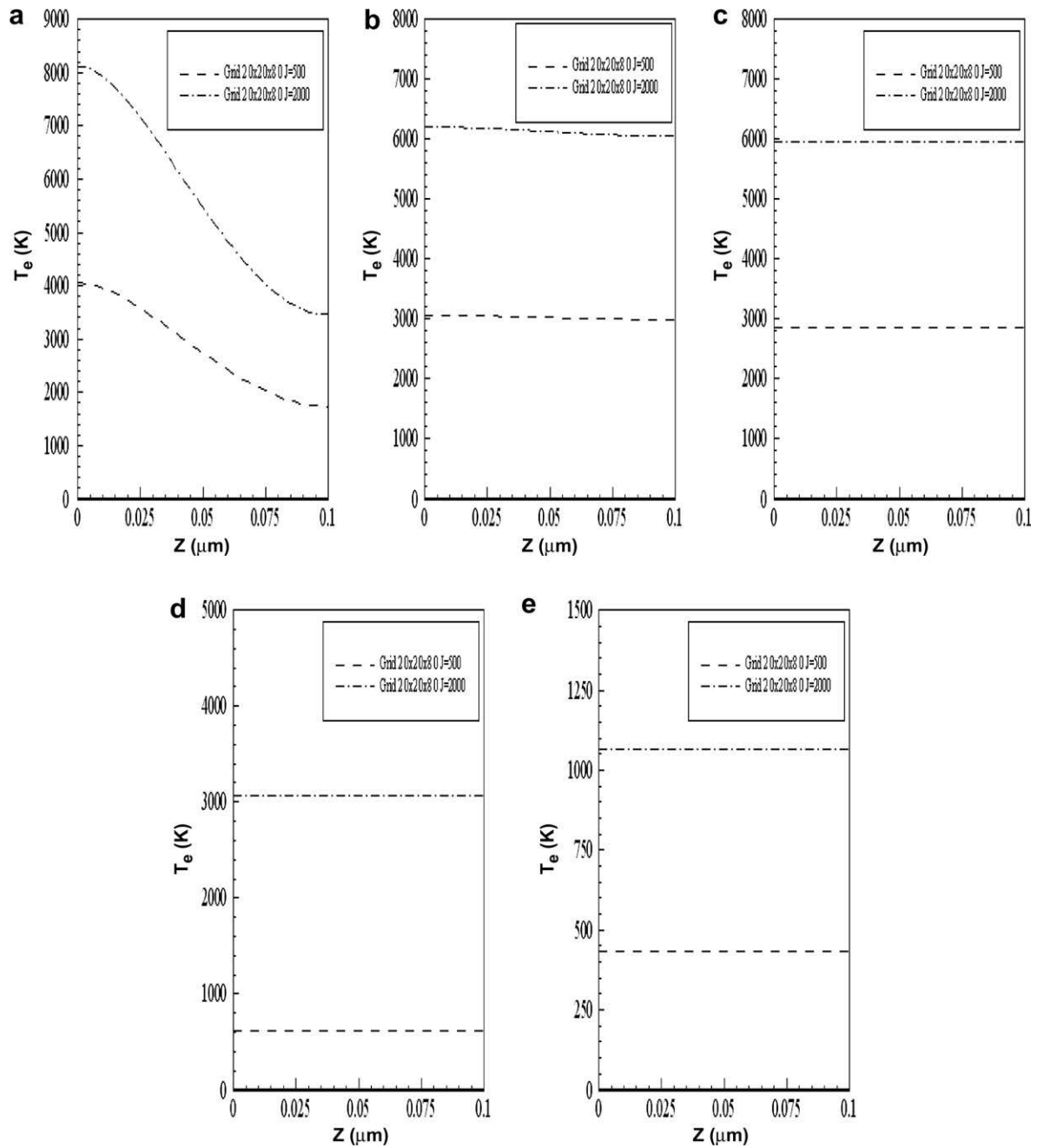


Fig. 4. Electron temperature profiles along  $z$  at  $(x_{\text{center}}, y_{\text{center}})$  at different times: (a)  $t = 0.25$  ps, (b)  $t = 0.5$  ps, (c)  $t = 1$  ps, (d)  $t = 10$  ps and (e)  $t = 20$  ps with a mesh of  $20 \times 20 \times 80$  and two different laser fluences  $J$  of  $500 \text{ J/m}^2$  and  $J$  of  $2000 \text{ J/m}^2$ .

$$\begin{aligned} & \rho \frac{1}{\Delta t} \Delta_{-t} v_3^{n+1}(i, j, k + \frac{1}{2}) \\ &= \frac{\partial \sigma_z^{n+1}(i, j, k + \frac{1}{2})}{\partial z} + \frac{\partial \sigma_{xz}^{n+1}(i, j, k + \frac{1}{2})}{\partial x} \\ &+ \frac{\partial \sigma_{yz}^{n+1}(i, j, k + \frac{1}{2})}{\partial y} + A \frac{1}{\Delta z} \delta_z (T_e^2)^{n+1}(i, j, k + \frac{1}{2}). \end{aligned} \quad (23)$$

On the other hand, the finite difference schemes for rest of the governing equations can be seen as generalizations of the schemes described in [27] to the 3D case. We summarize these generalizations below:

$$\frac{1}{\Delta t} \Delta_{-t} e_x^{n+1}(i, j, k) = \frac{1}{\Delta x} \delta_x v_1^{n+1}(i, j, k), \quad (24a)$$

$$\frac{1}{\Delta t} \Delta_{-t} e_y^{n+1}(i, j, k) = \frac{1}{\Delta y} \delta_y v_2^{n+1}(i, j, k), \quad (24b)$$

$$\frac{1}{\Delta t} \Delta_{-t} e_z^{n+1}(i, j, k) = \frac{1}{\Delta z} \delta_z v_3^{n+1}(i, j, k), \quad (24c)$$

$$\begin{aligned} & \frac{1}{\Delta t} \Delta_{-t} \gamma_{xy}^{n+1}(i + \frac{1}{2}, j + \frac{1}{2}, k) \\ &= \frac{1}{\Delta y} \delta_y v_1^{n+1}(i + \frac{1}{2}, j + \frac{1}{2}, k) + \frac{1}{\Delta x} \delta_x v_2^{n+1}(i + \frac{1}{2}, j + \frac{1}{2}, k), \end{aligned} \quad (25a)$$

$$\begin{aligned} & \frac{1}{\Delta t} \Delta_{-i} \gamma_{xz}^{n+1} \left( i + \frac{1}{2}, j, k + \frac{1}{2} \right) \\ &= \frac{1}{\Delta z} \delta_z v_1^{n+1} \left( i + \frac{1}{2}, j, k + \frac{1}{2} \right) + \frac{1}{\Delta x} \delta_x v_3^{n+1} \left( i + \frac{1}{2}, j, k + \frac{1}{2} \right), \end{aligned} \quad (25b)$$

$$\begin{aligned} & \frac{1}{\Delta t} \Delta_{-i} \gamma_{yz}^{n+1} \left( i, j + \frac{1}{2}, k + \frac{1}{2} \right) \\ &= \frac{1}{\Delta z} \delta_z v_2^{n+1} \left( i, j + \frac{1}{2}, k + \frac{1}{2} \right) + \frac{1}{\Delta y} \delta_y v_3^{n+1} \left( i, j + \frac{1}{2}, k + \frac{1}{2} \right), \end{aligned} \quad (25c)$$

$$\begin{aligned} \sigma_x^{n+1}(i, j, k) &= \lambda [\varepsilon_x^{n+1}(i, j, k) + \varepsilon_y^{n+1}(i, j, k) + \varepsilon_z^{n+1}(i, j, k)] + 2\mu \varepsilon_x^{n+1}(i, j, k) \\ &\quad - (3\lambda + 2\mu) \alpha_T [T_1^{n+1}(i, j, k) - T_0], \end{aligned} \quad (26a)$$

$$\begin{aligned} \sigma_y^{n+1}(i, j, k) &= \lambda [\varepsilon_x^{n+1}(i, j, k) + \varepsilon_y^{n+1}(i, j, k) + \varepsilon_z^{n+1}(i, j, k)] + 2\mu \varepsilon_y^{n+1}(i, j, k) \\ &\quad - (3\lambda + 2\mu) \alpha_T [T_1^{n+1}(i, j, k) - T_0], \end{aligned} \quad (26b)$$

$$\begin{aligned} \sigma_z^{n+1}(i, j, k) &= \lambda [\varepsilon_x^{n+1}(i, j, k) + \varepsilon_y^{n+1}(i, j, k) + \varepsilon_z^{n+1}(i, j, k)] + 2\mu \varepsilon_z^{n+1}(i, j, k) \\ &\quad - (3\lambda + 2\mu) \alpha_T [T_1^{n+1}(i, j, k) - T_0], \end{aligned} \quad (26c)$$

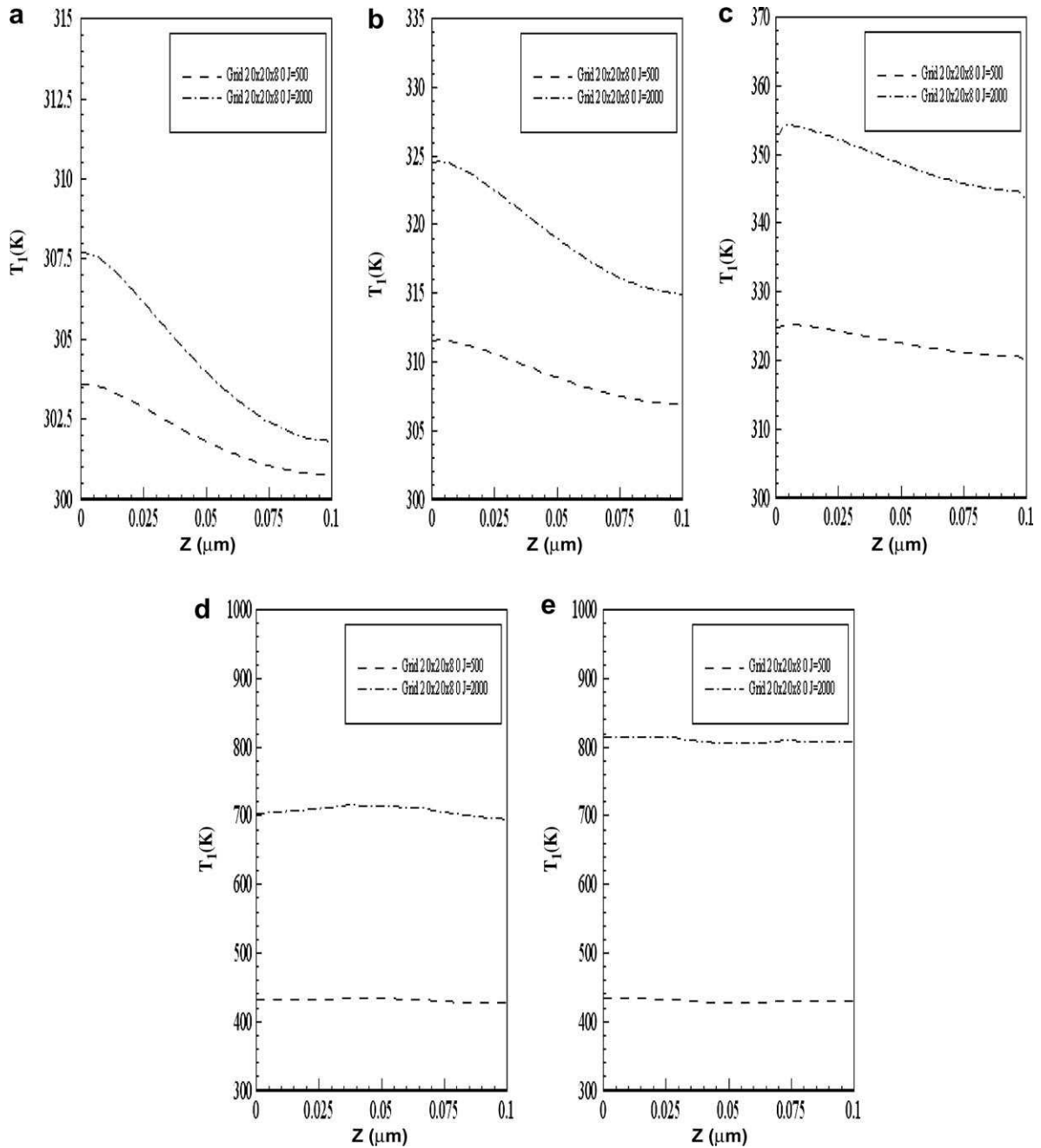


Fig. 5. Lattice temperature profiles along  $z$  at  $(x_{\text{center}}, y_{\text{center}})$  at different times: (a)  $t = 0.25$  ps, (b)  $t = 0.5$  ps, (c)  $t = 1$  ps, (d)  $t = 10$  ps and (e)  $t = 20$  ps with a mesh of  $20 \times 20 \times 80$  and two different laser fluences  $J$  of  $500 \text{ J/m}^2$  and  $J$  of  $2000 \text{ J/m}^2$ .

$$\sigma_{xy}^{n+1}(i+\frac{1}{2}, j+\frac{1}{2}, k) = \mu \gamma_{xy}^{n+1}(i+\frac{1}{2}, j+\frac{1}{2}, k), \quad (27a)$$

$$\sigma_{xz}^{n+1}(i+\frac{1}{2}, j, k+\frac{1}{2}) = \mu \gamma_{xz}^{n+1}(i+\frac{1}{2}, j, k+\frac{1}{2}), \quad (27b)$$

$$\sigma_{yz}^{n+1}(i, j+\frac{1}{2}, k+\frac{1}{2}) = \mu \gamma_{yz}^{n+1}(i, j+\frac{1}{2}, k+\frac{1}{2}), \quad (27c)$$

$$C_{e0} \frac{T_e^{n+1}(i, j, k) + T_e^n(i, j, k)}{2T_0} \cdot \frac{1}{\Delta t} \Delta_{-t} T_e^{n+1}(i, j, k) \\ = \frac{1}{2\Delta x^2} [k_e^{n+1}(i+\frac{1}{2}, j, k) \delta_x T_e^{n+1}(i+\frac{1}{2}, j, k) \\ - k_e^{n+1}(i-\frac{1}{2}, j, k) \delta_x T_e^{n+1}(i-\frac{1}{2}, j, k)]$$

$$+ \frac{1}{2\Delta x^2} [k_e^n(i+\frac{1}{2}, j, k) \delta_x T_e^n(i+\frac{1}{2}, j, k) \\ - k_e^n(i-\frac{1}{2}, j, k) \delta_x T_e^n(i-\frac{1}{2}, j, k)] \\ + \frac{1}{2\Delta y^2} [k_e^{n+1}(i, j+\frac{1}{2}, k) \delta_y T_e^{n+1}(i, j+\frac{1}{2}, k) \\ - k_e^{n+1}(i, j-\frac{1}{2}, k) \delta_y T_e^{n+1}(i, j-\frac{1}{2}, k)] \\ + \frac{1}{2\Delta y^2} [k_e^n(i, j+\frac{1}{2}, k) \delta_y T_e^n(i, j+\frac{1}{2}, k) \\ - k_e^n(i, j-\frac{1}{2}, k) \delta_y T_e^n(i, j-\frac{1}{2}, k)]$$

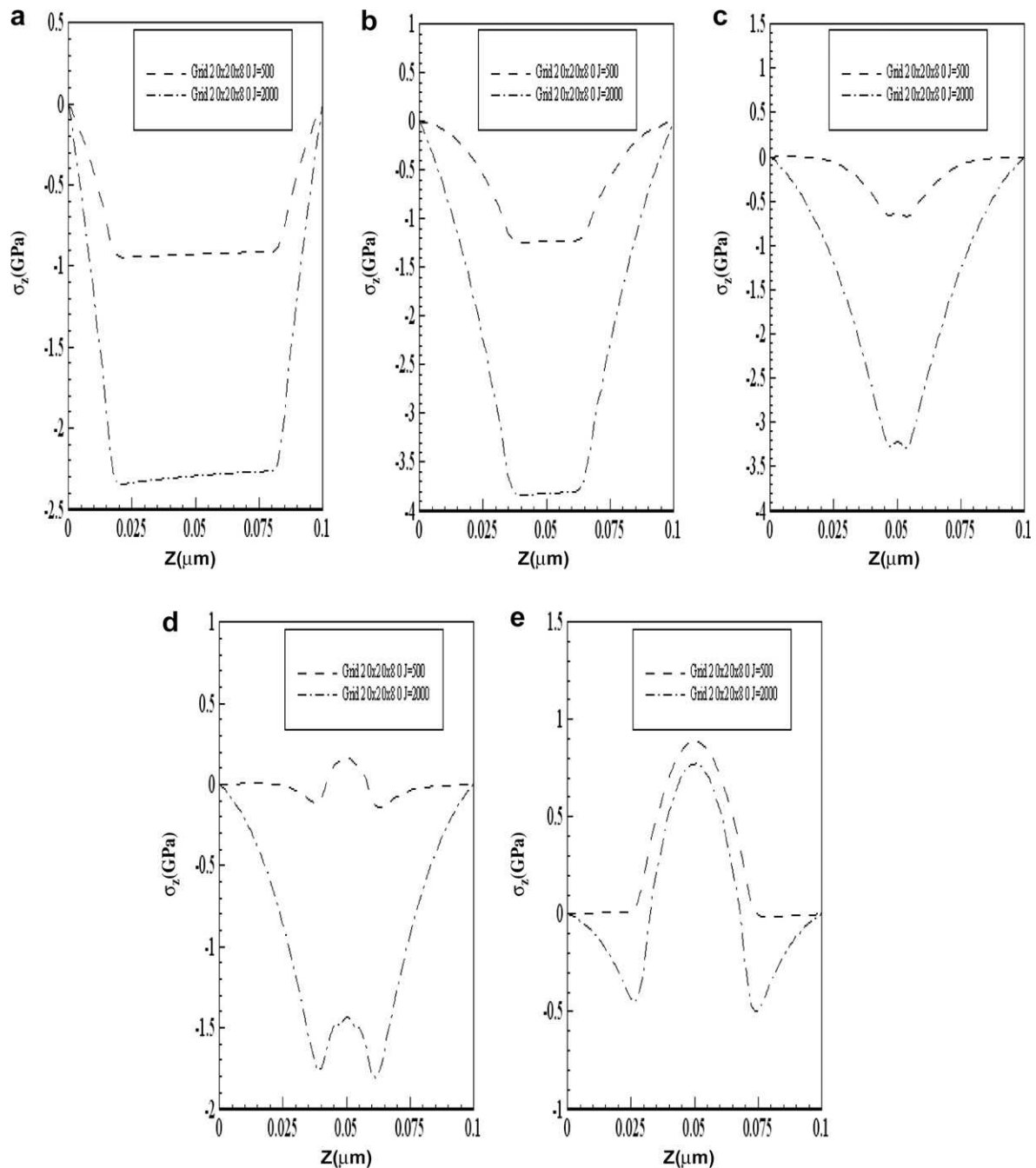


Fig. 6. Normal stress ( $\sigma_z$ ) profiles along  $z$  at  $(x_{\text{center}}, y_{\text{center}})$  at different times: (a)  $t = 5$  ps, (b)  $t = 10$  ps, (c)  $t = 15$  ps, (d)  $t = 17$  ps and (e)  $t = 20$  ps with a mesh of  $20 \times 20 \times 80$  and two different laser fluences  $J$  of  $500 \text{ J/m}^2$  and  $2000 \text{ J/m}^2$ .

$$\begin{aligned}
& + \frac{1}{2\Delta z^2} [k_e^{n+1}(i, j, k + \frac{1}{2}) \delta_z T_e^{n+1}(i, j, k + \frac{1}{2}) \\
& - k_e^{n+1}(i, j, k - \frac{1}{2}) \delta_z T_e^{n+1}(i, j, k - \frac{1}{2})] \\
& + \frac{1}{2\Delta z^2} [k_e^n(i, j, k + \frac{1}{2}) \delta_z T_e^n(i, j, k + \frac{1}{2}) \\
& - k_e^n(i, j, k - \frac{1}{2}) \delta_z T_e^n(i, j, k - \frac{1}{2})] \\
& - G \left[ \frac{T_e^{n+1}(i, j, k) + T_e^n(i, j, k)}{2} - \frac{T_1^{n+1}(i, j, k) + T_1^n(i, j, k)}{2} \right] \\
& + Q^{n+\frac{1}{2}}(i, j, k),
\end{aligned} \tag{28}$$

$$\begin{aligned}
& C_1 \frac{1}{\Delta t} \Delta_{-t} T_1^{n+1}(i, j, k) \\
& = G \left[ \frac{T_e^{n+1}(i, j, k) + T_e^n(i, j, k)}{2} - \frac{T_1^{n+1}(i, j, k) + T_1^n(i, j, k)}{2} \right] \\
& - (3\lambda + 2\mu) \alpha_T T_0 \frac{1}{\Delta t} [\Delta_{-t} \varepsilon_x^{n+1}(i, j, k) + \Delta_{-t} \varepsilon_y^{n+1}(i, j, k) \\
& + \Delta_{-t} \varepsilon_z^{n+1}(i, j, k)],
\end{aligned} \tag{29}$$

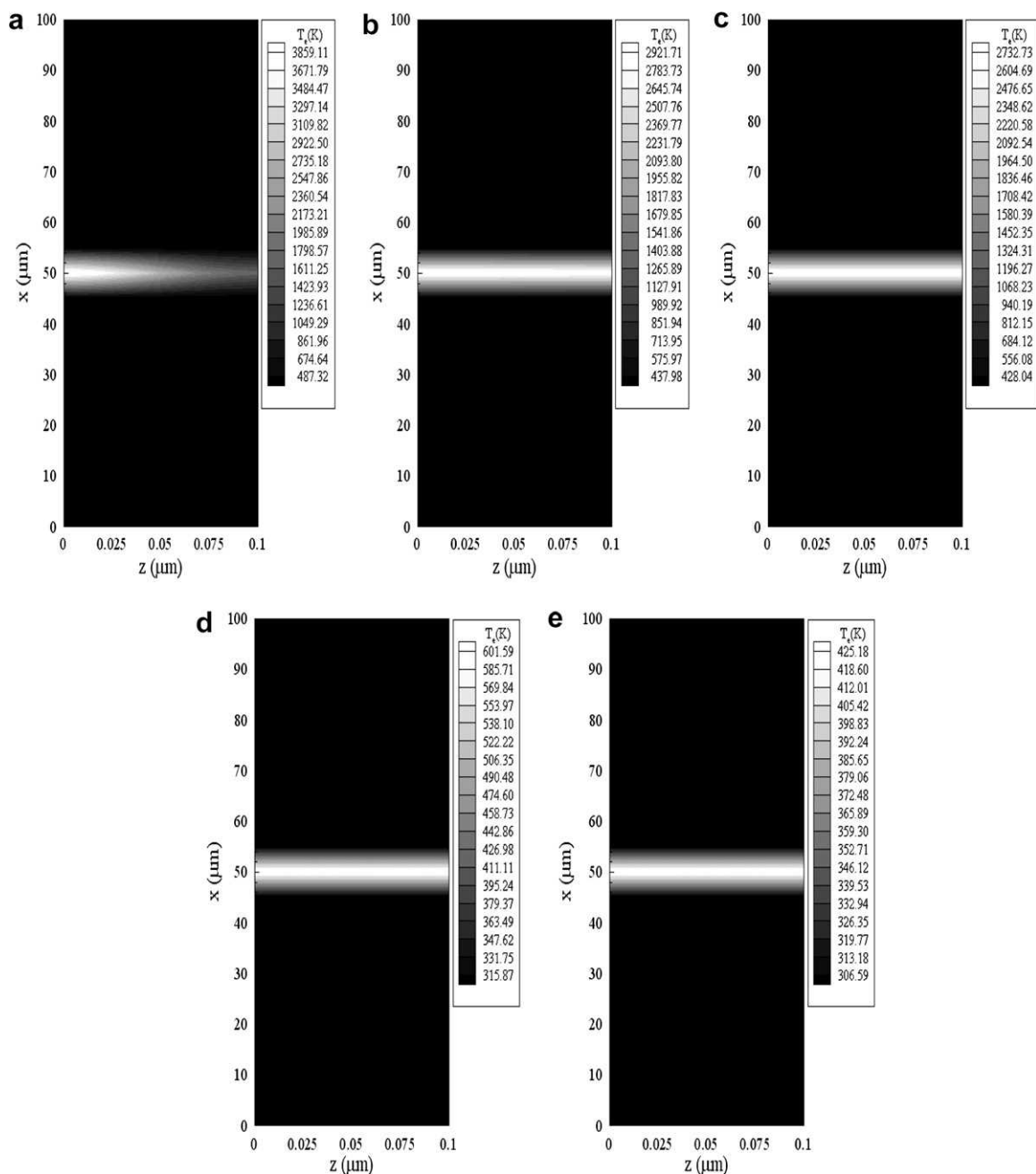


Fig. 7. Contours of electron temperature profiles in the cross-section of  $y = 50 \mu\text{m}$  at different times: (a)  $t = 0.25 \text{ ps}$ , (b)  $t = 0.5 \text{ ps}$ , (c)  $t = 1 \text{ ps}$ , (d)  $t = 10 \text{ ps}$ , and (e)  $t = 20 \text{ ps}$  with a mesh of  $20 \times 20 \times 80$  and laser fluence  $J$  of  $500 \text{ J/m}^2$ .



$$\frac{1}{\Delta t} \Delta_{-t} u^{n+1}(i + \frac{1}{2}, j, k) = v_1^{n+1}(i + \frac{1}{2}, j, k), \quad (30a)$$

$$\frac{1}{\Delta t} \Delta_{-t} v^{n+1}(i, j + \frac{1}{2}, k) = v_2^{n+1}(i, j + \frac{1}{2}, k), \quad (30b)$$

$$\frac{1}{\Delta t} \Delta_{-t} w^{n+1}(i, j, k + \frac{1}{2}) = v_3^{n+1}(i, j, k + \frac{1}{2}). \quad (30c)$$

To complete the formulation of our numerical method, we now turn our attention to the approximation of boundary and initial conditions:

$$\sigma_x^n(1, j, k) = \sigma_x^n(N_x + 1, j, k) = 0, \quad 1 \leq j \leq N_y + 1, 1 \leq k \leq N_z + 1; \quad (31a)$$

$$\sigma_{xy}^n(1 + \frac{1}{2}, j + \frac{1}{2}, k) = \sigma_{xy}^n(N_x + \frac{1}{2}, j + \frac{1}{2}, k) = 0, \quad 1 \leq j \leq N_y, 1 \leq k \leq N_z; \quad (31b)$$

$$\sigma_{xz}^n(1 + \frac{1}{2}, j, k + \frac{1}{2}) = \sigma_{xz}^n(N_x + \frac{1}{2}, j, k + \frac{1}{2}) = 0, \quad 1 \leq j \leq N_y, 1 \leq k \leq N_z; \quad (31c)$$

$$\sigma_{yz}^n(1, j + \frac{1}{2}, k + \frac{1}{2}) = \sigma_{yz}^n(N_x, j + \frac{1}{2}, k + \frac{1}{2}) = 0, \quad 1 \leq j \leq N_y, 1 \leq k \leq N_z; \quad (31d)$$

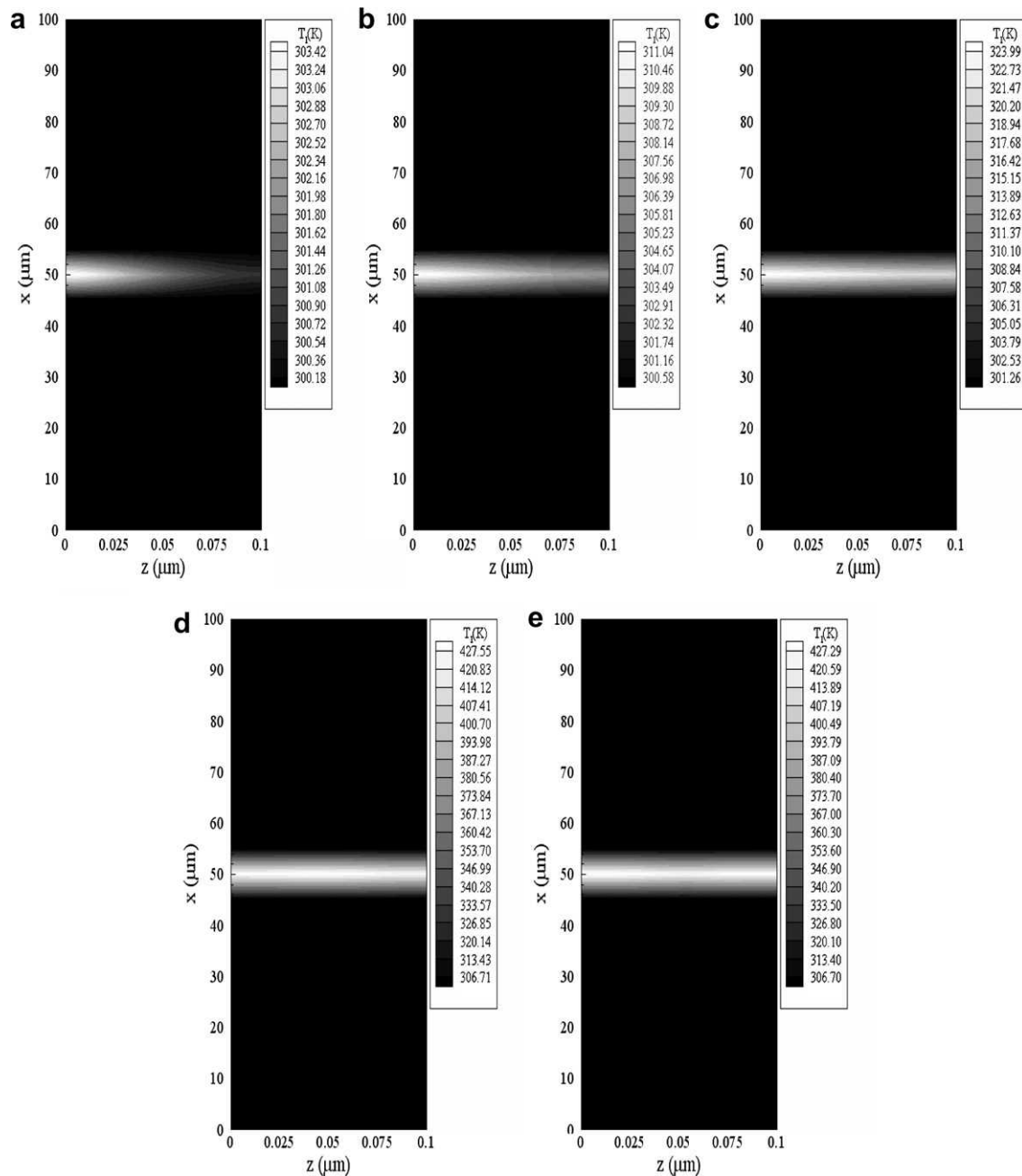


Fig. 8. Contours of lattice temperature profiles in the cross-section of  $y = 50 \mu\text{m}$  at different times: (a)  $t = 0.25 \text{ ps}$ , (b)  $t = 0.5 \text{ ps}$ , (c)  $t = 1 \text{ ps}$ , (d)  $t = 10 \text{ ps}$ , and (e)  $t = 20 \text{ ps}$  with a mesh of  $20 \times 20 \times 80$  and laser fluence  $J$  of  $500 \text{ J/m}^2$ .

$$\sigma_y^n(i, 1, k) = \sigma_y^n(i, N_y + 1, k) = 0, \quad 1 \leq i \leq N_x + 1, \quad 1 \leq k \leq N_z + 1; \quad (32a)$$

$$\sigma_{xy}^n(i + \frac{1}{2}, 1 + \frac{1}{2}, k) = \sigma_{xy}^n(i + \frac{1}{2}, N_y + \frac{1}{2}, k) = 0, \quad 1 \leq i \leq N_x, \quad 1 \leq k \leq N_z; \quad (32b)$$

$$\sigma_{xz}^n(i + \frac{1}{2}, 1, k + \frac{1}{2}) = \sigma_{xz}^n(i + \frac{1}{2}, N_y, k + \frac{1}{2}) = 0, \quad 1 \leq i \leq N_x, \quad 1 \leq k \leq N_z; \quad (32c)$$

$$\sigma_{yz}^n(i, 1 + \frac{1}{2}, k + \frac{1}{2}) = \sigma_{yz}^n(i, N_y + \frac{1}{2}, k + \frac{1}{2}) = 0, \quad 1 \leq i \leq N_x, \quad 1 \leq k \leq N_z; \quad (32d)$$

$$\sigma_z^n(i, j, 1) = \sigma_z^n(i, j, N_z + 1) = 0, \quad 1 \leq i \leq N_x + 1, \quad 1 \leq j \leq N_y + 1; \quad (33a)$$

$$\sigma_{xy}^n(i + \frac{1}{2}, j + \frac{1}{2}, 1) = \sigma_{xy}^n(i + \frac{1}{2}, j + \frac{1}{2}, N_z) = 0, \quad 1 \leq i \leq N_x, \quad 1 \leq j \leq N_y; \quad (33b)$$

$$\sigma_{xz}^n(i + \frac{1}{2}, j, 1 + \frac{1}{2}) = \sigma_{xz}^n(i + \frac{1}{2}, j, N_z + \frac{1}{2}) = 0, \quad 1 \leq i \leq N_x, \quad 1 \leq j \leq N_y; \quad (33c)$$

$$\sigma_{yz}^n(i, j + \frac{1}{2}, 1 + \frac{1}{2}) = \sigma_{yz}^n(i, j + \frac{1}{2}, N_z + \frac{1}{2}) = 0, \quad 1 \leq i \leq N_x, \quad 1 \leq j \leq N_y; \quad (33d)$$

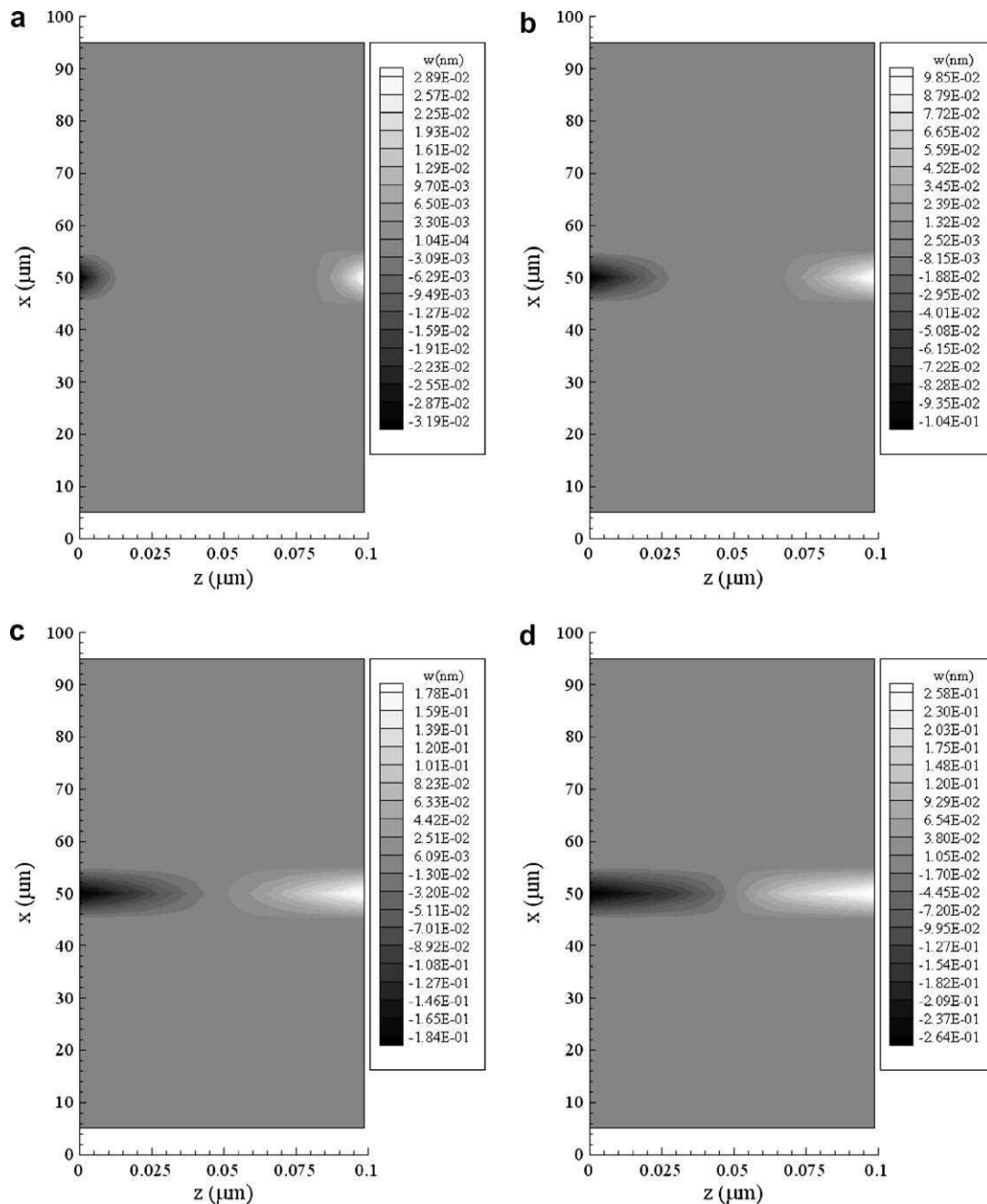


Fig. 9. Contours of displacement ( $w$ ) profiles in the cross-section of  $y = 50 \mu\text{m}$  at different times: (a)  $t = 5 \text{ ps}$ , (b)  $t = 10 \text{ ps}$ , (c)  $t = 15 \text{ ps}$ , and (d)  $t = 20 \text{ ps}$  with a mesh of  $20 \times 20 \times 80$  and laser fluence  $J$  of  $500 \text{ J/m}^2$ .

$$T_e^n(1, j, k) = T_e^n(2, j, k), \quad T_e^n(N_x + 1, j, k) = T_e^n(N_x, j, k); \quad (34a)$$

$$T_e^n(i, 1, k) = T_e^n(i, 2, k), \quad T_e^n(i, N_y + 1, k) = T_e^n(i, N_y, k); \quad (34b)$$

$$T_e^n(i, j, 1) = T_e^n(i, j, 2), \quad T_e^n(i, j, N_z + 1) = T_e^n(i, j, N_z); \quad (34c)$$

$$T_1^n(1, j, k) = T_1^n(2, j, k), \quad T_1^n(N_x + 1, j, k) = T_1^n(N_x, j, k); \quad (35a)$$

$$T_1^n(i, 1, k) = T_1^n(i, 2, k), \quad T_1^n(i, N_y + 1, k) = T_1^n(i, N_y, k); \quad (35b)$$

$$T_1^n(i, j, 1) = T_1^n(i, j, 2), \quad T_1^n(i, j, N_z + 1) = T_1^n(i, j, N_z); \quad (35c)$$

where  $1 \leq i \leq N_x + 1$ ,  $1 \leq j \leq N_y + 1$ ,  $1 \leq k \leq N_z + 1$ , for any time level  $n$ . The initial conditions are approximated as

$$u^0(i + \frac{1}{2}, j, k) = v^0(i, j + \frac{1}{2}, k) = w^0(i, j, k + \frac{1}{2}) = 0, \quad (36a)$$

$$v_1^0(i + \frac{1}{2}, j, k) = v_2^0(i, j + \frac{1}{2}, k) = v_3^0(i, j, k + \frac{1}{2}) = 0, \quad (36b)$$

$$T_e^0(i, j, k) = T_1^0(i, j, k) = T_0, \quad (36c)$$

$$\varepsilon_x^0(i + \frac{1}{2}, j, k) = \varepsilon_y^0(i, j + \frac{1}{2}, k) = \varepsilon_z^0(i, j, k + \frac{1}{2}) = 0, \quad (36d)$$

$$\sigma_x^0(i + \frac{1}{2}, j, k) = \sigma_y^0(i, j + \frac{1}{2}, k) = \sigma_z^0(i, j, k + \frac{1}{2}) = 0, \quad (36e)$$

$$\sigma_{xy}^0(i + \frac{1}{2}, j + \frac{1}{2}, k) = \gamma_{xy}^0(i + \frac{1}{2}, j + \frac{1}{2}, k) = 0, \quad (36f)$$

$$\sigma_{xz}^0(i + \frac{1}{2}, j, k + \frac{1}{2}) = \gamma_{xz}^0(i + \frac{1}{2}, j, k + \frac{1}{2}) = 0, \quad (36g)$$

$$\sigma_{yz}^0(i, j + \frac{1}{2}, k + \frac{1}{2}) = \gamma_{yz}^0(i, j + \frac{1}{2}, k + \frac{1}{2}) = 0. \quad (36h)$$

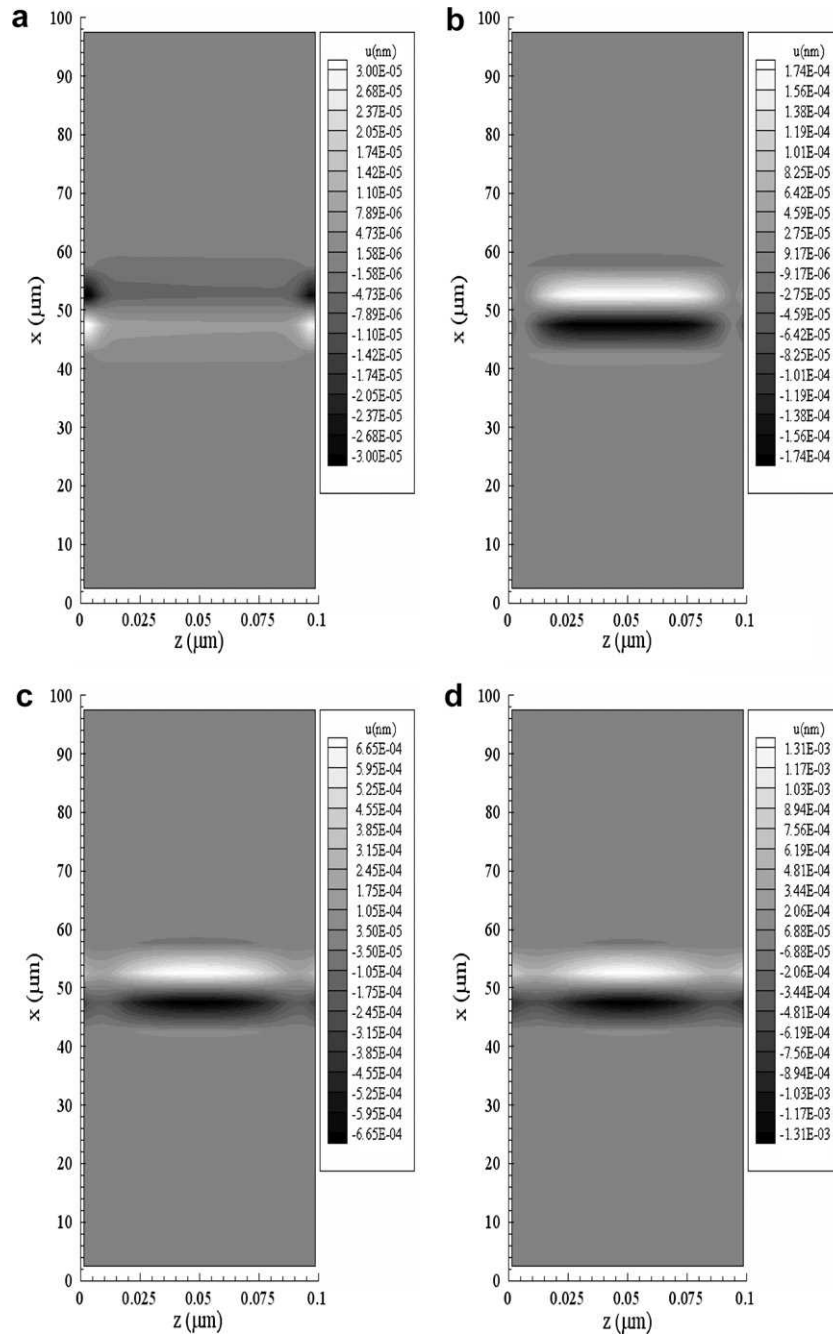


Fig. 10. Contours of displacement ( $u$ ) profiles in the cross-section of  $y = 50 \mu\text{m}$  at different times: (a)  $t = 5 \text{ ps}$ , (b)  $t = 10 \text{ ps}$ , (c)  $t = 15 \text{ ps}$ , and (d)  $t = 20 \text{ ps}$  with a mesh of  $20 \times 20 \times 80$  and laser fluence  $J$  of  $500 \text{ J/m}^2$ .

where  $1 \leq i \leq N_x + 1$ ,  $1 \leq j \leq N_y + 1$ ,  $1 \leq k \leq N_z + 1$ , for any time level  $n$ .

It should be pointed out that Eqs. (21)–(23) are nonlinear since the terms  $\delta_x(T_c^2)^{n+1}(i + \frac{1}{2}, j, k)$ ,  $\delta_y(T_c^2)^{n+1}(i, j + \frac{1}{2}, k)$  and  $\delta_z(T_c^2)^{n+1}(i, j, k + \frac{1}{2})$  are nonlinear. Also, it can be seen that Eq. (28) is nonlinear. Therefore, the above scheme must be solved iteratively. An iterative method for solving the above scheme at time level  $n + 1$  is developed as follows:

Step 1. Set the values  $\epsilon_x^{n+1}$ ,  $\epsilon_y^{n+1}$ ,  $\epsilon_z^{n+1}$ ,  $\gamma_{xy}^{n+1}$ ,  $\gamma_{xz}^{n+1}$  and  $\gamma_{yz}^{n+1}$ , solve Eqs. (28) and (29) iteratively for  $T_c^{n+1}$  and  $T_1^{n+1}$ .

Step 2. Solve for  $\sigma_x^{n+1}$ ,  $\sigma_y^{n+1}$ ,  $\sigma_z^{n+1}$ ,  $\sigma_{xy}^{n+1}$ ,  $\sigma_{xz}^{n+1}$  and  $\sigma_{yz}^{n+1}$  using Eqs. (26) and (27).

Step 3. Solve for derivatives of  $\sigma_x^{n+1}$ ,  $\sigma_y^{n+1}$ ,  $\sigma_z^{n+1}$ ,  $\sigma_{xy}^{n+1}$ ,  $\sigma_{xz}^{n+1}$  and  $\sigma_{yz}^{n+1}$  using Eqs. (19), (20) or similar equations.

Step 4. Solve for  $v_1^{n+1}$ ,  $v_2^{n+1}$  and  $v_3^{n+1}$  using Eqs. (21)–(23).

Step 5. Update  $\epsilon_x^{n+1}$ ,  $\epsilon_y^{n+1}$ ,  $\epsilon_z^{n+1}$ ,  $\gamma_{xy}^{n+1}$ ,  $\gamma_{xz}^{n+1}$  and  $\gamma_{yz}^{n+1}$  using Eqs. (24) and (25).

Given the required accuracy  $\epsilon_1$  (for temperature) and  $\epsilon_2$  (for strain), repeat the above steps until a convergent solution is obtained based on the following criteria

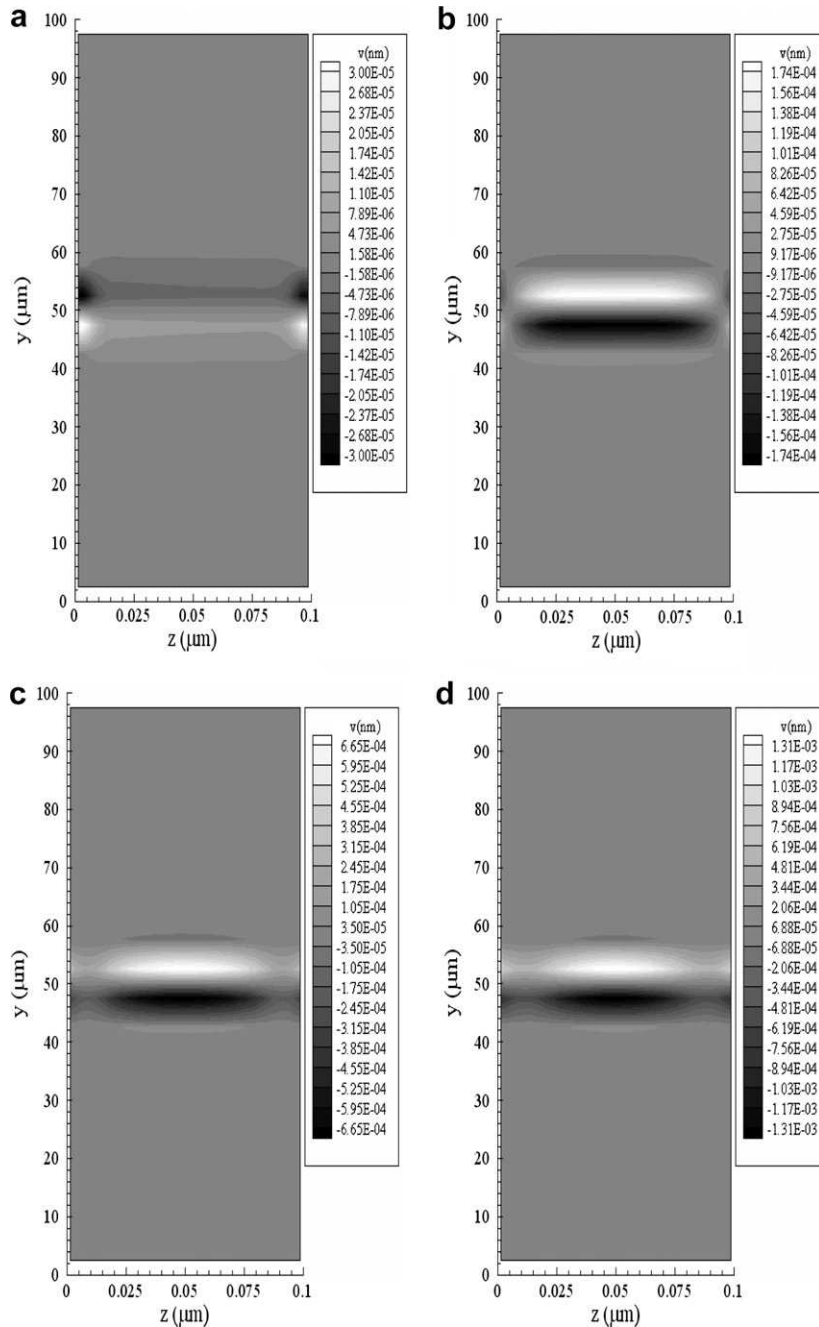


Fig. 11. Contours of displacement ( $v$ ) profiles in the cross-section of  $x = 50 \mu\text{m}$  at different times: (a)  $t = 5 \text{ ps}$ , (b)  $t = 10 \text{ ps}$ , (c)  $t = 15 \text{ ps}$ , and (d)  $t = 20 \text{ ps}$  with a mesh of  $20 \times 20 \times 80$  and laser fluence  $J$  of  $500 \text{ J/m}^2$ .

$$|T_e^{n+1}(i, j, k) - T_e^n(i, j, k)| \leq \epsilon_1, \quad (37a)$$

$$|\epsilon_x^{n+1}(i, j, k) - \epsilon_x^n(i, j, k)| \leq \epsilon_2, \quad (37b)$$

$$|\epsilon_y^{n+1}(i, j, k) - \epsilon_y^n(i, j, k)| \leq \epsilon_2, \quad (37c)$$

$$|\epsilon_z^{n+1}(i, j, k) - \epsilon_z^n(i, j, k)| \leq \epsilon_2, \quad (37d)$$

#### 4. Numerical examples

To test the applicability of the developed numerical scheme, we investigated the temperature rise and thermal deformation in a thin film with the dimensions  $100 \mu\text{m} \times 100 \mu\text{m} \times 0.1 \mu\text{m}$ , as shown in Fig. 1. The thermophysical properties for gold are listed in Table 1 [1,24,35]. Three meshes of  $20 \times 20 \times 40$ ,  $20 \times 20 \times 80$ ,  $20 \times 20 \times 100$  were chosen in order to test the convergence of the scheme. The time increment was chosen to be 0.005 ps and  $T_0$  was set to

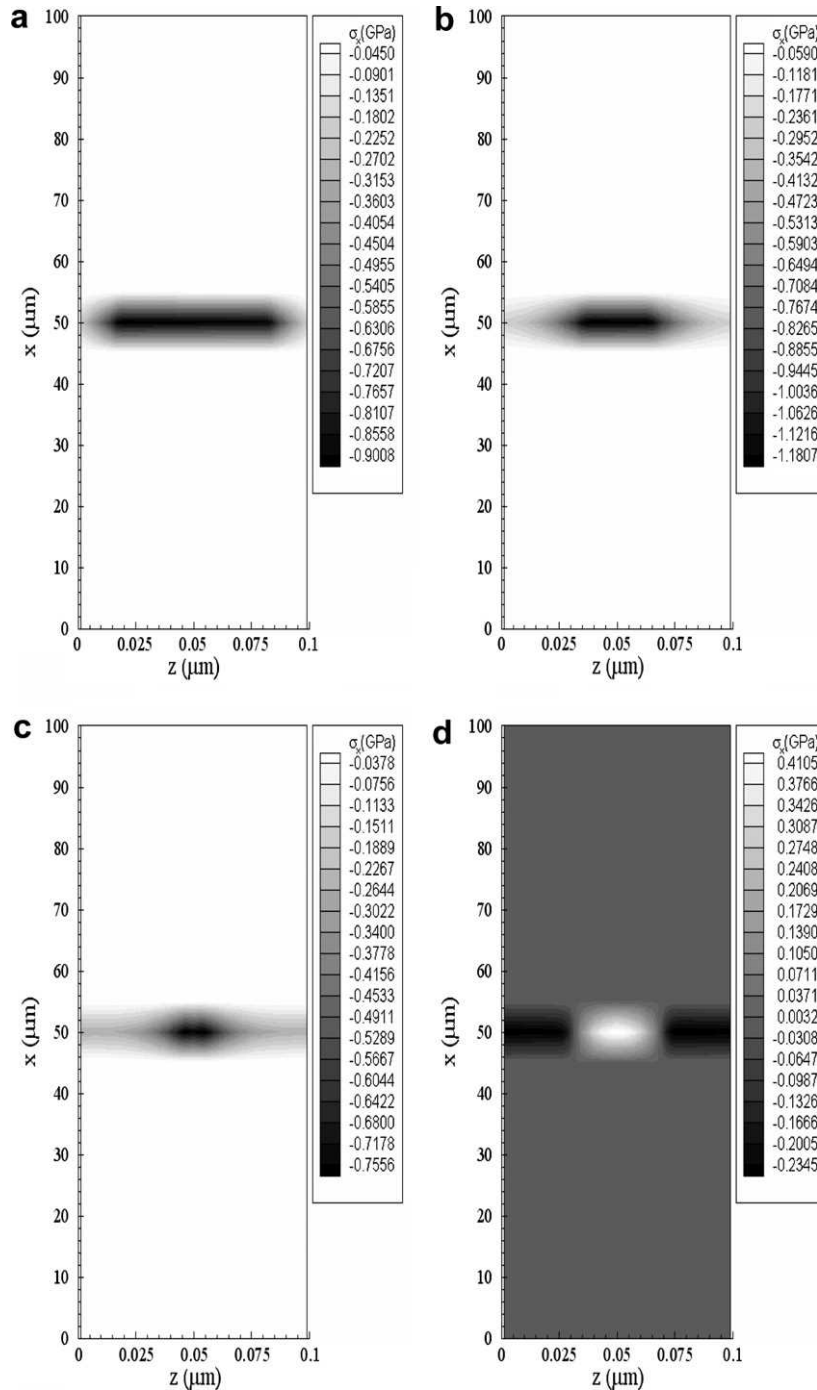


Fig. 12. Contours of normal stress ( $\sigma_x$ ) profiles in the cross-section of  $y = 50 \mu\text{m}$  at different times: (a)  $t = 5$  ps, (b)  $t = 10$  ps, (c)  $t = 15$  ps, and (d)  $t = 20$  ps with a mesh of  $20 \times 20 \times 80$  and laser fluence  $J$  of  $500 \text{ J/m}^2$ .

be 300 K. Two different values of laser fluences ( $J = 500 \text{ J/m}^2$ ,  $2000 \text{ J/m}^2$ ) were chosen to study the hot electron-blast force. The convergence criteria were chosen to be  $\epsilon_1 = 10^{-8}$  for temperature and  $\epsilon_2 = 10^{-16}$  for deformation.

We assumed that the laser was focused on the center of the film surface. Fig. 3a shows the change in electron temperature ( $\Delta T_e/(\Delta T_e)_{\max}$ ) at the center ( $x_{\text{center}} = 50 \mu\text{m}$ ,  $y_{\text{center}} = 50 \mu\text{m}$  and  $z = 0 \mu\text{m}$ ) with laser fluences  $J = 500 \text{ J/m}^2$ . The maximum temperature rise of  $T_e$  (i.e.,

$(\Delta T_e)_{\max}$ ) is about 3763 K, which is close to that obtained in [34]. Fig. 3b shows the displacement ( $w$ ) at the center ( $x_{\text{center}}, y_{\text{center}}, z$ ) versus time. It can be seen from both figures that mesh size had no significant effect on the solution and hence the solution is convergent.

Figs. 4 and 5 show electron temperature and lattice temperature along  $z$  at ( $x_{\text{center}}, y_{\text{center}}$ ) with two different laser fluences ( $J = 500 \text{ J/m}^2$  and  $2000 \text{ J/m}^2$ ) at different times (a)  $t = 0.25 \text{ ps}$ , (b)  $t = 0.5 \text{ ps}$ , (c)  $t = 1 \text{ ps}$ , (d)  $t = 10 \text{ ps}$ ,

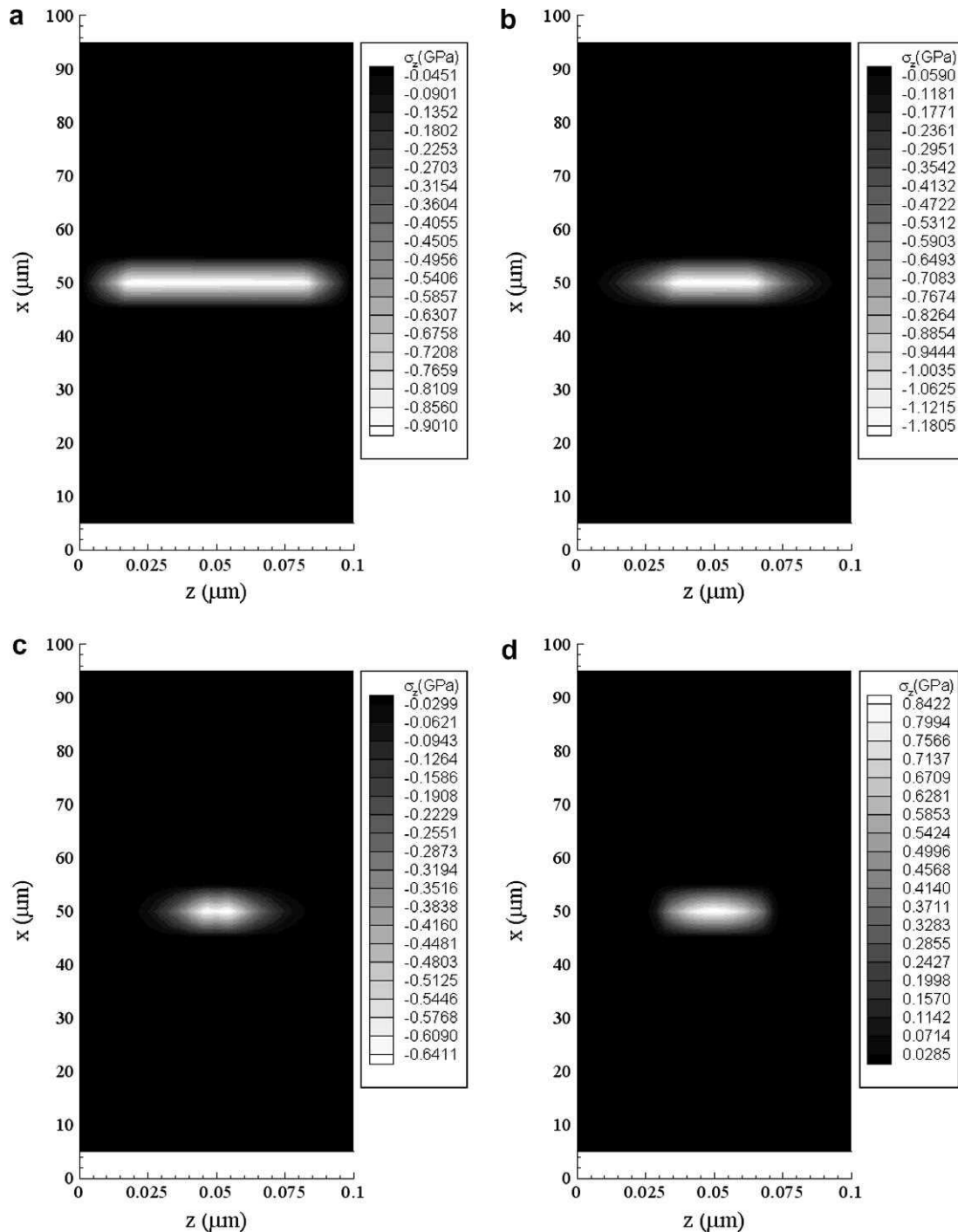


Fig. 13. Contours of normal stress ( $\sigma_z$ ) profiles in the cross-section of  $y = 50 \mu\text{m}$  at different times: (a)  $t = 5 \text{ ps}$ , (b)  $t = 10 \text{ ps}$ , (c)  $t = 15 \text{ ps}$ , and (d)  $t = 20 \text{ ps}$  with a mesh of  $20 \times 20 \times 80$  and laser fluence  $J$  of  $500 \text{ J/m}^2$ .

and (e)  $t = 20$  ps, respectively. It can be seen that the electron temperature rises to its maximum at the beginning and then decreases while the lattice temperature rises gradually with time.

Fig. 6 shows normal stress  $\sigma_z$  along  $z$  at  $(x_{\text{center}}, y_{\text{center}})$  at different times (a)  $t = 5$  ps, (b)  $t = 10$  ps, (c)  $t = 15$  ps, (d)  $t = 17$  ps and (e)  $t = 20$  ps with a mesh of  $20 \times 20 \times 80$  and two different laser fluences ( $J = 500 \text{ J/m}^2$  and  $2000 \text{ J/m}^2$ ). Usually, numerical oscillations appear near

the peak of the curve, as shown in Fig. 5 [27]. It can be seen from Fig. 6 (particularly, Fig. 6d–e) that the normal stress  $\sigma_z$  does not show non-physical oscillations near the peak of the curve.

Figs. 7–14 were plotted based on the results obtained in a mesh of  $20 \times 20 \times 80$  with a laser fluence of  $J = 500 \text{ J/m}^2$ . Figs. 7 and 8 show contours of electron temperature profile and lattice temperature profile in the cross-section of  $y = y_{\text{center}}$  at different times (a)  $t = 0.25$  ps,

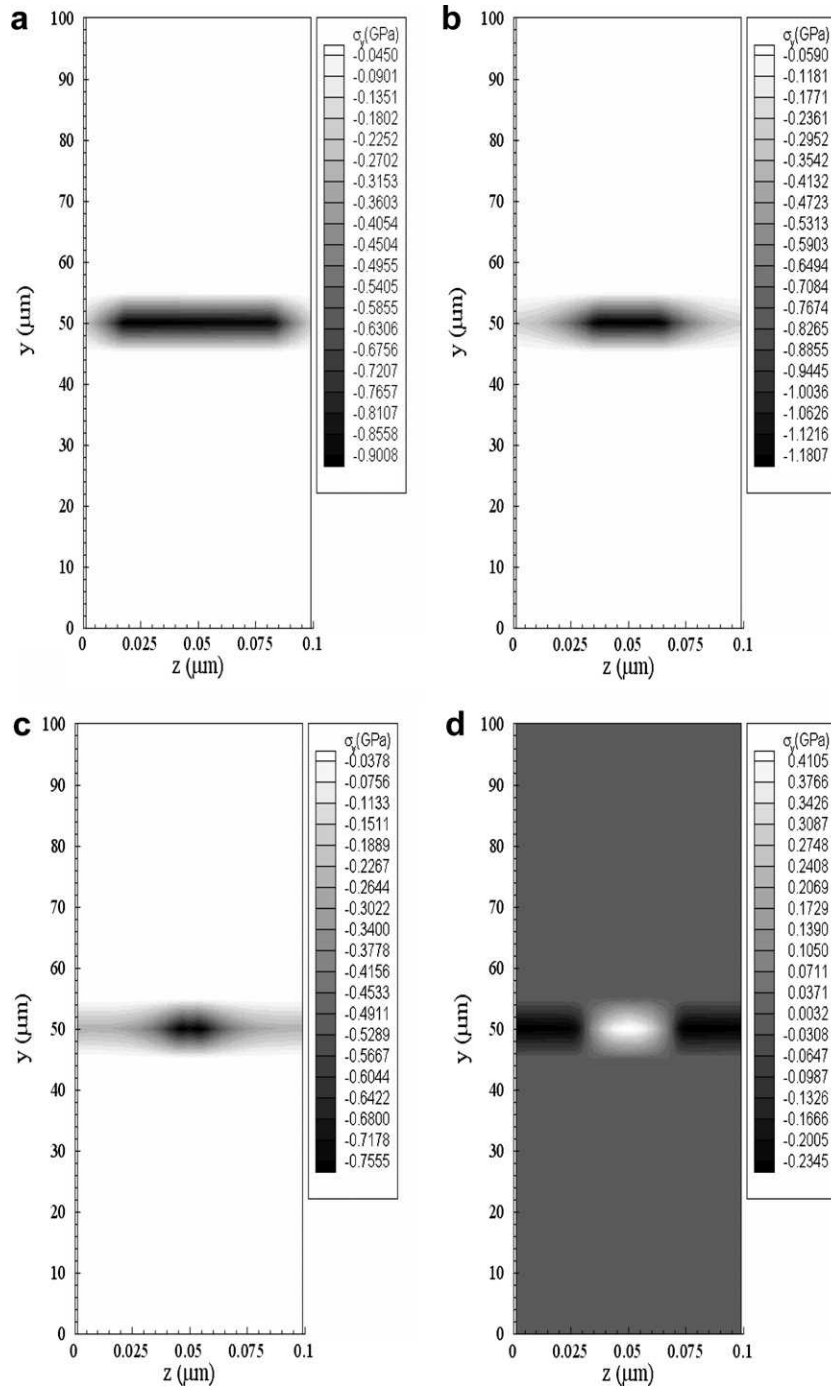


Fig. 14. Contours of normal stress ( $\sigma_y$ ) profiles in the cross-section of  $x = 50 \mu\text{m}$  at different times: (a)  $t = 5$  ps, (b)  $t = 10$  ps, (c)  $t = 15$  ps, and (d)  $t = 20$  ps with a mesh of  $20 \times 20 \times 80$  and laser fluence  $J$  of  $500 \text{ J/m}^2$ .



(b)  $t = 0.5$  ps, (c)  $t = 1$  ps, (d)  $t = 10$  ps, and (e)  $t = 20$  ps, respectively. It can be seen from both figures that the heat is mainly transferred along the  $z$  direction. This result illustrates the fact that the femtosecond lasers are an ideal candidate for precise thermal processing of functional nanophase materials. Figs. 9–14 show contours of displacements ( $u, v, w$ ) and normal stresses ( $\sigma_x, \sigma_y, \sigma_z$ ) in the cross-section of  $y = y_{\text{center}}$  at different times (a)  $t = 5$  ps, (b)  $t = 10$  ps, (c)  $t = 15$  ps, and (d)  $t = 20$  ps, respectively. It can be seen from Figs. 9–11 that the central part of the film is expanding because displacement changes from negative to positive along the center line in the  $z$  direction, and along  $x$  and  $y$  directions, respectively. Similar stress alterations are observed from Figs. 12–14.

## 5. Conclusion

We have developed a finite difference method for studying thermal deformation in a 3D thin film exposed to ultrashort pulsed lasers. The method, based on the parabolic two-step heat transport equations, accounts for the coupling effect between lattice temperature and strain rate, as well as for the hot electron-blast effect in momentum transfer. By replacing the displacement components in the dynamic equations of motion using the velocity components, developing a fourth-order compact method for evaluating stress derivatives in the dynamic equations of motion, and employing a staggered grid, we have developed a numerical method that allows us to avoid non-physical oscillations in the solution. Numerical results show the displacement and stress alterations at the center along the  $z$  direction, and along  $x$  and  $y$  directions, which reveal that the central part of thin film expands. Further research will focus on 3D double-layered cases where the interface could be either perfect thermal contact or imperfect thermal contact.

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