Phase transition induced by CW-laser in a finite silver selenide (Ag$_2$Se) according to (HHCE) model

M K El-Adawi$^1$ and S A Shalaby

Physics Department, Faculty of Education, Ain Shams University, Cairo, Egypt

$^1$Corresponding author, Email: adawish1@hotmail.com

Abstract. Thermal effects induced in a finite silver selenide slab by CW laser source are studied. The hyperbolic heat conduction equation (HHCE) in dimensionless form is solved using Laplace integral transform technique. Different laser power densities are considered. Expression for the temperature field within the target is obtained. As an illustrative example, the critical time required to initiate phase transition and that required to initiate melting are computed for different pulses.

1. Introduction

Heating sources of high power densities such as lasers have found numerous applications related to material processing techniques, such as spot wilding, laser cutting, drilling of metals [1, 2, 3]. Laser sources are also used in medicine [4]. In semiconductor industry many other applications are developed including industry both local diffusions and alloying to form p – n junctions. The most spectacular effects include a change of phase of the absorbing materials [5, 6]. Laser heating has always stimulated the interest of increasing number of investigators [7–13]. In many applications it is particularly important to find the temperature field inside an impacted medium. Moreover, it is useful to determine the critical time required to initiate phase transition in the heated target. The determination of the critical time required to initiate melting is also very important especially in studying the two phase heating problems. For such cases it may be necessary to find the rate of melting, the thickness of the molten layer and their functional dependence on the laser exposure time. The present trial is devoted to study analytically the problem of laser heating a finite homogeneous silver selenide (Ag$_2$Se) slab. The hyperbolic heat conduction equation (HHCE) is solved. According to such a model, heat propagates in the medium with a finite velocity. The chosen target is of great importance as a thermoelectric power generator material. It has also applications in the field of switching devices.

It is worth to note that the considered material (Ag$_2$Se) undergoes a polymorphic phase transition at (403 ± 2)$^\circ$K. It has two phases one below 400$^\circ$K and is identified as $\beta$ - Ag$_2$Se phase with orthorhombic structure and acts as a semiconducting materials, while, the other phase is at higher temperature and is called $\alpha$ - Ag$_2$Se phase with body – centered – cubic (bcc) form, and it has metallic nature.

Equations in dimensionless scales are solved using Laplace integral transform technique. Computations with different CW – fluxes having different power densities and different effective exposure intervals are considered.

2. Analysis

A finite homogenous slab of silver selenide (Ag$_2$Se) of thickness "d", m initially at equilibrium temperature $\theta = (T – T_0) = 0$, is heated by CW laser, where, $T_0$ is the ambient temperature and $\theta$, is the excess temperature relative to the ambient temperature. The thermal and the optical properties of the
material are assumed to be temperature independent. The slab is insulated at the rear surface. The laser CW flux is incident perpendicularly to the front surface. It is assumed that heat losses due to convection and radiation are neglected. The heat flow is considered to be one dimensional. The x-axis normal to the free surface of the slab is taken in the direction of the incident laser flux.

In setting the problem it is assumed that a part of the incident energy is reflected at the front surface and a part is absorbed by the target material. According to the considered model a thermal relaxation time \( t_k \) is assumed. The governing equations can be written as follows:

The modified Fourier equation (Cattaneo equation) is considered in the form:

\[
t_k \frac{\partial q(x,t)}{\partial t} + q(x,t) = -\lambda \nabla T(x,t)
\]

where,

\[
t_k = \frac{\alpha}{W^2}
\]

is the thermal relaxation time. \( \alpha = \frac{\lambda}{\rho c_p} \) is the thermal diffusivity in terms of: the thermal conductivity \( \lambda \), the density \( \rho \), the specific heat \( c_p \) and the speed of the propagation of the thermal wave in the medium \( W \). Equation (1) with the following conservation energy equation:

\[
- \nabla \cdot q = \rho c_p \frac{\partial T}{\partial t}
\]

leads to the hyperbolic conduction equation (HHCE) in the form:

\[
t_k \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \nabla^2 T.
\]

Considering the following dimensionless scales:

\[
X = \frac{Wx}{2\alpha},
\]

\[
Y = \frac{Wy}{2\alpha},
\]

\[
Z = \frac{Wz}{2\alpha},
\]

\[
\theta = \frac{T - T_0}{T_m - T_0},
\]

\[
\phi = \frac{q}{W \rho c_p (T_m - T_0)},
\]

where \( T_m \) is the melting temperature and \( R \) is the reflectivity at the front surface.

Let \( q_0 \) be the considered CW laser source at the front surface, taken in the form of a step function [14]. One obtains Cattaneo equation in dimensionless form as:

\[
\frac{\partial \phi}{\partial \tau} + 2\phi = -\nabla \theta, \quad \tau = \frac{t}{2t_k}
\]

The energy conservation equation in the dimensionless scale attains the form:

\[
\frac{\partial \theta}{\partial \tau} = -\nabla \phi
\]

And the hyperbolic heat conduction equation (HHCE) in dimensionless form is:
\[
\frac{\partial^2 \theta}{\partial \tau^2} + 2 \frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial X^2} \tag{12}
\]

Equation (12) is subjected to the following dimensionless initial and boundary conditions:

At \( \tau = 0 \rightarrow \) \( \theta(X,0) = 0 \) \hspace{1cm} \tag{13}

At \( X = X_d \rightarrow \) \( \frac{\partial \theta}{\partial X}(X_d,\tau) = 0 \) \hspace{1cm} \tag{14}

At \( X = 0 \rightarrow \) \( \left. \frac{\partial \theta}{\partial X} \right|_{X=0} = -2\phi_0 \) \hspace{1cm} \tag{15}

Equation (14) indicates that the rear surface of the target is thermally insulated. Laplace integral transform technique is applied to solve equation (12). Taking Laplace transform on equation (12) w.r.t. the time \( \tau \) one gets:

\[
\frac{\partial^2}{\partial X^2} \bar{\theta}(X,s) - (s^2 + 2s)\bar{\theta}(X,s) = 0 \tag{16}
\]

The solution of equation (16) is as follows :

\[
\bar{\theta}(X,s) = Ae^{\sqrt{s(s+2)}X} + Be^{-\sqrt{s(s+2)}X} \tag{17}
\]

At \( X = 0 \) one gets:

\[
\left. \frac{\partial \theta}{\partial X} \right|_{X=0} = A\sqrt{s(s+2)} - B\sqrt{s(s+2)} \tag{18}
\]

At \( X = X_d \) one gets :

\[
Ae^{\sqrt{s(s+2)}X_d} - Be^{-\sqrt{s(s+2)}X_d} = 0 \tag{19}
\]

Taking Laplace transform to the boundary condition equation (15) with respect to time at \( X = 0 \) one gets:

\[
\left. \frac{\partial \bar{\theta}(0,s)}{\partial X} \right|_{X=0} = -\frac{2\phi_0}{s} \tag{20}
\]

\[
\phi_0 = \frac{q_0(1-R)}{Wp \rho c_p(T_m - T_0)} \tag{21}
\]

Moreover, comparing equations (18) and (20) one gets at \( X = 0 \) the relation :

\[
(A - B) = -\frac{2\phi_0}{s\sqrt{s(s+2)}} \tag{22}
\]

To get \( A \) and \( B \), one has to solve equations (19) and (22) simultaneously.

This gives:
\[
B = \frac{2\phi_0 e^{\frac{\sqrt{s(s+2)} X_d}}}{2s\sqrt{s(s+2)} \sinh \sqrt{s(s+2)} X_d}
\] (23)

\[
A = \frac{+2\phi_0 e^{-\frac{\sqrt{s(s+2)} X_d}}}{2s\sqrt{s(s+2)} \sinh \sqrt{s(s+2)} X_d}
\] (24)

Substituting for A and B in equation (17) one gets:

\[
\bar{\theta}(X, s) = \frac{2\phi_0}{s\sqrt{s(s+2)}} \left\{ e^{\frac{\sqrt{s(s+2)} (X_d - X)}{s}} + e^{-\frac{\sqrt{s(s+2)} (X_d - X)}{s}} \right\}
\] (25)

\[
\bar{\theta}(X, s) = \frac{2\phi_0}{s\sqrt{s(s+2)}} \left[ e^{\sqrt{s(s+2)} X_d} - e^{-\sqrt{s(s+2)} X_d} \right]
\] (26)

Considering
\[
\frac{1}{1-a} = \sum_{n=0}^{\infty} a^n, \quad |a| < 1 \quad [14]
\] (27)

Thus
\[
\frac{1}{1-e^{2\sqrt{s(s+2)} X_d}} = \sum_{n=0}^{\infty} e^{-2n\sqrt{s(s+2)} X_d}
\] (28)

This is makes it possible to get the solution in the form:

\[
\bar{\theta}(X, s) = \sum_{n=0}^{\infty} \frac{2\phi_0 e^{-\frac{\sqrt{s(s+2)} (2n X_d + X)}}}{s\sqrt{s(s+2)}}
\] (29)

This equation can be rewritten as:

\[
\bar{\theta}(X, s) = \sum_{n=0}^{\infty} \left[ 2\phi_0 \cdot f_n(s) \right]
\] (30)

where,

\[
f_n(s) = \frac{e^{-\sqrt{s(s+2)} (2n X_d + X)}}{\sqrt{s(s+2)}}
\] (31)

Considering the standard inverse Laplace's transform tables, the solution can be obtained in the form [16, 17, 18, and 19]:

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Substituting for \(A\) and \(B\) in equation (17) one gets:

\[
\bar{\theta}(X, s) = \frac{2\phi_0}{s\sqrt{s(s+2)}} \left\{ e^{\frac{\sqrt{s(s+2)} (X_d - X)}{s}} + e^{-\frac{\sqrt{s(s+2)} (X_d - X)}{s}} \right\}
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\bar{\theta}(X, s) = \frac{2\phi_0}{s\sqrt{s(s+2)}} \left[ e^{\sqrt{s(s+2)} X_d} - e^{-\sqrt{s(s+2)} X_d} \right]
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\] (31)

Considering the standard inverse Laplace's transform tables, the solution can be obtained in the form [16, 17, 18, and 19]:

---
\[ \theta(X, \tau) = 2 \phi_0 \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \int_{0}^{\infty} e^{-\tau} \left[ \frac{(X + 2nX_d)^2}{2^{2m}} \right] \ d\tau \]  

(32)

It is better for practical considerations to get a simple form of expression (32). For this reason we consider the case for \( m = 1 \) and \( n = 1 \), this gives:

\[ \theta(X, \tau) = 2\phi_0 \int_{0}^{\tau} e^{-\tau} \left[ \frac{W}{2\alpha} \right] \left( x + 2nx_d \right)^2 \cdot d\tau \]  

(33)

Performing integrations in equation (33) and considering the case for which \( x=0 \) (i.e. at the front surface) one gets:

\[ \theta(0, \tau) = \frac{2\phi_0}{4} \left[ 2 - e^{-\tau^2} \right] \]  

\[ + \left( \frac{W}{2\alpha} \right)^2 \left( 4x_d^2 \right) \left( e^{-\tau} - 1 \right) \]  

(34)

3. Computations

As an illustrative example, the function \( \theta(0, t) \) (Eq. 34) is computed for silver selenide (Ag\(_2\)Se) slab for \( m = 1 \) and \( n = 1 \). Different thicknesses are considered:

\( x_d = 0.10, 0.25, 0.30 \) and \( 0.40 \) \( \mu \)m .

Different CW laser power densities are also considered:

\( q_0 = 10^9, \ 2 \times 10^9 \) and \( 2.05 \times 10^9 \frac{W}{m^2} \)

\( \phi_0 \), is computed according to eq. (21).

For the considered case \([20, 21]\):

- \( \rho = 8200 \text{ kg/m}^3 \), \( \lambda = 1.08 \text{ W/m.K} \)
- \( \alpha = 3.9 \times 10^{-7} \text{ m}^2/\text{sec.} \)
- \( c_p = 277 \text{ J/kg.K} \),
- \( T_m = 855^\circ \text{K}, \ T_{ph} = 403 \pm 2 \text{ K} \), \([22]\).

The obtained results are given in table (1).
Table (1): The temperature of the front surface of the target as a function of exposure time and the thickness for different CW laser power densities.

| q, W/m² | 1E9 θ(0,t), K | 1E9 θ(0,t), K | 1E9 θ(0,t), K |
|---------|----------------|----------------|----------------|
| x, μm   | 0.10           | 0.25           | 0.30           |
| t, us   |                |                |                |
| 2       | 34.11          | 14.04          | 3.53           |
| 4       | 147.48         | 120.04         | 105.66         |
| 5       | 209.96         | 180.77         | 165.52         |
| 6       | 266.69         | 236.53         | 220.73         |
| 8       | 353.91         | 322.76         | 306.44         |
| 9.9     | 405.45         |                |                |
| 10      | 407.42         | 376.03         | 359.39         |
| 12      | 430.97         | 405.34         | 388.76         |
| 14      | 452.27         | 420.56         | 403.90         |
| 16      | 459.77         | 428.04         | 411.42         |
| 18      |                |                | 414.9          |
| 20      | 464.95         | 433.26         |                |

| q, W/m² | 2E9 θ(0,t), K | 2E9 θ(0,t), K | 2E9 θ(0,t), K |
|---------|---------------|---------------|---------------|
| x, μm   | 0.10          | 0.25          | 0.30          |
| t, us   |               |               |               |
| 2       | 68.21         | 28.09         | 7.07          |
| 4       | 294.96        | 240.07        | 211.32        |
| 5       | 419.93        | 361.55        | 331.03        |
| 5.38    |               | 405.57        |               |
| 5.65    |               | 404.40        |               |
| 6       | 533.37        | 473.03        | 441.46        |
| 8       | 707.83        | 645.51        | 612.87        |
| 10      | 814.85        | 752.06        | 718.78        |
| 12      | 861.94        | 810.70        | 777.52        |
| 14      | 904.53        | 841.11        | 807.89        |
| 16      | 919.54        | 856.08        | 822.84        |
| 18      |               | 829.92        |               |
| 20      | 929.9         | 866.52        | 833.18        |

| q, W/m² | 2.05E9 θ(0,t), K | 2.05E9 θ(0,t), K | 2.05E9 θ(0,t), K |
|---------|------------------|------------------|------------------|
| x, μm   | 0.10             | 0.25             | 0.30             |
| t, us   |                  |                  |                  |
| 2       | 69.92            | 28.79            | 7.24             |
| 4       | 302.34           | 246.08           | 216.61           |
| 5       | 430.32           | 370.60           | 339.31           |
| 5.27    |                  | 402.84           |                  |
| 5.30    |                  | 406.37           |                  |
| 6       | 546.71           | 484.88           | 452.49           |
| 8       | 725.52           | 661.65           | 628.19           |
| 10      | 835.23           | 707.86           | 736.75           |
| 12      | 883.49           | 830.96           | 796.96           |
| 13.45   | 855.60           |                  |                  |
| 13.70   | 858.73           |                  |                  |
| 14      | 927.15           | 862.14           | 828.09           |
| 16      | 942.52           | 877.48           | 843.41           |
| 18      |                  | 850.66           |                  |
| 20      | 953.17           | 888.18           | 854.00           |

The dependence of the time required to initiate phase transition \( t_{ph} \) on the thickness of the targets at laser power densities \( q_0 = (1.2, 2.05) \times 10^9 W/m^2 \) as examples are given in table (2).
Table (2): The time required to initiate phase transition "\( t_{ph} \)" as a function of the laser power density \( q_0 \), W / m\(^2\) and the thickness of the irradiated target.

| \( X_d \), \( \mu \text{m} \) | \( q_0 = 10^9 \text{ W} / \text{m}^2 \) | \( q_0 = 2 \times 10^9 \text{ W} / \text{m}^2 \) | \( q_0 = 2.05 \times 10^9 \text{ W} / \text{m}^2 \) |
|-----------------|-----------------|-----------------|-----------------|
|                 | \( t_{ph} \), \( \mu \text{s} \) | \( t_{ph} \), \( \mu \text{s} \) | \( t_{ph} \), \( \mu \text{s} \) |
| 0.10            | 9.9             | 4.87            | 4.78            |
| 0.25            | 12.0            | 5.38            | 5.27            |
| 0.30            | 14.0            | 5.65            | 5.55            |
| 0.40            | --              | 6.45            | 6.33            |

From table (2) it is revealed to have nonlinear dependence between the thickness and "\( t_{ph} \)" (figure 1).

Figure 1. The dependence of the time required to initiate phase transition "\( t_{ph} \)" on the thickness of the targets at laser power densities \( q_0 = (1,2,2.05) \times 10^9 \text{ W} / \text{m}^2 \)

Moreover, the dependence of the time required to initiate melting "\( t_{m} \)" on the thickness of the targets at laser power density \( q_0 = (2.05) \times 10^9 \text{ W} / \text{m}^2 \) as an example is given in table (3) and illustrated graphically in (figure 2).

Table (3). The time required to initiate melting "\( t_{m} \)" as a function of the thickness of the irradiated target for \( q_0 = 2.05 \times 10^9 \text{ W} / \text{m}^2 \).

| \( X_d \), \( \mu \text{m} \) | \( t_{m} \), \( \mu \text{s} \) |
|-----------------|-----------------|
| 0.10            | 10.5            |
| 0.25            | 13.45           |
| 0.30            | 20              |
It is revealed to have also nonlinear dependence between the thickness and "t_m" for certain laser irradiance.

\[ q_0 = 2.05 \times 10^9 \text{ W/m}^2 \]

Figure 2: The dependence of the time required to initiate melting "t_m" on the thickness of the targets

4. Discussion
The general expressions for \( \Theta(X, \tau) \) equation (32) and that for special case \( m = 1 \) and \( n = 1 \), equation (33) reveal the linear dependence on the laser power density \( q_0 \text{ W/m}^2 \). Moreover, in order to get positive values of \( \theta(0, t) \) according to equation (34), the following condition must be fulfilled:

\[
\left\{ 2 - e^{-\tau} (\tau^2 + 2\tau + 2) \right\} > \left\{ \frac{W}{2\alpha} \right\}^2 \left( 4x_d^2(1 - e^{-\tau}) \right)
\]

Computations reveal also that as \( \tau \to \infty \) the function \( \theta(0, \tau) \) attains asymptotic behavior. The value of such temperature may be less than either of \( t_{ph} \) or \( t_m \). Computations reveal also that such asymptotic time increases with the thickness of the target while it attains lower values as the laser power density of the laser source increases.

5. Conclusions
As a result of the present study, the following conclusions are clarified:

1. The temperature of the irradiated target does depend linearly on the laser power density \( q_0 \text{ W/m}^2 \) of the source.
2. The dependence of both \( t_{ph} \) or \( t_m \) on the thickness of the target is not linear.
3. A particular value of laser source \( q_0 \text{ W/m}^2 \) is required to initiate both phase transition and melting for a certain thickness of the considered target.

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