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Two-phase isochoric Stefan problem for ultrafast processes

P.A. Krasnova [a,*], P.R. Levashov [a,b]

[a] Joint Institute for High Temperatures RAS, Izhorskaya 13 Bldg. 2, Moscow 125412, Russia
[b] Tomsk State University, 36 Lenin Prospekt, Tomsk 634050, Russia

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ABSTRACT

We establish a modification of the one-dimensional two-phase Stefan problem which is promising for the investigation of ultrafast processes in solids lasting less than the time of electron–phonon relaxation. Under such conditions the heat equations should be solved separately for ions and electrons at constant volume. We discuss the system of equations and boundary conditions for this special case and derive the computational scheme for the numerical solution. To demonstrate our new approach we calculate the electronic and ionic temperatures in an aluminum target subjected to a femtosecond laser pulse.

1. Introduction

A classical Stefan problem naturally appears in slow processes with phase transitions [1]. Indeed, Stefan himself considered the problem of ice formation in the polar seas; he found an approximate solution of the heat conductivity equation with constant coefficients: the thickness of ice layer was proportional to the square root of time passed. Further improvement of the model resulted in the so-called one-phase Stefan problem: the heat conductivity equation is solved only in one domain, the left boundary is at given temperature function, the domain and its right boundary is at phase transition temperature. A special Stefan condition is set at the right boundary: the heat flux through this boundary causes the growth of the new phase. The solution of the one-phase Stefan problem was found by Stefan at constant temperature at the left boundary. Again, the thickness of the new phase was proportional to the square root of the time passed; the temperature distribution was given by the error function [2].

Analytical solutions for the Neumann condition at the left boundary are found only for some special cases, for example, for the exponentially decaying with time [3,5] or power function of time [6] boundary heat flux. Consideration of the heat propagation in two phases separated by the moving boundary with the Stefan condition defined on it identifies the two-phase Stefan problem.

The one- and two-phase Stefan problems are examples of the so-called moving boundary problems (MBP): the boundary condition is set at the surface which position is defined by the solution of the problem. MBPs occurs in many areas of practical interest from material science to geophysics and plasma physics [7]. In particular, the melting and ablation processes under the laser heating can be considered as MBPs [8–10].

The non-linear Stefan problem (for example, if heat capacity or heat conductivity coefficients are temperature-dependent) can be treated analytically in some special cases [11,12], but is usually solved numerically; the overview of different approaches can be found in the book [4].

In some cases it is of importance to take into account the finite speed of heat propagation in matter, for example, in dielectric solids or other media with low value of the so-called second sound [13]. This leads to the introduction of the hyperbolic term into the heat equation and modification of the Fourier law; the corresponding statements of the Stefan problem have been considered in [14,15]. It is worth noting, however, that the hyperbolic heat equation is not compatible with the second law of thermodynamics because of the introduction of a new term into the definition of the heat flux [16].

The Stefan condition is simply a particular case of energy conservation [17]; both phases are incompressible and non-moving. However, in slow processes at constant pressure there can be a considerable density change in a phase transition; this effect was taken into account by some investigators [4]. On the other hand, the appearance of ultrafast femtosecond lasers made it possible to study very fast processes in which the change of density is negligible because the average displacement of atoms is insignificant during the time of experiment [18–22]. So it is of interest to consider the case of ultrafast isochoric heating with a phase transition (melting) and establish the corresponding Stefan problem. The

* Corresponding author. Tel.: +7 495 4842456.
E-mail address: pakrasnova@gmail.com (P.A. Krasnova).

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main idea of this paper is to formulate the modified two-phase Stefan problem and to study the peculiarities of a numerical solution to this problem by example of aluminum with a realistic equation of state. In particular, we consider the distribution of electron and ion temperatures as well as the time dependence of the position of the phase boundary between the liquid and solid phases.

2. Model

The classical 1D two-phase Stefan problem [4] considers the heat propagation in the domain $0 \leqslant x \leqslant H$ in which the phase transition of the first order takes place and the boundary between two phases propagates from $x = 0$ to H (Fig. 1). The defining equation system for the 1D case includes thermal conductivity equations for two phases: liquid (with label l) and solid (with label s):

$$\rho c_l \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_l \frac{\partial T}{\partial x}\right), \quad 0 \leqslant x < x_m; \tag{1}$$

$$\rho c_s \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_s \frac{\partial T}{\partial x}\right), \quad x_m < x \leqslant H; \tag{2}$$

boundary conditions:

$$-\kappa_l \left.\frac{\partial T}{\partial x}\right|_{x=0} = q_0(t); \tag{3}$$

$$-\kappa_s \left.\frac{\partial T}{\partial x}\right|_{x=H} = q_H(t); \tag{4}$$

Stefan conditions:

$$T(x_m(t), t) = T_m = const; \tag{5}$$

$$\alpha\rho \frac{dx_m}{dt} = \kappa_l \left.\frac{\partial T}{\partial x}\right|_{x=x_m-0} - \kappa_s \left.\frac{\partial T}{\partial x}\right|_{x=x_m+0}; \tag{6}$$

and initial conditions:

$$x_m(0) = 0; \tag{7}$$

$$T(x, 0) = \omega(x). \tag{8}$$

Here $T(x,t)$ is the function of the one-dimensional temperature distribution; ρ—the density, κ_l, c_l and κ_s, c_s are the thermal conductivity and specific heat capacity coefficients for the liquid and solid phase, respectively. The function $x_m = x_m(t)$ indicates the point dividing the solid and liquid parts of the domain; q_0 and q_H are the heat fluxes at the boundaries; T_m—the melting temperature; α—the specific melting energy; $\omega(x)$—the initial temperature distribution.

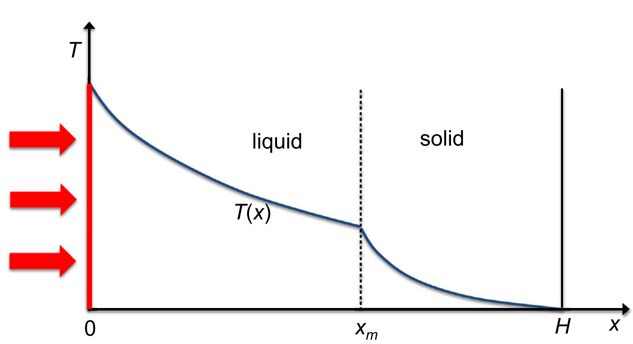

Fig. 1. Distribution of temperature in a target subjected to heating.

The evolution of a target heating by a femtosecond laser pulse can be considered in the classical 1D two-temperature form when the material motion is ignored [18]:

$$\frac{\partial(\rho E_e)}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_e \frac{\partial T_e}{\partial x}\right) - G_{ei}(T_e - T_i), \tag{9}$$

$$\frac{\partial(\rho E_i)}{\partial t} = G_{ei}(T_e - T_i), \quad 0 \leqslant x \leqslant H. \tag{10}$$

Here E_e and E_i are the specific energies of electrons and ions, respectively, κ_e is the electron thermal conductivity, T_e and T_i are the temperatures of electrons and ions, respectively; G_{ei} is the electron–phonon energy exchange coefficient. In this model the heat conductivity of ions is neglected in comparison with the electronic one; ions are heated by the energy exchange with electrons. This leads to the delay between the electronic temperature gradient which is created by the laser radiation absorption, and the ionic heat flux, which is responsible for the heating of matter. The temperatures of ions and electrons equalizes during the relaxation time, so this lag tends to zero. This is to some extent similar to the solution of the hyperbolic heat equation in which there is always the delay between the heat flux and the temperature gradient [13]. However, the description of heat propagation in ions by a hyperbolic heat equation is physically incomplete as the heat in metals is conducted by electrons. Therefore the velocity of speed distribution in the target is very high and this process for electrons is adequately described by the parabolic heat equation. The laser radiation is absorbed by electrons, so the heat flux at $x = 0$ is introduced for electrons as a boundary condition (see Fig. 1); for ions the heat flux at the domain boundaries is 0. This approach is valid for low and moderate ultrashort laser intensities $I_L \lesssim 10^{13}$ W/cm^2.

Combining the Stefan problem (1)–(8) and the two-temperature model (9), (10) we have to write out the thermal conductivity equations for the electronic and ionic subsystems regarding the discontinuity of the parameters at x_m:

$$\kappa_e = \begin{cases} \kappa_{el}, & 0 \leqslant x < x_m, \\ \kappa_{es}, & x_m < x \leqslant H; \end{cases}$$

$$c_e = \begin{cases} c_{el}, & 0 \leqslant x < x_m, \\ c_{es}, & x_m < x \leqslant H; \end{cases}$$

$$c_i = \begin{cases} c_{il}, & 0 \leqslant x < x_m, \\ c_{is}, & x_m < x \leqslant H. \end{cases}$$

The thermal conductivity equation and the boundary conditions for the ions will be stated similar to the Stefan problem (1)–(8) because the melting process is governed by the behavior of the ionic subsystem. Electron (ion) thermal capacities of solid c_{es} (c_{is}) and liquid c_{el} (c_{il}) states are known from an equation of state. As a result of these assumptions we obtain the following set of equations:

$$\rho c_{il} \frac{\partial T_i}{\partial t} = G_{ei}(T_e - T_i), \quad 0 \leqslant x < x_m; \tag{11}$$

$$\rho c_{is} \frac{\partial T_i}{\partial t} = G_{ei}(T_e - T_i), \quad x_m < x \leqslant H; \tag{12}$$

$$\rho c_{el} \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_{el} \frac{\partial T_e}{\partial x}\right) - G_{ei}(T_e - T_i), \quad 0 \leqslant x < x_m; \tag{13}$$

$$\rho c_{es} \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_{es} \frac{\partial T_e}{\partial x}\right) - G_{ei}(T_e - T_i), \quad x_m < x \leqslant H \tag{14}$$

with boundary conditions: