Optimal control of laser hardening

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Abstract

We present a mathematical model for the laser surface hardening of steel. It consists of a nonlinear heat equation coupled with a system of five ordinary differential equations to describe the volume fractions of the occuring phases.

Existence, regularity and stability results are discussed.

Since the resulting hardness can be estimated by the volume fraction of martensite, we formulate the problem of surface hardening in terms of an optimal control problem. To avoid surface melting, which would decrease the workpiece's quality, state constraints for the temperature are included.

We prove differentiability of the solution operator and derive necessary conditions for optimality.

1 Introduction

In this paper we present a mathematical model for the laser surface hardening of steel. In this process a laser beam moves along the surface of a workpiece (cf. fig. 1). The laser radiation is absorbed by the workpiece, leading to a rapid heating of its boundary layers. Then, the workpiece is quenched by 'self–cooling' of the workpiece, which is accompanied by a growth of the surface hardness. To increase the scanning width, the laser beam performs an additional oscillating movement orthogonal to the principle moving direction. Compared to other surface heat treatment procedures, like induction hardening, laser hardening has the advantage that it can be applied to workpieces with very complicated geometries or to harden curved edges.

The reason for the possibility to change the hardness of steel by thermal treatment originates from the occuring phase transitions, depicted in figure 2. At room temperature, in

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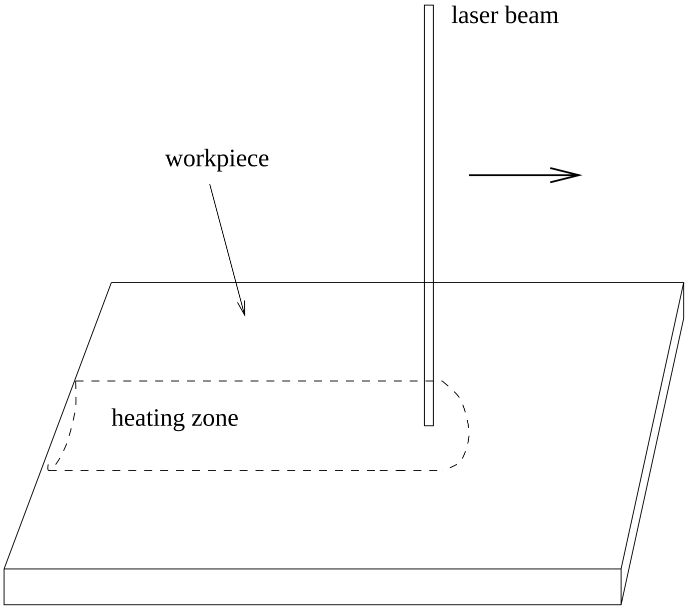

Figure 1: Sketch of a laser hardening process

general, steel is a mixture of ferrite, pearlite, bainite and martensite. Upon heating, these phases are transformed to austenite. Then, during cooling, austenite is transformed back to a mixture of ferrite, pearlite, bainite and martensite.
The actual phase distribution at the end of the heat treatment depends on the cooling strategy. In the case of laser hardening, owing to high cooling rates most of the austenite is transformed to martensite by a diffusionless phase transition leading to the desired increase of hardness.

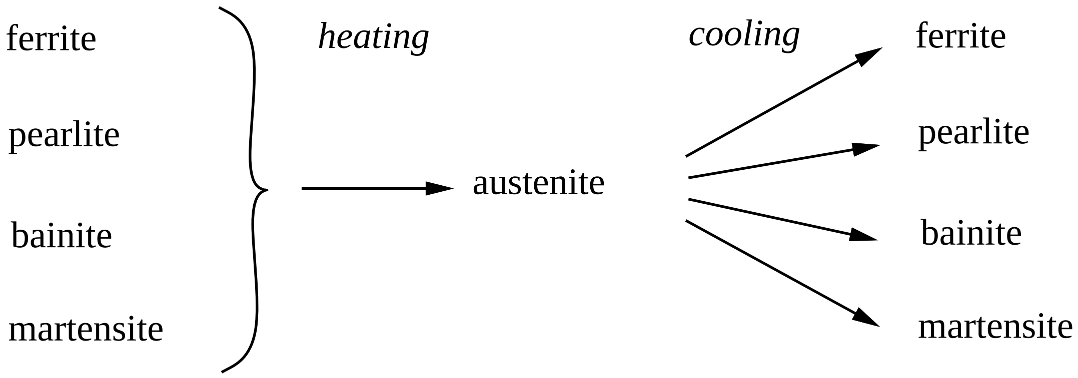

Figure 2: Possible phase transitions in steel

Mathematical models for phase transitions in steel have been considered e.g. in [1], [4], [5], [11]. In [3], numerical results for laser surface hardening are presented. For a survey on mathematical models for laser material treatments, we refer to [9].
The paper is organized as follows: in Section 2, we describe the mathematical model,

Section 3 contains existence and stability results. In the last section we investigate the control problem.

2 Model equations

2.1 The phase transitions

For a detailed description of the following model for phase transitions during surface hardening, we refer to [3]. A simplified version has recently been used in connection with the mathematical modeling of induction heat treatments [6].
We introduce the following assumptions:

z_0: volume fraction of austenite,

$z_1, ..., z_4$: relative volume fractions of ferrite, pearlite, bainite, martensite, which have been transformed from z_0,

A_s: critical temperature, above which the formation of austenite starts,

M_s: critical temperature, below which the formation of martensite starts ($M_s < A_s$).

We describe the evolution of volume fractions for given temperature evolution $\theta(.)$ by the following initial–value problem:

$$\begin{aligned}
z_0(0) &= z_{00} \in (0,1), && && (2.1a)\\
z_i(0) &= 0, && i = 1, ..., 4, && (2.1b)\\
z_{0,t}(t) &= \frac{1}{\tau(\theta)}\Big(a_{eq}(\theta(t)) - z_0(t)\Big)\,\mathcal{H}(\theta(t) - A_s) - \sum_{j=1}^{4} z_{j,t}(t) && && (2.1c)\\
z_{i,t}(t) &= -z_0(t)\ln(z_0(t))\,g_i(t, z(t), \theta(t))\,\mathcal{H}(A_s - \theta(t)), && i = 1, ..., 3, && (2.1d)\\
z_{4,t}(t) &= z_0(t)\mathcal{H}(-\theta_t) g_4(t, z(t), \theta(t))\,\mathcal{H}(M_s - \theta(t)), && && (2.1e)
\end{aligned}$$

where we assume

(A1) $\mathcal{H} \in C^\infty(\mathrm{I\!R})$, monotone regularization of the heaviside graph, satisfying $\mathcal{H}(0) = 0$ (cf. [10]),

(A2) $a_{eq} \in C^{1,1}(\mathrm{I\!R})$, $a_{eq}(x) \in [0,1]$ for all $x \in \mathrm{I\!R}$,

(A3) $\tau \in C^{1,1}(\mathrm{I\!R})$, $m \le \tau(x) \le M$ for all $x \in \mathrm{I\!R}$, and constants $0 < m < M$,

(A4) $g_i \in C^{1,1}(D)$, $i = 1, \ldots, 4$, $\quad D = [0,T] \times [0,1]^5 \times \mathrm{I\!R}$, moreover

$0 \le g_i \le M, \quad$ for all $(t, z, \theta) \in D$ and a constant $M > 0$.

Remark 2.1 *(1) a_{eq} has been introduced by Leblond and Deveaux [8], to account for equilibrium fractions of austenite less than one.*
(2) $\mathcal{H}(-\theta_t)$ prevents the formation of martensite, if the temperature is not decreasing.

2.2 Energy balance equation

Using Fourier's law of heat conduction and neglecting mechanical effects, we consider the following heat transfer equation:

$$\rho c\theta_t - k\Delta\theta = \tilde{F}_1[\theta] + \tilde{F}_2[\theta], \qquad \text{in } Q_T = \Omega \times (0,T), \tag{2.2}$$

where $\Omega \subset \mathbb{R}^3$ with smooth boundary.
The positive constants ρ, c and k denote density, specific heat at constant pressure and heat conductivity, respectively. The heat sources $\tilde{F}_1$, $\tilde{F}_2$ will take care of the latent heats of the phase transitions and the heating owing to laser radiation.
Since the self–cooling of the workpiece is the primary quenching effect in surface hardening, we assume the workpiece to be thermally isolated, i.e. we complete (2.2) by

$$\frac{\partial\theta}{\partial\nu} = 0 \qquad \text{in } \Sigma_T := \partial\Omega \times (0,T),$$

and the initial condition

$$\theta(.,0) = \theta_0, \qquad \text{in } \Omega.$$

We assume that the laser radiation is volumetrically absorbed by the workpiece (for details, we refer again to [3]). Thus, we define

$$\tilde{F}_2[\theta] := \alpha(\theta)u,$$

where α measures the temperature dependent absorptivity of the workpiece's surface, and u is the radiation intensity inside the workpiece. Clearly, u decreases with increasing distance from the surface.
To simplify the exposition, we assume that the latent heat of all phase transitions has the same value L. Then, $\tilde{F}_1$ in (2.2) can be written as follows:

$$\begin{aligned} \tilde{F}_1[\theta] &= -\rho L z_{0,t} \\ &= \rho L\Big(- F_1[\theta]A(\theta_t) + F_2[\theta]\Big), \end{aligned} \tag{2.3}$$

with

$$F_1[\theta] := z_0 g_4(t,z,\theta)\mathcal{H}(M_s - \theta), \tag{2.4}$$

$$F_2[\theta] := -\frac{1}{\tau(\theta)}\Big(a_{eq}(\theta) - z_0\Big)\mathcal{H}(\theta - A_s) - z_0\ln(z_0)\mathcal{H}(A_s - \theta)\sum_{i=1}^{3} g_i(t,z,\theta), \tag{2.5}$$

$$A(\theta_t) := -\mathcal{H}(-\theta_t). \tag{2.6}$$

We end up with the following nonlinear problem for laser surface hardening:

$$\theta_t + F_1[\theta]A(\theta_t) - \Delta\theta = F_2[\theta] + \alpha(\theta)u, \qquad \text{in } Q_T, \tag{2.7a}$$
$$\frac{\partial\theta}{\partial\nu} = 0, \qquad \text{in } \Sigma_T, \tag{2.7b}$$
$$\theta(.,0) = \theta_0, \qquad \text{in } \Omega, \tag{2.7c}$$

where F_1, F_2 are defined by (2.4), (2.5), and z is the solution to (2.1a–e).
To simplify notations we have normed all physical constants to one.

Remark 2.2 *In view of (2.1c), (2.3) means that latent heat is consumed during the formation of austenite ($z_{0,t} > 0$), and released during the transformation back to ferrite, pearlite, bainite and martensite ($z_{0,t} < 0$).*

3 Existence and stability results

3.1 Existence of a strong solution to (2.7a–c)

In the sequel, we will extensively use Sobolev spaces $W_q^{2,1}(Q_T)$, $q \geq 1$ (cf. [7]), defined by

$$W_q^{2,1}(Q_T) := W^{1,q}(0,T;L^q(\Omega)) \cap L^q(0,T;W^{2,q}(\Omega)).$$

Note that in three space dimensions for $q > 5/2$ we have

$$W_q^{2,1}(Q_T) \subset C^\beta(\bar{Q}_T) \qquad \text{with } 0 \leq \beta < 2 - 5/q. \tag{3.1}$$

We assume

(A5) $\alpha \in C^{1,1}(\mathbb{R})$,

(A6) $u \in W^{1,4}(0,T;L^4(\Omega)) \cap L^9(Q_T)$, $u(.,0) = 0$, a.e. in Ω,

(A7) θ_0 constant,

then we have the following result:

Theorem 3.1 *Assume (A1)–(A7), then (2.7a–c) has a unique solution $\theta \in W_9^{2,1}(Q_T)$. Moreover, we have $\theta_t \in W_4^{2,1}(Q_T)$.*

To prove the theorem, we need the following

Lemma 3.1 *Assume (A1)–(A4), and let $\theta \in W^{1,p}(0,T;L^p(\Omega))$, $p \in [1,\infty]$, then the following are valid:*

(1) (2.1a–e) has a unique solution $z \in [W^{1,\infty}(0,T;L^\infty(\Omega))]^5$.

(2) There are constants c_*, c^*, *independent of* θ, *such that*

$$0 < c_* < z_0(x,t) < c^*, \qquad a.e.\ in\ Q_T.$$

(3) Let $\theta_i \in W^{1,p}(0,T;L^p(\Omega))$, *i=1,2, and* z^i *the corresponding solutions to (2.1a-e), then there exist constants* $L_i > 0$, *such that*

$$\sup_{t\in(0,T)} \|F_i[\theta_1](.,t) - F_i[\theta_2](.,t)\|^q_{L^p(\Omega)} \le L_i \|\theta_1 - \theta_2\|^q_{W^{1,p}(0,T;L^p(\Omega))},$$

for any $q \in [1,\infty)$, *where* F_i, $i = 1,2$ *are defined in (2.4), (2.5).*

Proof:
Let $\theta \in W^{1,1}(0,T;L^1(\Omega))$ and $x \in \Omega \setminus N$ fixed, with $N \subset \Omega$ of zero measure. In view of (A1)–(A4), (2.1a–e) has a unique local solution.
Inserting (2.1d), i=1,. . . ,3 and (2.1e) into (2.1c), we obtain

$$z_{0,t}(t,x) = \frac{1}{\tau(\theta)}\Big(a_{eq}(\theta) - z_0(t,x)\Big)\mathcal{H}(\theta - A_s) + z_0(t,x)\mathcal{H}(A_s - \theta)\times$$
$$\Big(-\mathcal{H}(-\theta_t)g_4(t,z,\theta)\mathcal{H}(M_s-\theta) + \ln(z_0(t,x))\sum_{i=1}^{3} g_i(t,z,\theta)\Big),$$

where we have omitted the dependency of θ and z on (x,t). Using differential inequalities and (A1)–(A4), one obtains first

$$z_0(t,x) \le c^* < 1 \qquad \text{for all } t \in [0,T]. \tag{3.2}$$

Substituting $y = 1 - z_0$ and using (3.2), we get

$$0 \le y_t \le -(1-y)\ln(1-y)\Big(c_1 - \frac{c_2}{\ln(c^*)}\Big),$$

with positive constants c_1, c_2. Hence, using again differential inequalities and (A1)–(A4), we find $y(t,x) \le c_T < 1$ and thereby

$$z_0(t,x) \ge c_* > 0 \qquad \text{for all } t \in [0,T].$$

In view of (A2)–(A4), c_*, c^* are independent of θ. This proves (1) and (2). Assertion (3) follows directly from (A1)–(A4) and Gronwall's lemma. □

Proof of Theorem 3.1:
Proving existence of a unique solution in the space $H^1(0,T;L^2(\Omega))$ is a standard application of the contraction mapping principle. Using Lemma 3.1, this can be done exactly as in [5], Theorem 3.1.

Moreover, in view of (A6) and Lemma 3.1, standard regularity results for linear parabolic equations (cf. Theorem IV.9.1 in [7]) imply that

$$\theta \in W_9^{2,1}(Q_T).$$

Now, let θ be the solution to (2.7a–c). Owing to (A2)–(A4) and Lemma 3.1, we have $F_i[\theta] \in W^{1,9}(0,T;L^9(\Omega))$, $\; i = 1,2$, with derivative

$$\frac{\partial}{\partial t} F_i[\theta] = f_{i1} + f_{i2}\theta_t,$$

and $f_{ij} \in L^\infty(Q)$, $i,j = 1,2$, depending on θ.
Next, we differentiate (2.7a–b) formally with respect to t to obtain

$$\begin{aligned} \theta_{tt} + F_1[\theta]A'(\theta_t)\theta_{tt} - \Delta\theta_t & \\ = \;& f_{21} + \alpha u_t - f_{11}A(\theta_t) + \big(f_{22} + \alpha' u - f_{12}A(\theta_t)\big)\theta_t, \quad \text{in } Q_T, \quad (3.3a) \\ \frac{\partial \theta_t}{\partial \nu} = \;& 0, \quad \text{in } \Sigma, \quad (3.3b) \\ \theta_t(.,0) = \;& \big(I + F_1[\theta_0]A(.)\big)^{-1} F_2[\theta_0], \quad \text{in } \Omega. \quad (3.3c) \end{aligned}$$

(3.3c) has been derived from (2.7a) using (A6).
Since we have θ_t, $u \in L^9(Q)$, the right–hand side of (3.3a) is in $L^{9/2}(Q_T)$. Thus, according to [12], the solution to (3.3a–c) is continuous, i.e. we have $\theta_t \in C(\bar{Q_T})$. Hence, we can again apply Theorem IV.9.1 in [7] to obtain

$$\theta_t \in W_4^{2,1}(Q_T),$$

which finishes the proof. □

3.2 Stability estimates

We have the following stability result.

Theorem 3.2 *Assume (A1)–(A7) and let θ_i, $i = 1,2$, be the solution to (2.7a–c) with respect to $u_i \in W^{1,4}(0,T;L^4(\Omega)) \cap L^9(Q_T)$. Then, there exists a constant $C > 0$ such that*

$$\|\theta_1 - \theta_2\|_{H^{2,1}(Q_T)} + \|\theta_{1,t} - \theta_{2,t}\|_{C(0,T;H^1(\Omega))\cap H^1(0,T;L^2(\Omega))} \le C\|u_1 - u_2\|_{W^{1,4}(0,T;L^4(\Omega))}.$$

To prove Theorem 3.2, we need the following result, which is an easy consequence of Lemma 3.1 and (A1)–(A4).

Lemma 3.2 *Assume (A1)–(A4) and let θ_i, $i = 1, 2$, as in Theorem 3.2, then there exist constants $L_i > 0$, such that*

$$\int_0^t \Big\| \frac{\partial F_i[\theta_1]}{\partial s}(.,s) - \frac{\partial F_i[\theta_2]}{\partial s}(.,s)\Big\|^2_{L^2(\Omega)} ds \le L_i \|\theta_1 - \theta_2\|^2_{H^1(0,T;L^2(\Omega))} ds,$$

where F_i, $i = 1, 2$ are defined in (2.4), (2.5).

Proof of Theorem 3.2:
Defining $\theta := \theta_1 - \theta_2$ and $u := u_1 - u_2$, we insert θ_1, θ_2 into (2.7a), subtract both equations, and test with θ_t to obtain:

$$\begin{aligned}
&\int_0^t \int_\Omega \theta_s^2 dx ds + \int_0^t \int_\Omega F_1[\theta_1]\Big(A(\theta_{1,s}) - A(\theta_{2,s})\Big)\theta_s dx ds + \frac{1}{2}\int_\Omega |\nabla\theta(t)|^2 dx \\
&= \; -\int_0^t \int_\Omega A(\theta_{2,s})\Big(F_1[\theta_1] - F_1[\theta_2]\Big)\theta_s dx ds + \int_0^t \int_\Omega \alpha(\theta_1) u \theta_s dx ds + \int_0^t \int_\Omega u_2\Big(\alpha(\theta_1) - \alpha(\theta_2)\Big)\theta_s dx ds \\
&\quad + \int_0^t \int_\Omega \Big(F_2[\theta_1] - F_2[\theta_2]\Big)\theta_s dx ds =: I_1 + \ldots + I_4.
\end{aligned}$$

Using the inequalities of Hölder and Young, Lemma 3.1 and (A5), we obtain:

$$\begin{aligned}
|I_1| &\le \frac{1}{5}\int_0^t \int_\Omega \theta_s^2 dx ds + c_1 \int_0^t \|\theta\|^2_{H^1(0,s;L^2(\Omega))} ds, \\
|I_2| &\le \frac{1}{5}\int_0^t \int_\Omega \theta_s^2 dx ds + c_2 \int_0^t \int_\Omega u^2 dx ds, \\
|I_3| &\le \frac{1}{5}\int_0^t \int_\Omega \theta_s^2 dx ds + c_3 \int_0^t \|u_2\|^2_{L^4(\Omega)} \cdot \|\theta\|^2_{H^1(\Omega)} ds, \\
|I_4| &\le \frac{1}{5}\int_0^t \int_\Omega \theta_s^2 dx ds + c_4 \int_0^t \|\theta\|^2_{H^1(0,s;L^2(\Omega))} ds.
\end{aligned}$$

Thanks to the monotonicity of A, applying Gronwall's lemma leads to

$$\int_0^t \int_\Omega \theta_s^2 dx ds + \int_\Omega |\nabla\theta(t)|^2 dx \le c_5 \int_0^t \int_\Omega u^2 dx ds.$$

Testing with $-\Delta\theta$ and making the same computations as before we get

$$\int_0^t \int_\Omega |\Delta\theta|^2 dx ds \le c_6 \int_0^t \int_\Omega u^2 dx ds.$$

Hence, in view of (2.7b), we end up with

$$\|\theta\|_{H^{2,1}(Q_T)} \le c_7 \|u\|_{L^2(Q_T)}. \tag{3.4}$$

Next, we differentiate (2.7a-c) formally with respect to t (cf. (3.3a-c)), insert θ_1, θ_2, subtract the equations and test with θ_{tt} to obtain

$$\begin{aligned}
&\int_0^t\int_\Omega \theta_{ss}^2 dxds + \int_0^t\int_\Omega \Big(F_1[\theta_1]A'(\theta_{1,s})\theta_{1,ss} - F_1[\theta_2]A'(\theta_{2,s})\theta_{2,ss}\Big)\theta_{ss}dxds + \frac{1}{2}\int_\Omega |\nabla\theta_t|^2 dx \\
= \;& -\int_0^t\int_\Omega \Big(A(\theta_{1,s})\frac{\partial F_1[\theta_1]}{\partial s} - A(\theta_{2,s})\frac{\partial F_1[\theta_2]}{\partial s}\Big)\theta_{ss}dxds \\
& + \int_0^t\int_\Omega \Big(\frac{\partial F_2[\theta_1]}{\partial s} - \frac{\partial F_2[\theta_2]}{\partial s}\Big)\theta_{ss}dxds + \int_0^t\int_\Omega \Big(\alpha(\theta_1)u_{1,s} - \alpha(\theta_2)u_{2,s}\Big)\theta_{ss}dxds \\
& + \int_0^t\int_\Omega \Big(\alpha'(\theta_1)u_1\theta_{1,s} - \alpha'(\theta_2)u_2\theta_{2,s}\Big)\theta_{ss}dxds =: I_1 + \ldots I_4.
\end{aligned} \tag{3.5}$$

We estimate term by term, using Hölder's and Young's inequalities, (A1)–(A6), Lemmas 3.1 and 3.2, (3.4) and the embedding $H^1(\Omega) \subset L^4(\Omega)$. The second term in (3.5) gives

$$\begin{aligned}
&\int_0^t\int_\Omega \Big(F_1[\theta_1]A'(\theta_{1,s})\theta_{1,ss} - F_1[\theta_2]A'(\theta_{2,s})\theta_{2,ss}\Big)\theta_{ss}dxds \\
= \;& \int_0^t\int_\Omega F_1[\theta_1]A'(\theta_{1,s})\theta_{ss}^2 dxds + \int_0^t\int_\Omega \theta_{2,ss}F_1[\theta_1]\Big(A'(\theta_{1,s}) - (A'(\theta_{2,s})\Big)\theta_{ss}dxds \\
& + \int_0^t\int_\Omega \theta_{2,ss}A'(\theta_{2,s})\Big(F_1[\theta_1] - F_1[\theta_2]\Big)\theta_{ss}dxds \\
\ge \;& -\frac{1}{6}\int_0^t\int_\Omega \theta_{ss}^2 dxds - c_8\int_0^t \|\theta_{2,ss}\|^2_{L^4(\Omega)} \cdot \|\theta_s\|^2_{H^1(\Omega)} ds \\
& - c_9\Big(\int_0^t \|\theta_{2,ss}\|^2_{L^4(\Omega)} ds\Big) \cdot \int_0^t \Big(\|\theta\|^2_{L^4(\Omega)} + \|\theta_s\|^2_{L^4(\Omega)}\Big) ds \\
\ge \;& -\frac{1}{6}\int_0^t\int_\Omega \theta_{ss}^2 dxds - c_{10}\int_0^t \Big(1 + \|\theta_{2,ss}\|^2_{L^4(\Omega)}\Big) \cdot \|\theta_s\|^2_{H^1(\Omega)} ds \\
& - c_{11}\int_0^t\int_\Omega u^2 dxds,
\end{aligned}$$

$$|I_1| \le \int_0^t\int_\Omega \Big|A(\theta_{1,s})\Big(\frac{\partial F_1[\theta_1]}{\partial s} - \frac{\partial F_1[\theta_2]}{\partial s}\Big)\theta_{ss}\Big| ds$$

$$
\begin{aligned}
&+\int_0^t\int_\Omega \Big|\frac{\partial F_1[\theta_2]}{\partial s}\Big(A(\theta_{1,s})-A(\theta_{2,s})\Big)\theta_{ss}\Big|ds\\
\le\ & \frac{1}{6}\int_0^t\int_\Omega \theta_{ss}^2 dxds + c_{12}\int_0^t\int_\Omega u^2 dxds + c_{13}\int_0^t \Big\|\frac{\partial F_1[\theta_2]}{\partial s}\Big\|^2_{L^4(\Omega)}\cdot\|\theta_s\|^2_{H^1(\Omega)}ds.
\end{aligned}
$$

In the same way, we obtain

$$
|I_2| \le \frac{1}{12}\int_0^t\int_\Omega \theta_{ss}^2 dxds + c_{14}\int_0^t\int_\Omega u^2 dxds,
$$

$$
\begin{aligned}
|I_3| \ &\le\ \int_0^t\int_\Omega \Big|u_{1,s}\Big(\alpha(\theta_1)-\alpha(\theta_2)\Big)\theta_{ss}\Big|dxds + \int_0^t\int_\Omega \Big|\alpha(\theta_2)u_s\theta_{ss}\Big|ds\\
&\le\ \frac{1}{6}\int_0^t\int_\Omega \theta_{ss}^2 ds + c_{15}\|u\|^2_{H^1(0,T;L^2(\Omega))},
\end{aligned}
$$

$$
\begin{aligned}
|I_4| \ &\le\ \int_0^t\int_\Omega \Big|\alpha'(\theta_1)u_1\theta_s\theta_{ss}\Big|dxdt + \int_0^t\int_\Omega \Big|u_1\theta_{2,s}\Big(\alpha'(\theta_1)-\alpha'(\theta_2)\Big)\theta_{ss}\Big|dxds\\
&\quad + \int_0^t\int_\Omega \Big|\theta_{2,s}\alpha'(\theta_2)u\theta_{ss}\Big|dxds\\
&\le\ \frac{1}{4}\int_0^t\int_\Omega \theta_{ss}^2 ds + c_{16}\int_0^t \|u_1\|^2_{L^4(\Omega)}\cdot\|\theta_s\|^2_{L^4(\Omega)}ds\\
&\quad + c_{17}\int_0^t \|\theta_{2,s}\|^2_{L^8(\Omega)}\cdot\|u_1\|^2_{L^8(\Omega)}\cdot\|\theta\|^2_{L^4(\Omega)}ds\\
&\quad + c_{18}\int_0^t \|\theta_{2,s}\|^2_{L^4(\Omega)}\cdot\|u\|^2_{L^4(\Omega)}ds\\
&\le\ \frac{1}{4}\int_0^t\int_\Omega \theta_{ss}^2 ds + c_{16}\int_0^t \|u_1\|^2_{L^4(\Omega)}\cdot\|\theta_s\|^2_{L^4(\Omega)}ds\\
&\quad + c_{19}\int_0^t\int_\Omega u^2 dxds + c_{20}\|u\|^2_{L^4(Q_T)}.
\end{aligned}
$$

Altogether, we end up with

$$
\begin{aligned}
\frac{1}{6}\int_0^t\int_\Omega \theta_{ss}^2 ds + \frac{1}{2}\int_\Omega |\nabla\theta_t|^2 dx \ &\le\ c_{21}\|u\|^2_{H^1(0,T;L^2(\Omega))} + c_{22}\|u\|^2_{L^4(Q_T)} + \int_0^t g(s)\|\theta_s\|^2_{H^1(\Omega)}ds\\
&\le\ c_{23}\|u\|^2_{W^{1,4}(0,T;L^4(\Omega))} + \int_0^t g(s)\|\theta_s\|^2_{H^1(\Omega)}ds,
\end{aligned}
$$

with a positive, nondecreasing function $g \in L^1(0,T)$. Applying Gronwall's lemma finishes the proof. $\square$

Remark 3.1 *Using the embedding $H^1(\Omega) \subset L^6(\Omega)$, a particular consequence of Theorem 3.2 is*

$$\|\theta_1 - \theta_2\|_{W^{1,6}(0,T;L^6(\Omega))} \leq \tilde{C}\|u_1 - u_2\|_{W^{1,4}(0,T;L^4(\Omega))}. \tag{3.6}$$

4 Optimal control

4.1 Problem statement

The aim of laser heat treatments is to increase the surface hardness of the workpiece. Therefore we have to control the volume fraction of martensite, i.e. we consider the following cost functional

$$J(u) = \frac{\beta_1}{2}\int_\Omega \Big(z_4(x,T) - \tilde{m}(x)\Big)^2 dx + \frac{\beta_2}{2}\int_0^T\int_\Omega u^2 dx dt.$$

In order to maintain the quality of the workpiece, it is of the utmost importance to avoid surface melting. To this end, we have to introduce the state constraint

$$\theta(x,t) \leq \theta_m, \qquad \text{a.e. in } Q_T, \tag{4.1}$$

where θ_m is the melting temperature of the workpiece.
Then, the control problem for laser surface hardening takes the following form:

$$\left.\begin{array}{l} \text{Minimize } J(u) \\ \text{subject to (2.7a-c),} \\ \text{the constraint (4.1), and} \\ u \in U_{ad}, \end{array}\right\} \tag{4.2}$$

with the convex set of admissible controls $U_{ad} \subset W^{1,4}(0,T;L^4(\Omega)) \cap L^9(Q_T)$, satisfying $u(.,0) = 0$ a.e. in Ω for all $u \in U_{ad}$.

4.2 Differentiability of the solution operator

In view of Lemma 3.1, the solution to (2.1a-e) defines an operator

$$\tilde{z} \,:\, \theta \mapsto \Big(\tilde{z}[\theta]\Big)(x,t) = z(x,t),$$

where z is the unique solution to (2.1a–e) for given temperature evolution θ. In the sequel, we will identify $\tilde{z}$ with z.

Lemma 4.1 *Assume (A1)–(A4), then*

$$z : W^{1,p}(0,T;L^p(\Omega)) \longrightarrow [C(0,T;L^p(\Omega))]^5$$

is Fréchet–differentiable for any $p \in [2,\infty]$.

Proof:
The proof is a standard application of the implicit function theorem (cf. [13], Theorem 4B), hence we will only sketch it:
(I) Let $G : U \subset W^{1,p}(0,T;L^p(\Omega)) \times [C(0,T;L^p(\Omega))]^5 \longrightarrow [C(0,T;L^1(\Omega))]^5$ be defined by

$$G(\theta, z) = z - z^0 - \int_0^t f(\xi, z(\xi), \theta(\xi))d\xi,$$

where f is the right–hand side of (2.1c-e) and $z^0 = (z_{00}, 0, 0, 0, 0)^T$ is the vector of initial values, defined in (2.1a–b).
According to Lemma 3.1, for given $\theta \in W^{1,p}(0,T;L^p(\Omega))$ (2.1a–e) has a unique solution such that G is well-defined on a neighbourhood $U \subset W^{1,p}(0,T;L^p(\Omega)) \times [C(0,T;L^p(\Omega))]^5$ of θ.
Using the mean–value theorem and (A1)–(A4), one proves now that
(II) G is differentiable with respect to z, with

$$G_z[h] = h - \int_0^t f_z \cdot h d\xi,$$

for all $h \in [C(0,T;L^p(\Omega))]^5$, s.t. $(\theta, z+h) \in U$.
Thanks to (A1)–(A4) and Lemma 3.1(2), f is differentiable with respect to z, and the mean–value theorem gives

$$f(t, z+h, \theta) - f(t, z, \theta) = f_z(t, z+\mu h, \theta) \cdot h,$$

with $\mu \in (0,1)$ for (x,t) a.e. in Q_T. Hence, we get

$$\begin{aligned}
&\int_\Omega \Big|G(\theta, z+h) - G(\theta, z) - G_z[h]\Big|dx \\
&\qquad \le \int_0^t \int_\Omega \Big|f(\xi, z+h, \theta) - f(\xi, z, \theta) - f_z \cdot h\Big|dxd\xi \\
&\qquad \le c_1 \int_0^t \int_\Omega |h|^2 dxd\xi \le c_2 \|h\|^2_{C(0,T;L^p(\Omega))}.
\end{aligned}$$

In the same manner it is proved that

(III) G is differentiable with respect to θ, with

$$G_\theta[h] = -\int_0^t f_\theta \cdot h d\xi - \int_0^t f_{\theta_t} \cdot h_\xi d\xi,$$

for all $h \in W^{1,p}(0,T;L^p(\Omega))$, s.t. $(\theta + h, z) \in U$. Here, f_{θ_t} denotes the partial derivative of f with respect to the time derivative of θ.
Next, we have to show that
(IV) $G_z[h] = f$ has a unique solution for any $f \in [C(0,T;L^1(\Omega))]^5$.
This can be done using a contraction mapping argument.
In view of (A1)–(A4) and (II)–(IV), G, G_z and G_θ are continuous, hence the implicit function theorem shows that z is continuously differentiable with derivative

$$z_\theta[h] = -G_z^{-1} G_\theta[h].$$

□

Using Lemma 4.1, (A1)–(A4), and the product rule, we obtain easily

Lemma 4.2 *Assume (A1)–(A4), then $F_i : W_p^{2,1}(Q_T) \longrightarrow W_{p/2}^{2,1}(Q_T)$, $i = 1, 2$, and $p \in [2, \infty)$, as defined in (2.4), (2.5) are Fréchet–differentiable, satisfying*

$$F_{i,\theta}[h] = g_{i1} \cdot h + g_{i2} \cdot z_\theta[h],$$

where $g_{i1} \in L^\infty(Q)$ and $g_{i2} \in [L^\infty(Q)]^5$ for $i = 1, 2$.

Now, we can prove the differentiability of the solution operator.

Theorem 4.1 *Assume (A1)–(A7) and let $S : U_{ad} \longrightarrow W_3^{2,1}(Q_T)$, $u \mapsto S(u) = \theta$ be the solution operator to (2.7a–c).*
Then, S is differentiable, and for any h satisfying $u + h \in U_{ad}$, its directional derivative $\psi = S_u(u)[h]$ is the solution to the following linear problem:

$$\begin{aligned} (1 + F_1[\theta]A'(\theta_t))\psi_t - \Delta\psi + \Big(A(\theta_t)F_{1,\theta}[\theta] - F_{2,\theta}[\theta] - u\alpha'(\theta)\Big)[\psi] &= \alpha(\theta)h, & (4.3a)\\ \frac{\partial\psi}{\partial\nu} &= 0, & (4.3b)\\ \psi(.,0) &= 0. & (4.3c) \end{aligned}$$

Proof:
(I) (4.3a–c) has a unique solution $\psi \in W_3^{2,1}(Q_T)$.
Let $K_T = \{f \in W_3^{2,1}(Q_T) \,\big|\, f(.,0) = 0,\ \|f\|_{W_3^{2,1}(Q_T)} < M\}$, with a constant $M > 0$, and define

$$\mathcal{F} : K_T \longrightarrow W_3^{2,1}(Q_T), \qquad \mathcal{F}[\hat{\psi}] = \psi,$$

where ψ is the solution to

$$
\begin{aligned}
(1+F_1[\theta]A'(\theta_t))\psi_t - \Delta\psi + \Big(A(\theta_t)F_{1,\theta}[\theta] - F_{2,\theta}[\theta] - u\alpha'(\theta)\Big)[\hat{\psi}] &= \alpha(\theta)h, &(4.4a)\\
\frac{\partial\psi}{\partial\nu} &= 0, &(4.4b)\\
\psi(.,0) &= 0. &(4.4c)
\end{aligned}
$$

Since $\theta_t \in C(\bar{Q_T})$, according to Theorem IV.9.1 of [7], (4.4a-c) has a unique solution satisfying

$$
\begin{aligned}
\|\psi\|^3_{W_3^{2,1}(Q_T)} &\le 4\|\alpha(\theta)h\|^3_{L^3(Q_T)} + 4\Big\|\Big(A(\theta_t)F_{1,\theta}[\theta] - F_{2,\theta}[\theta] - u\alpha'(\theta)\Big)[\hat{\psi}]\Big\|^3_{L^3(Q_T)}\\
&\le 4\|\alpha(\theta)h\|^3_{L^3(Q_T)} + c_1\Big(\|\hat{\psi}\|^3_{L^3(Q_T)} + \|z_\theta[\hat{\psi}]\|^3_{L^3(Q_T)} + \|u\hat{\psi}\|^3_{L^3(Q_T)}\Big)\\
&\le 4\|\alpha(\theta)h\|^3_{L^3(Q_T)} + c_2\Big(T + \|u\|^3_{L^6(Q_T)}\Big)\|\hat{\psi}\|^3_{W_3^{2,1}(Q_T)}. \qquad (4.5)
\end{aligned}
$$

Here, we have used Lemmas 4.1 and 4.2 as well as the embeddings $W_3^{2,1}(Q_T) \subset C(0,T;L^3(\Omega))$ and $W_3^{2,1}(Q_T) \subset L^6(Q_T)$. Choosing $M > 4\|\alpha(\theta)h\|_{L^3(Q_T)}$, there exists a $T^+ > 0$ such that $\mathcal{F}$ is a self–mapping on K_{T^+}. Because of the linearity of the F–derivatives, $\mathcal{F}$ is also a contraction, if T^+ has been chosen small enough. Applying the contraction mapping theorem, we obtain a unique solution ψ to (4.3a–c).

(II) Let $q := S[u+h] - S[u] - \psi$, then $\|q\|_{W_3^{2,1}(Q_T)} = o(\|h\|_{W^{1,4}(0,T,L^4(\Omega))\cap L^6(Q_T)})$.
We define $\theta^h := S[u+h]$ and $\theta := S[u]$. Then, q solves the following linear problem

$$
\begin{aligned}
(1+F_1[\theta]A'(\theta_t))q_t - \Delta q + \Big(A(\theta_t)F_{1,\theta}[\theta] - F_{2,\theta}[\theta] - u\alpha'(\theta)\Big)[q] &= G(\theta,\theta^h), &(4.6a)\\
\frac{\partial q}{\partial\nu} &= 0, &(4.6b)\\
q(.,0) &= 0, &(4.6c)
\end{aligned}
$$

with

$$
\begin{aligned}
G(\theta,\theta^h) = -F_1[\theta]\Big(&A(\theta^h_t) - A(\theta_t) - A'(\theta_t)(\theta^h_t - \theta_t)\Big)\\
&-A(\theta^h_t)\Big(F_1[\theta^h] - F_1[\theta] - F_{1,\theta}[\theta][\theta^h - \theta]\Big)\\
&-\Big(A(\theta^h_t) - A(\theta_t)\Big)F_{1,\theta}[\theta][\theta^h - \theta]\Big)\\
&+(F_2[\theta^h] - F_2[\theta] - F_{2,\theta}[\theta][\theta^h - \theta]\\
&+u\Big(\alpha(\theta^h) - \alpha(\theta) - \alpha'(\theta)(\theta^h - \theta)\Big)\\
&+h\Big(\alpha(\theta^h) - \alpha(\theta)\Big).
\end{aligned}
$$

Using again Theorem 9.1 in [7] and reasoning as in (4.5), we get

$$
\|q\|^3_{W_3^{2,1}(Q_T)} \le 4\int_0^T \Big\|\Big(A(\theta_s)F_{1,\theta}[\theta] - F_{2,\theta}[\theta] - u\alpha'(\theta)\Big)[q]\Big\|^3_{L^3(\Omega)} ds + 4\|G(\theta,\theta^h)\|^3_{L^3(Q_T)}
$$

$$\leq \quad c_3 \int_0^T \|q\|^3_{W_3^{2,1}(Q_s)} ds + 4\|G(\theta,\theta^h)\|^3_{L^3(Q_T)}.$$

Invoking Gronwall's lemma, we end up with

$$\|q\|_{W_3^{2,1}(Q_T)} \leq c_4 \|G(\theta,\theta^h)\|_{L^3(Q_T)}.$$

Now, using (A1), (A5) and Lemma 4.1, we obtain

$$\begin{aligned}\|G(\theta,\theta^h)\|_{L^3(\Omega)} \quad &\leq \quad o\Big(\|\theta-\theta^h\|_{W^{1,6}(0,T;L^6(\Omega))}\Big) + c_5\|u\|_{L^9(Q_T)}\|\theta-\theta^h\|^2_{L^9(Q_T)} \\ &\quad + c_6\|h\|_{L^6(Q_T)}\|\theta-\theta^h\|_{L^6(Q_T)}.\end{aligned}$$

Applying the stability result of Theorem 3.2 and the embedding $H^{2,1}(Q_T) \subset L^9(Q_T)$ finishes the proof. □

4.3 Necessary conditions of optimality

We begin with some notations. Let

$$K = \{\eta \in C(\bar{Q_T}))\,\Big|\,\eta \leq \theta_m\}.$$

For a control $u+h$, with $u, u+h \in U_{ad}$, we denote by $[\theta^h, z^h]$ the solution to (2.1a-e) and (2.7a–c), and by $[\psi, w]$ the solution to the linearized system (4.3a-c) and

$$w_t \;=\; f_z w + f_\theta \psi, \qquad \text{in } Q_T, \tag{4.7a}$$

$$w(.,0) \;=\; 0, \qquad \text{in } \Omega, \tag{4.7b}$$

where again f is the right–hand side of (2.1c–e). According to Theorem 4.1 and (3.1), the solution operator $S : U_{ad} \to C(\bar{Q_T})$ and the cost functional J are differentiable with

$$S'(u)[h] = \psi,$$

and

$$J'(u)[h] = \beta_1 \int_\Omega \Big(z_4(x,T) - \tilde{m}(x)\Big) w_4(x,T)\,dx + \beta_2 \int_0^T \int_\Omega uh\,dxdt.$$

We will now derive optimality conditions for the non–convex optimization problem under consideration using an abstract result for the existence of Lagrange multipliers by Casas (cf. [2], Theorem 5.2).

¿From the abstract result it follows that there exist

$$\lambda \geq 0 \text{ and a Borel measure } \mu \geq 0 \text{ such that}$$

$$\lambda + \|\mu\|_{\mathcal{M}(\bar{Q_T})} > 0,$$

$$\int (\eta - \theta) d\mu \leq 0 \text{ for all } \eta \in K,$$

$$\lambda J'(u)[v-u] + \int S'(u)[v-u] d\mu \geq 0 \text{ for all } v \in U_{ad}.$$

Here $u \in U_{ad}$ denotes an optimal control, $\theta = \theta(u), z_4 = z_4(u)$ and the second conditon means that the measure μ is supported on the set

$$\Xi = \{(x,t) \in \bar{Q} \,\Big|\, \theta(x,t) = \theta_m\} \tag{4.8}$$

which is closed since $\theta \in C(\bar{Q})$.

The multiplier $\lambda = 1$ provided there exists an admissible control $v \in U_{ad}$ such that the following Slater condition is satisfied,

$$\theta(u; x,t) + \psi(u; x,t)(v-u) < \theta_m$$

for all $(x,t) \in \bar{Q} = \bar{Q}_T$, where $\psi(u)(v-u) = S'(u)[v-u]$. In the sequel, we assume for simplicity that the Slater condition is satisfied.

To simplify the third optimality condition we introduce the adjoint state equations. To this end, for any given $\eta \in V_1, \xi = (\xi_0, ..., \xi_4) \in V_2$, we denote by

$$\Psi[(\eta,\xi)] = \beta_1 \int\limits_{\Omega} \Big(z_4(x,T) - \tilde{m}(x)\Big)\xi_4(x,T)\, dx + \int \eta d\mu$$

the linear form which is defined on the space $V = V_1 \times V_2$, which will be specified below. We assume that the spaces V_1 and V_2 are selected in such a way that the linear form $\Psi[(\eta,\xi)]$ is continuous on the space V, i.e.

$$\left| \int \eta d\mu \right| \leq C_1 \|\eta\|_{V_1},$$

$$\left| \int\limits_{\Omega} \Big(z_4(x,T) - \tilde{m}(x)\Big)\xi_4(x,T)\, dx \right| \leq C_2 \|\xi\|_{V_2}.$$

The linearized state equations are rewritten in the following form

$$\psi \in V_1 \ : \ \mathcal{L}_{11}(\psi) = \alpha(\theta) h \text{ in } Q_T,$$

$$w \in V_2 \ : \ \mathcal{L}_{21}(\psi) + \mathcal{L}_{22}(w) = 0 \text{ in } Q_T,$$

where

$$\mathcal{L}_{11}(\psi) = (1 + F_1[\theta]A'(\theta_t))\psi_t - \Delta\psi + \Big(A(\theta_t)F_{1,\theta}[\theta] - F_{2,\theta}[\theta] - u\alpha'(\theta)\Big)[\psi],$$

$$\mathcal{L}_{21}(\psi) = -f_\theta \psi,$$

$$\mathcal{L}_{22}(w) = w_t - f_z w,$$

and we set

$$V_1 = \{\eta \in W_3^{2,1}(Q_T) | \eta(0) = 0 \text{ in } \Omega, \frac{\partial \eta}{\partial \nu} = 0 \text{ in } \Sigma_T\}.$$

For the choice made for the space V_1, the space V_2 can be defined e.g. in the following way. We have to satisfy two conditions by the definition. First, that the linearized state $w(h) \in V_2$, the second that the linear form

$$\xi \;\to\; \int_\Omega \Big(z_4(x,T) - \tilde{m}(x)\Big)\xi_4(x,T)\,dx$$

is continuous on the space V_2. Since the linearized state is regular, i.e. satisfies the equation

$$\mathcal{L}_{22}(w) = \mathcal{L}_{21}(\psi) \text{ in } Q \text{ with the initial condition } w(0) = 0 \text{ in } \Omega,$$

we can select

$$V_2 = \{\xi \in C(0,T;[L^1(\Omega)]^5) | \xi(0) = 0, \mathcal{L}_{22}(\xi) \in [L^2(Q)]^5\},$$

with the norm

$$\|\xi\|_{V_2} = \|\mathcal{L}_{22}(\xi)\|_{[L^2(Q)]^5},$$

therefore

$$\mathcal{L}_{21}(\eta) + \mathcal{L}_{22}(\xi) \in [L^2(Q)]^5 \text{ for all } \eta \in V_1, \xi \in V_2.$$

We introduce the linear mapping

$$\mathcal{L} \;:\; V \to W$$

of the following form

$$\mathcal{L}(\eta,\xi) = \begin{pmatrix} \mathcal{L}_{11}(\eta) \\ \mathcal{L}_{21}(\eta) + \mathcal{L}_{22}(\xi) \end{pmatrix} \tag{4.9}$$

where $V = V_1 \times V_2$, $W = W_1 \times W_2$ and $W_1 = L^3(Q)$, $W_2 = [L^2(Q)]^5$. Then an adjoint state $(p,r) \in W' = L^{\frac{3}{2}}(Q) \times [L^2(Q) vipssokol]^5$ satisfies the following equation

$$\langle (p,r), \mathcal{L}(\eta,\xi)\rangle_{W' \times W} = \Psi[(\eta,\xi)] \text{ for all } (\eta,\xi) \in V_1 \times V_2.$$

The existence and uniqueness of the pair $(p,r) \in W'$ follows by an application of the representation theorem for linear and continuous functionals on the space V.
Using the adjoint state, it follows that

$$J'(u)[h] + \int S'(u)[h] d\mu = \Psi[(\psi[h], w[h])] + \beta_2 \int_0^T \int_\Omega uh\,dxdt$$

$$= \langle (p,r), \mathcal{L}(\psi[h], w[h]) \rangle_{W' \times W} + \beta_2 \int_0^T \int_\Omega uh \, dxdt$$

in view of (4.3a)

$$= \int_0^T \int_\Omega \alpha(\theta) hp dxdt + \beta_2 \int_0^T \int_\Omega uh \, dxdt.$$

The adjoint state $(p,r) \in L^{\frac{3}{2}}(Q_T) \times [L^2(Q_T)]^5$ is given by a solution to the following system

$$\int_0^T \int_\Omega \Big[(1 + F_1[\theta] A'(\theta_t))\eta_t - \Delta\eta + \Big(A(\theta_t) F_{1,\theta}[\theta] - F_{2,\theta}[\theta] - u\alpha'(\theta) \Big) \eta \Big] \, p dxdt$$
$$- \int_0^T \int_\Omega f_\theta \eta r \, dxdt = \int \eta d\mu \qquad (4.10a)$$

$$\int_0^T \int_\Omega [\xi_t - f_z \xi] r dxdt + \beta_1 \int_\Omega \Big(z_4(x,T) - \tilde{m}(x) \Big) \xi_4(x,T) \, dx = 0 \qquad (4.10b)$$

for all $\eta \in V_1$, $\xi \in V_2$.

Since the existence of an optimal control is a consequence of standard compactness arguments, which we omit here, the following necessary optimality conditions hold for the control problem under consideration:

Theorem 4.2 *There exists an optimal control $u \in U_{ad}$ which minimizes the cost functional $J(u)$ over the set of admissible controls and subject to the state constraint $\theta \in K$. If the Slater condition is satisfied, then there exists a Borel measure $\mu \geq 0$ supported on the set Ξ and the adjoint state $(p,r) \in L^{\frac{3}{2}}(Q_T) \times [L^2(Q_T)]^5$ such that the state equations (2.7a-c), the adjoint state equations (4.10a-b) and the following optimality condition is satisfied:*

$$\int_0^T \int_\Omega \alpha(\theta) p(v-u) dxdt + \beta_2 \int_0^T \int_\Omega u(v-u) \, dxdt \geq 0$$

for all $v \in U_{ad}$.

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