# Error Analysis of an Evolution Equation for Microstructure


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## Introduction

Microstructure in metal alloys sometimes occurs when the martensitic variants (favoured crystal orientations at low temperature) "mix" to achieve an overall lower energy for the bulk crystal. This is explained with a stored-energy functional with two or more "wells" corresponding to each of the martensitic variants. In order to satisfy other physical constraints different regions within the metal fall into the different energy wells while simultaneously minimising energy. In this project we are interested in trying to model a (simple) dynamical process that might explain the observed properties of microstructure and how it appears when a metal is cooled from its austenitic phase (favoured crystal orientation at high temperature) to its martensitic phase.

## Problem

Consider the problem

$$\begin{aligned} \Delta u_t + \operatorname{div}(\sigma(\nabla u)) &= 0 && \text{in } \Omega = (0,1)^2, \\ u &= 0 && \text{on } \partial\Omega, \\ u &= u_0 \in H_0^1(\Omega) && \text{when } t = 0, \end{aligned}$$

$\sigma : \mathbb{R}^2 \to \mathbb{R}^2$ globally Lipschitz, $\sigma(p) \cdot p \geq c|p|^2 - d$ for $c > 0$, $d \geq 0$, and $\sigma = DW$, where $W$ is a double well potential. For example,

$$W(\nabla u) = \tfrac{1}{2}\tfrac{1}{u_x^2+1}(u_x^2 - 1)^2 + \tfrac{1}{2}u_y^2.$$

This problem can also be expressed as the $H_0^1(\Omega)$ gradient flow of $I(u) := \int_\Omega W(\nabla u)dx$, i.e. $u_t = -\nabla I(u)$ in $H_0^1(\Omega)$. The direction chosen by the dynamics is the direction of steepest descent. In our example, the solution would like to satisfy $u_x = \pm 1$, $u_y = 0$.

To study this problem it is useful to rewrite it as

$$u_t = F(u) \qquad \text{in } H_0^1(\Omega),$$

where $F(u) := -\Delta^{-1}\operatorname{div}(\sigma(\nabla u))$. $F : H_0^1(\Omega) \to H_0^1(\Omega)$ is Lipschitz.

## Main Question

What can we say about the long-time behaviour of solutions and the appearance of microstructure?

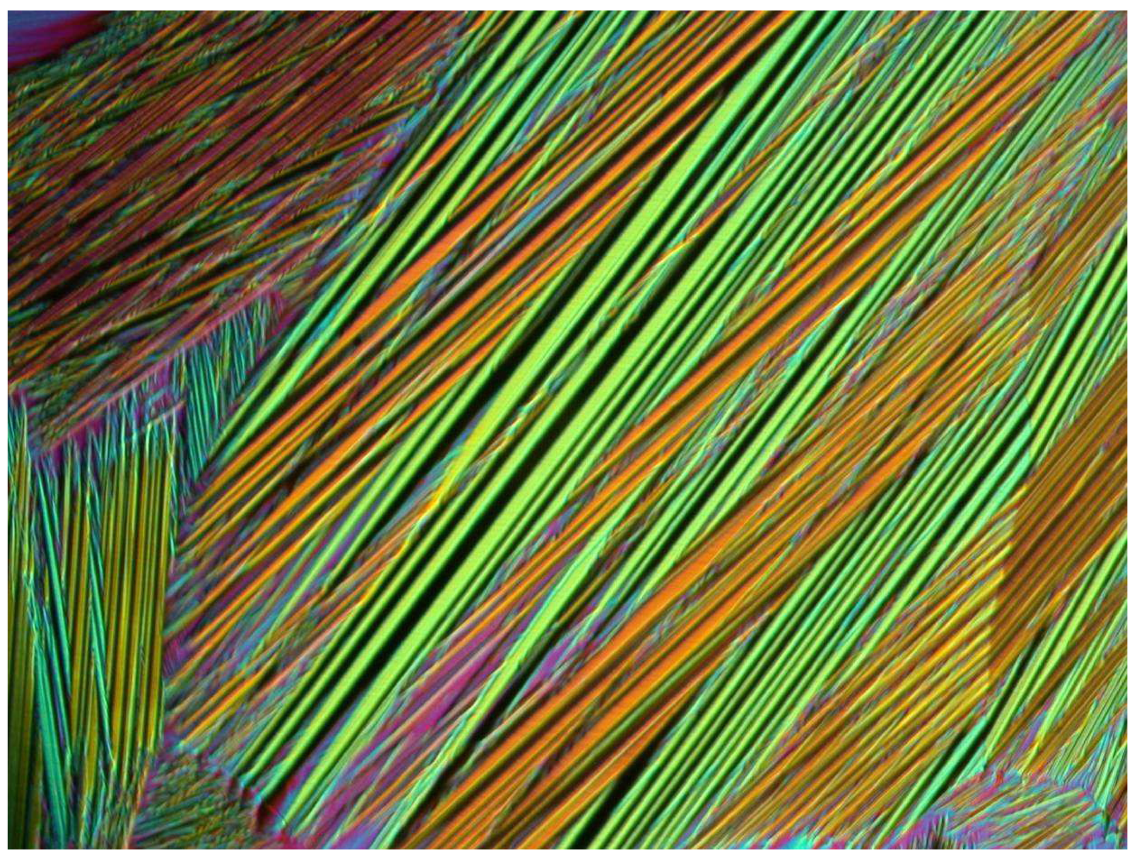

**Figure 1: Martensitic microstructure in CuZnAl (M. Morin, INSA de Lyon)**

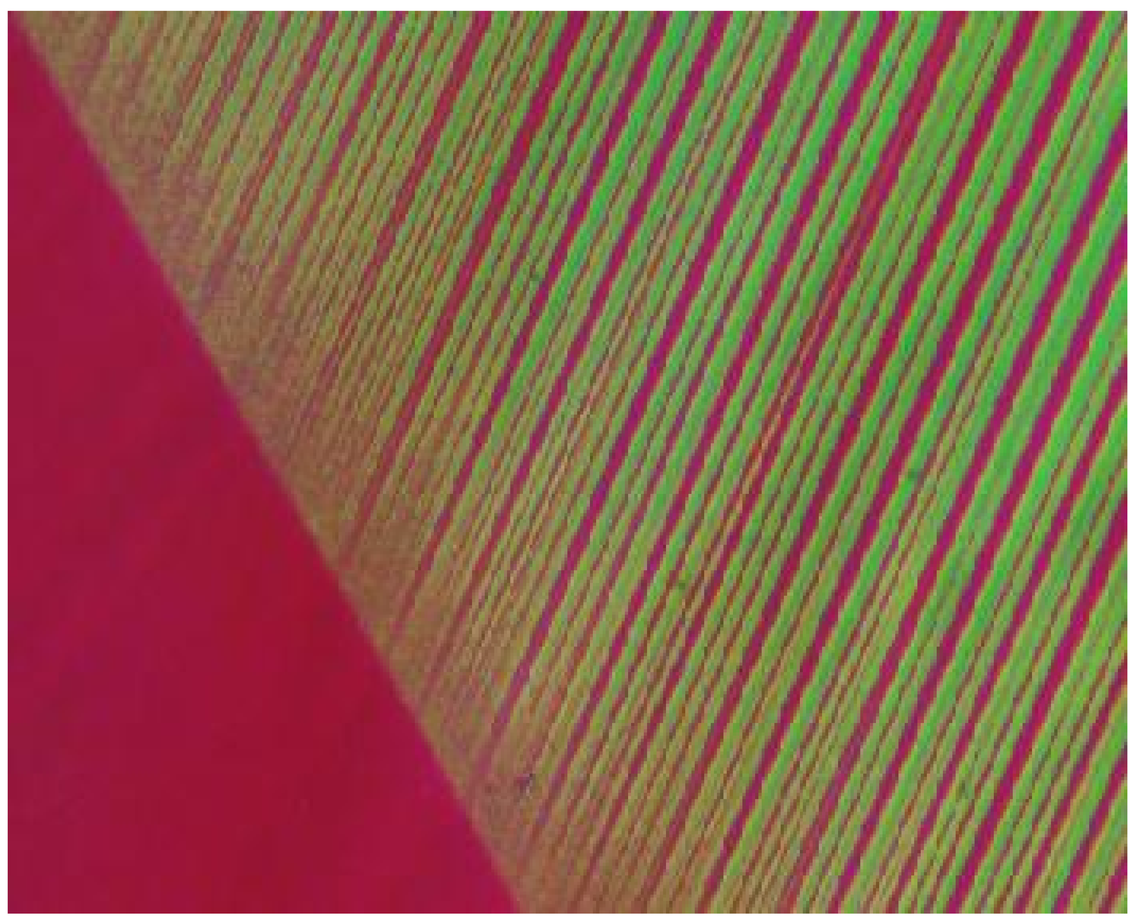

**Figure 2: Austenite/martensite boundary (R.D. James & C. Chu)**

## Theory

Standard theory and energy estimates (eg. Henry and Temam) $\Rightarrow \exists!$ solution

$$u(t) = u_0 + \int_0^t F(u(s))ds,$$

$u \in C^{0,1}([0,\infty), H_0^1(\Omega)) \cap L^\infty([0,\infty), H_0^1(\Omega))$, $u_t \in C^{0,1}((0,\infty), H_0^1(\Omega)) \cap L^\infty((0,\infty), H_0^1(\Omega))$, and

$$\int_\Omega W(\nabla u(t))dx + \int_0^t \|\nabla u_s(s)\|_{L^2(\Omega)}^2 ds = const. \qquad t \geq 0,$$

$\Rightarrow u_t \in L^2((0,\infty), H_0^1(\Omega))$ and $u_t \to 0$ in $H_0^1(\Omega)$ as $t \to 0$.

We have been unable to prove additional regularity or compactness. This limits what we can say about the long-time behaviour of solutions. Question remains: Are all solutions minimising sequences for $\int_\Omega W(\nabla u(x))dx$, or are some solutions attracted to rest points, for which $\int_\Omega W(\nabla u(x))dx > 0$?

## Numerics

Is the microstructure that we observe in Figure 3 a numerical artifact and can we bound the FEM error? Up to finite time it is possible to prove that $u_h \to u$ in $H_0^1(\Omega)$ as $h \to 0$ but we do not get a rate of convergence due to lack of additional regularity. Try regularizing problem...

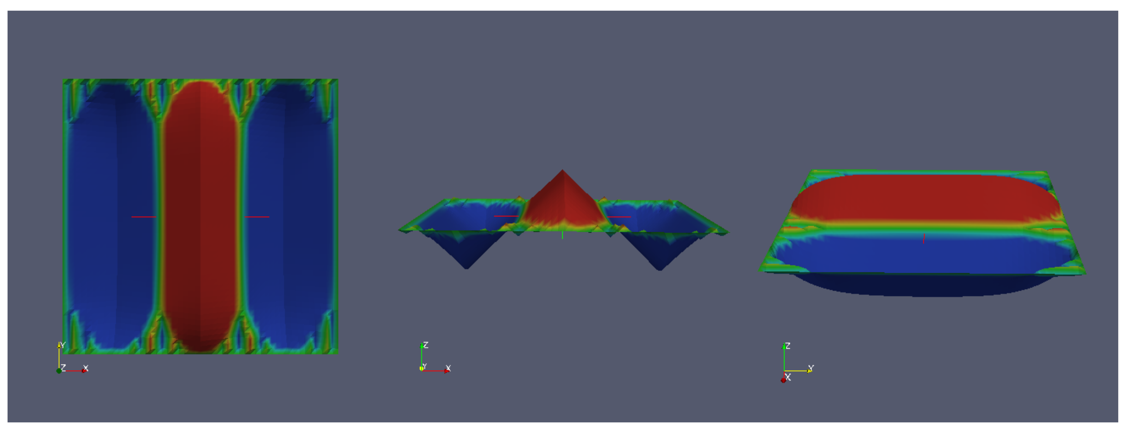

**Figure 3: Solution at $t = 15$, smooth $u_0$, standard FEM, implicit/explicit time discretization. Observe microstructure that appears from the boundary.**

## Regularized Problem

For $\epsilon > 0$ consider the problem

$$\begin{aligned} \Delta u_t - \epsilon\Delta^2 u + \operatorname{div}(\sigma(\nabla u)) &= 0 && \text{in } \Omega = (0,1)^2, \\ \Delta u = u &= 0 && \text{on } \partial\Omega, \\ u &= u_0 \in H_0^1(\Omega) && \text{at } t = 0. \end{aligned}$$

Rewrite as

$$u_t - \epsilon\Delta u = F(u) \qquad \text{in } H_0^1(\Omega). \tag{1}$$

In the gradient flow representation the additional term is bending energy, $I(u) = \int_\Omega W(\nabla u) + \frac{\epsilon}{2}(\Delta u)^2$. Using the same techniques as above we can prove similar results, e.g. $\exists!$ solution $u \in C([0,\infty), H_0^1(\Omega)) \cap C((0,\infty), V)$

$$u(t) = \mathrm{e}^{t\epsilon\Delta} u_0 + \int_0^t \mathrm{e}^{(t-s)\epsilon\Delta} F(u(s))ds$$

where $V := \{v \in H_0^1(\Omega) : \Delta v \in H_0^1(\Omega)\}$ and it is also possible to prove that for finite $T$, $\exists\, C > 0$ such that

$$\|u(t)\|_{H^1} \leq C \qquad t \in [0,\infty),$$

$$\|u(t)\|_{H^2} \leq \begin{cases} C\epsilon^{-1/2}t^{-1/2} & t \in (0,T], \\ C\epsilon^{-1/2} & t \in (T,\infty), \end{cases} \tag{2}$$

$$\|u_t(t)\|_{H^1} \leq \begin{cases} Ct^{-1} & t \in (0,T], \\ C & t \in (T,\infty). \end{cases} \tag{3}$$

Other results are also possible, eg. higher regularity, existence of a Lyapunov function, $u_t \to 0$ in $H^1$ as $t \to \infty$ and existence of a compact attractor of finite dimension (where the dimension depends on $\epsilon^{-1/2}$).

## Semi-discrete Problem

Let $V_h \subset H_0^1(\Omega)$ be finite dimensional and define $\Delta_h : V_h \to V_h$ by $(\Delta_h u_h, \phi_h)_{L^2} = -(\nabla u_h, \nabla\phi_h)_{L^2}$ for all $u_h, \phi_h \in V_h$. Also define the elliptic projection operator $R = R(h)$ and the $L^2$ projection operator $P = P(h)$ by

$$\begin{aligned} (\nabla(Ru - u), \nabla\phi_h)_{L^2} &= 0 && \forall\phi_h \in V_h, u \in H_0^1(\Omega) \\ (Pu - u, \phi_h)_{L^2} &= 0 && \forall\phi_h \in V_h, u \in H_0^1(\Omega). \end{aligned}$$

We have $\Delta_h R = P\Delta$. Assume

$$\begin{aligned} \|u - Ru\|_{L^2} + h\|u - Ru\|_{H^1} &\lesssim h^s\|u\|_{H^s} \\ \|u - Pu\|_{L^2} + h\|u - Pu\|_{H^1} &\lesssim h^s\|u\|_{H^s} \quad s = 1,2. \end{aligned} \tag{4}$$

Applying the Galerkin method to (1) we get: find $u_h \in C([0,\infty), V_h)$ such that $u = u_{0h} := Ru_0$ at $t = 0$ and

$$u_{h,t} - \epsilon\Delta_h u_h = F_h(u_h) \qquad \text{in } V_h \text{ for } t > 0,$$

where $F_h(u_h) := RF(u_h) = -\Delta_h^{-1}\operatorname{div}(\sigma(\nabla u_h))$. The same theory as earlier $\Rightarrow \exists!$ solution

$$u_h(t) = \mathrm{e}^{t\epsilon\Delta_h} u_{0h} + \int_0^t \mathrm{e}^{(t-s)\epsilon\Delta_h} F_h(u_h(s))ds.$$

Using the same techinques as earlier we get the similar regularity results for the solution to the semi-discrete problem (except the $H^2$ norm is replaced with $\|\Delta_h u_h\|_{L^2}$).

## Error Analysis

To analyse the error we follow standard theory (e.g. Larsson), but pay particular attention to the dependence on $\epsilon$, to show that

$$\|u_h(t) - u(t)\|_{H^1} \lesssim h\epsilon^{-1/2}t^{-1/2} \qquad t \in (0,T]. \tag{5}$$

A sketch of the proof is as follows. First split the error into two parts

$$e = u_h - u = \underbrace{u_h - Ru}_{\theta(t)\in V_h} + \underbrace{Ru - u}_{\rho(t)}.$$

$\rho(t)$ is just the elliptic projection error, and using (2) and (4) we get

$$\|\rho(t)\|_{H^1} \lesssim h\|u(t)\|_{H^2} \lesssim h\epsilon^{-1/2}t^{-1/2} \qquad \text{for } t \in (0,T].$$

$\theta(t)$ satisfies its own equation,

$$\theta_t - \epsilon\Delta_h\theta = F_h(u_h) - F_h(u) + (P - R)(u_t - F(u)).$$

with solution

$$\theta_h(t) = \mathrm{e}^{t\epsilon\Delta_h}\theta_{0h} + \int_0^t \mathrm{e}^{(t-s)\epsilon\Delta_h}\Big[F_h(u_h) - F_h(u) + (P-R)(u_s - F(u))\Big]ds.$$

$u_s(s)$ is not so well behaved for small $s$, see (3), so integrate by parts to get

$$\begin{aligned} \theta(t) = \mathrm{e}^{t\epsilon\Delta_h}\theta_0 & \\ &+ \int_0^t \mathrm{e}^{(t-s)\epsilon\Delta_h}\left[F_h(u_h(s)) - F_h(u(s))\right]ds \\ &- \int_0^t \mathrm{e}^{(t-s)\epsilon\Delta_h}(P-R)F(u(s))ds \\ &+ \mathrm{e}^{\frac{t}{2}\epsilon\Delta_h}(P-R)u(\tfrac{t}{2}) - \mathrm{e}^{t\epsilon\Delta_h}(P-R)u_0 \\ &+ \epsilon\int_0^{\frac{t}{2}} \Delta_h\,\mathrm{e}^{(t-s)\epsilon\Delta_h}(P-R)u(s)ds \\ &+ \int_{\frac{t}{2}}^t \mathrm{e}^{(t-s)\epsilon\Delta_h}(P-R)u_s(s)ds \end{aligned}$$

Now take $\|\cdot\|_{H^1}$ of each term separately and use (2), (3), (4) and the fact that $\|\Delta_h^\alpha\,\mathrm{e}^{t\epsilon\Delta_h}\| \lesssim \epsilon^{-\alpha}t^{-\alpha}$ for $\alpha \geq 0$ in either the $H^1$ or $L^2$ norm to get the result (5).

If we choose $h$ sufficiently small, $h^{2-2\delta} < \epsilon$ for some $\delta > 0$, then

$$\|u_{\epsilon h} - u_\epsilon\|_{H^1} \lesssim h^\delta t^{-1/2}$$

*independent of $\epsilon$.* Unfortunately we can only prove that $u_\epsilon \to u$ in $H_0^1(\Omega)$ as $\epsilon \to 0$ up to finite time . We do not have a rate of convergence for the regularization error.

## Numerics and Conclusions

Numerical simulations in Figure 4 suggest that too much regularization might prevent microstructure from appearing.

Other results that we have made some progress towards include: long-time convergence result for the convergence of attractors, bounding the discretization error in $L^2$ and existence of non-trivial rest points for the original PDE.

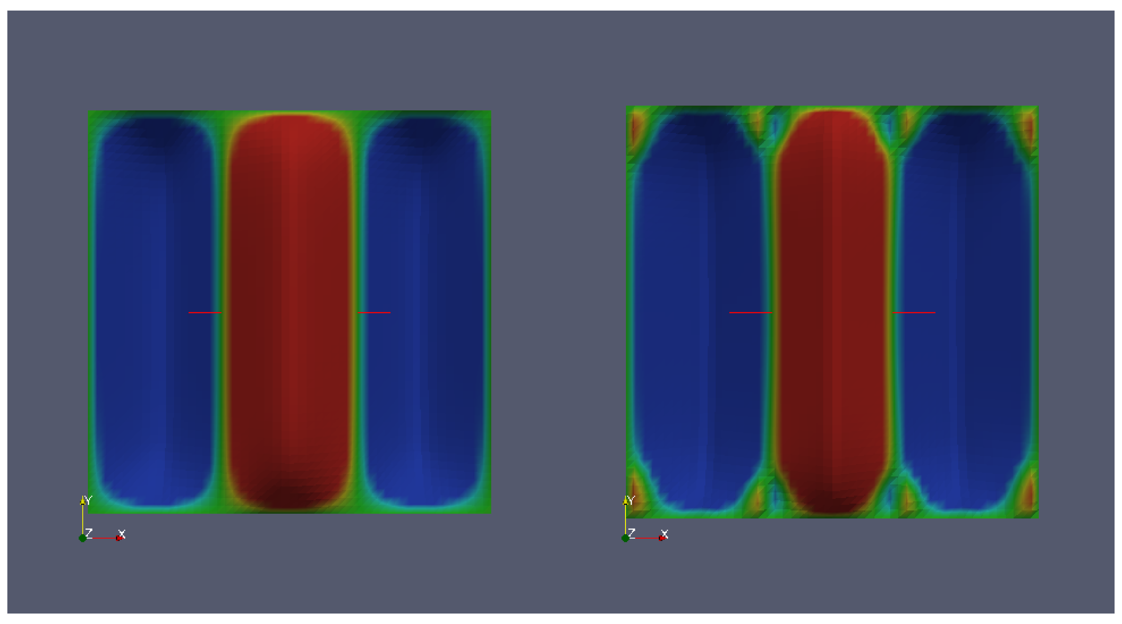

**Figure 4: left: $\epsilon = 10^{-3}$, right: $\epsilon = 10^{-4}$. $h = \frac{1}{50}$.**


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