# Numerical and analytical aspects of the pinning of martensitic phase boundaries

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We study the pinning and depinning behavior of interfaces immersed in a heterogeneous medium. For a fully elastic model of the martensitic phase transformation, we numerically estimate the critical depinning stress of a phase boundary intersecting a non-transforming inclusion in the material. In the limit of a nearly flat phase boundary, the elastic energy of the phase boundary can be approximated by an elliptic operator of order 1. For such an approximation we study the depinning transition near the critical point. Finally, we prove existence of a pinned solution for a parabolic model for the evolution of phase boundaries in a random environment.



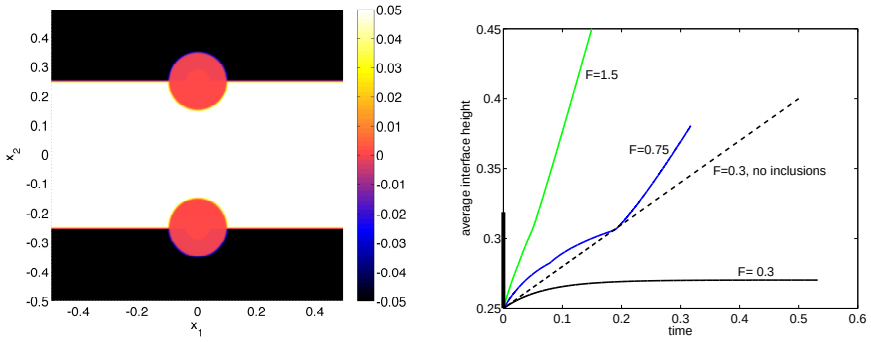
## 1 Introduction and model

The phenomenon of rate independent hysteresis is ubiquitous in phase transforming materials. Macroscopic models commonly incorporate hysteresis by using a rate independent evolution model for phase fractions or phase boundaries. Microscopic models, however, often assume a linear (viscous) dependence of the velocity of a phase boundary on the associated thermodynamic driving force. In this article, we wish to explore the question of whether, and if so how, rate independent hysteresis can emerge from the interaction of viscously evolving phase boundaries with a heterogeneous environment.

In section 2 we study a model for martensitic phase boundaries, where the heterogeneity consists of non-transforming inclusions in the material and provide a numerical estimate for the critical depinning stress. Then, an approximate model is derived and its behavior near the critical force is examined in section 3. Finally, in section 4, we study a generic model involving line-tension under the influence of a random environment.

## 2 Numerical estimate of the critical depinning force

To study the pinning of martensitic phase boundaries by non-transforming inclusions, we assume a linearly elastic material with its transformation strain depending on the material phase. For more information on such models, see [2]. For simplicity, we restrict ourselves to two




(a) Initial configuration of the transformation strain

(b) Evolution of the average height of the interfaces for different external loads.

**Fig. 1** Initial condition and evolution of the interface depending on the external load

phases and an anti-plane shear model of scalar displacement. For a given phase distribution, one can write the elastic energy of the system as

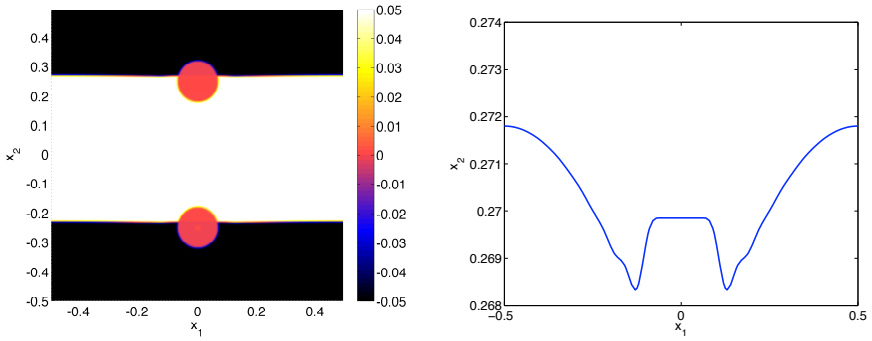
$$E_{\text{elastic}} = \min_u \int_\Omega \frac{1}{2} \left|\nabla u(x) - \xi_A(x)\right|^2 \, \mathrm{d}x,$$

where $u\colon \Omega \subset \mathbb{R}^{n+1} \to \mathbb{R}$ is the displacement field of sufficient regularity and endowed with suitable boundary conditions. The transformation strain $\xi_A$ fixes the phase distribution. We take it to be piecewise constant, assuming respective constants in the regions associated with each phase. In order to model the inclusions, we assign a third value to $\xi$ at the domain of the inclusions. Thus, taking $A \subset \Omega$ to be the domain occupied by the first phase, $\Omega \setminus A$ to be the domain occupied by the second phase, and $B \subset \Omega$ being the region occupied by inclusions, we write

$$\xi_A(x) = \begin{cases} \xi^+ & x \in A \setminus B \\ \xi^- & x \in (\Omega \setminus A) \setminus B \\ \xi^0 & x \in B. \end{cases}$$

A common course of action would be to minimize this elastic energy also with respect to $A$, thus finding the energy-minimizing phase-distribution, see for example [3]. We would like to follow a different route though: We study the viscous gradient flow of the boundary of $A$ with respect to the elastic energy and under the influence of a constant external driving force.

The first question that arises is whether or not the interface will assume a steady state at non-vanishing external driving force. In an attempt to answer this question, a two-dimensional numerical simulation of the interface evolution in the model described above has been developed using MATLAB. The transformation strain is chosen to be $\xi^\pm = \pm(0, 0.05)^{\mathrm{T}}$ and $\xi^A = 0$. On the domain $\Omega$, one-periodic in both $x_1$ and $x_2$, we place two inclusions at $x_1 = 0$ and $x_2 = \pm 0.25$. The inclusions occupy approximately three per cent of the area. For symmetry reasons it is clear that the situation depicted in Figure 1(a), where phase 1 is occupying the region $-0.25 \geq x_2 > 0.25$ is a stationary state if there is no force applied. Starting at this




(a) Transformation strain corresponding to a stuck interface. The strong elastic forces keep the phase boundary nearly flat.

(b) One of the splines describing the interface in its stuck state

**Fig. 2** The stuck phase boundary

initial state, we evolve the interface according to a gradient flow with respect to the energy, under varying external applied forces, until either a steady state is reached or the interfaces escape from the inclusions.

The two phase boundaries in the simulation are described by cubic periodic B-splines, in the present case with 32 knots. According to the position of the phase boundary, the transformation strain $\xi_E(x)$ is generated on a $256 \times 265$ grid. As one can see in Figure 1(a), the phase boundary and also the boundaries of the inclusions are smoothed out slightly. A purely piecewise constant transformation strain would lead to artificial pinning of the interface. The elastic energy calculated by solving the equilibrium equation for the displacement using the Fourier transform. We calculate the variation of the energy with respect to the position of the interface by numerically differentiating the elastic energy with respect to the position of the nodes of the B-spline defining the phase boundary. This generates a force for each node of the spline. To this force, we add a constant applied load $F$ and evolve the nodes of the spline by a first-order explicit step in time—higher order schemes would of course not be hard to implement, however, to answer the question whether the interface can become stuck a first order scheme is sufficient. The part of the phase boundary that is inside the inclusions is interpolated linearly, since no force acts on it.

Figure 1(b) shows the evolution of the average height of phase boundaries for different applied loads. The size of the inclusion is indicated by the black bar on the $x_2$-axis in the figure. For $F = 1.5$ and $F = 0.75$ (non-dimensionalized units), the interface is only slowed down slightly. For $F = 0.3$, we notice that the interface indeed becomes stuck. For comparison, the evolution of the interface at $F = 0.3$ without any inclusions in the domain is also shown. The interface gets stuck in the configuration shown in Figure 2. By starting the simulation with the two interfaces slightly displaced, it has also been verified that there is indeed an effect that pulls the interface back to the stuck state.

In order to give an estimate of the driving force necessary to release an interface from such an inclusion, one has to re-introduce physical units to the calculation. In this elastic case this

is not hard. By merit of the scale invariance of linear elasticity the only relevant quantities are the volume fraction of the inclusions and the elastic modulus. If we assume an elastic modulus of $100\,\mathrm{GPa}$, (in relation to the elastic modulus of the simulation, which was normalized to $1 \cdot 256^2$ non-dimensional units, due to the discretization) this leads to a critical pinning stress on the order of $1\,\mathrm{MPa}$. This compares very favorably to the critical stress found in [1].

## 3 Depinning transition in an approximate model

As one can see in Figure 2, due to the strong restoring force of the elastic energy, the interface remains almost completely flat, even when interacting with inclusions. In [7], an approximate model for a nearly flat interface, given as the graph of a function $g\colon \Omega \subset \mathbb{R}^n \to \mathbb{R}$ has been derived. Using the method of $\Gamma$-convergence, it was possible to show that the elastic energy of the system can be approximated by the $H^{1/2}$-seminorm of the function $g$ for a sufficiently flat interface. It is well known that the variation of the $H^{1/2}$-seminorm on a periodic domain yields the square root of the Laplace operator. We also make the assumption that the influence of the precipitates can be approximated by a local, smooth, nonlinear force term $\varphi\colon \mathbb{R}^{n+1} \to \mathbb{R}$ acting on the interface and study this simplified model for $n = 1$ with periodic boundary conditions. This leaves us with the governing equation

$$g_t(x,t) = -(-\Delta^{1/2})g(x,t) + \varphi(x, g(x)) + F. \tag{1}$$

We prove in [7] that for this equation there exists a critical depinning threshold $F^*$ so that, for $F \leq F^*$, there exists a stationary solution to (1) and for $F > F*$ there exists a time-space periodic propagating solution with average velocity $\bar{v}(F)$. In [6] it is proved that the depinning transition of a parabolic system (Laplacian instead of the square root of the Laplacian in (1)) exhibits—under certain non-degeneracy conditions—a power law behavior. In this case, close to the critical driving force, the average velocity $\bar{v} = 1/T$ of the unique space-time periodic solution is given by

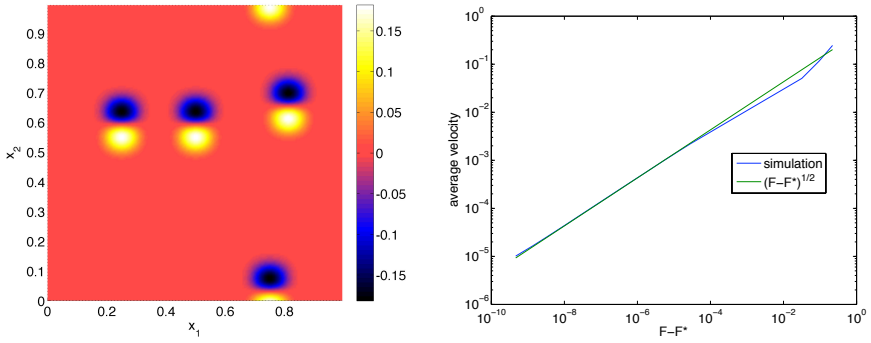
$$\bar{v} = C \cdot \sqrt{F - F^*} + o(\sqrt{F - F^*}), \tag{2}$$

where $C$ depends on the local forcing $\varphi$. In order to study this behavior in our non-local elasticity setting, a series of numerical simulations were conducted on a 2d periodic domain to examine the depinning behavior. The results show good agreement with a square-root power law behavior. It is important to note that the depinning behavior depends very sensitively on the discretization of the pinning force. In [6], the power law behavior is only proved if $\varphi \in C^2$. In fact, for a piecewise linear or piecewise constant approximation of the local pinning force, we do not see the same behavior.

### 3.1 The numerical method

Starting with an initial configuration $g(0) = 0$ and a fixed applied load $F$, we numerically integrate equation (1) using an explicit first-order Euler scheme[1]. The elastic force is calculated using Fourier transforms. The local pinning force is constructed using a cubic B-spline.

[1] An explanation might be in order. The timestep of the simulation has to be fairly small, since otherwise one will miss the peak of the pinning force $\varphi$, simply jumping over it in one timestep. The time integration nevertheless has to be fast, since the propagation becomes very slow near the depinning transition. For this reason we employ such a simplistic scheme.




(a) Force distribution used to examine the general depinning behavior.

(b) Power law of the depinning transition

**Fig. 3** Experiment 1, the general depinning behavior

Once the interface has traveled a certain length on average (and never became stuck on the way), the final time is recorded. In this way, a relation between the average velocity $\bar{v}$ and $F$ is obtained. The interface is considered stuck if the $L^2$ norm of the driving force $f$ drops below a certain threshold. This 'inner loop' is repeated with $F$ chosen each time through a bisection algorithm, thus giving new upper and lower bounds for the critical $F^*$ at each run. The program terminates after a certain accuracy for determining $F^*$ has been reached.

### 3.2 Simulations

As a standard example, we use a local driving force $\varphi(x_1, x_2) = \frac{\partial}{\partial x_2}\Phi(x_1, x_2)$, where $\Phi$ is a potential that has smooth dips of a fixed depth and radius at random points. We approximate $\varphi$ by a cubic $C^2$ spline curve. The exact force used in this simulation is depicted in Figure 3(a). In Figure 3(b), the relation between the average velocity, compared to a square-root power law is shown. The fit over almost three decades is excellent and at the very high end of the applied force one can see that the velocity turns toward a linear dependence on the applied force, as expected.

## 4 Random obstacles

The periodic arrangement of obstacles treated in Section 3 is of course a great simplification. The in many cases more realistic problem of interface evolution in a random environment has received much attention from physicists (see [8] for an overview). Rigorous results, however, are still scarce. We will study a similar problem as in Section 3, but go back to the simpler case of line tension instead of the square root of the Laplacian.

The essential difficulty in studying an equation for interface evolution in a random environment, in this case

$$u_t(x,t,\omega) = \Delta u(x,t,\omega) + f(x, u(x,t,\omega), \omega) + F, \quad \omega \in \Omega \text{ (probability space)}, \quad (3)$$

stems from the fact that the randomness appears in the nonlinear term in the equation. It is thus necessary to make some assumptions on $f\colon \mathbb{R}^n \times \mathbb{R} \times \Omega \to \mathbb{R}$. A particular model of interest is that of smooth obstacles of fixed shape $\phi\colon \mathbb{R}^n \times \mathbb{R} \to [-1,0]$, $\phi(x,y) = -1$ for $|x|^2 + y^2 \leq r_0^2$, $\phi(x,y) = 0$ for $|x|^2 + y^2 \geq r_1^2$, $\phi \in C_c^\infty$. The centers of the obstacles are distributed by a $n+1$-dimensional Poisson process $(x_k, y_k)$ and the obstacles have random strength, so that $f(x,y,\omega) = \sum_k f_k(\omega)\phi(x - x_k(\omega), y - y_k(\omega))$.

For such a model for an interface evolving in a random environment, the existence of pinned solutions at finite driving force was proved [5]. To provide a barrier for the moving interface, we constructed a positive, steady-state supersolution. The construction depends on the existence, after rescaling, of a Lipschitz hypersurface separating the domain into a top and a bottom part, consisting of boxes that contain at least one obstacle of sufficient strength. This was proved in [4].

**Theorem 4.1** (Lipschitz percolation) *Consider site percolation in $\mathbb{Z}^{n+1}$ and declare a site open with probability $p \in (0,1)$ independent of each other. There exists $p_c < 1$ so that for $p > p_c$, there exists a 1-Lipschitz function $w\colon \mathbb{Z}^n \to \mathbb{N}_0$ so that $w(z)$ open for all $z \in \mathbb{Z}^n$.*

From this Lipschitz percolation result one can construct a supersolution $v \geq 0$ to (3). In a first step, one has to rescale $\mathbb{R}^n \times \mathbb{R}$ into boxes so that in each box there is a large enough obstacle with probability $p > p_c$, leaving space between the boxes in $x$-direction. Then one uses a parabola-solution inside the obstacles, a solution of $\Delta v = F_1 < 0$ outside the obstacles on ring-shaped domains, as well as a gluing function in the spaces between the boxes in order to take the function $v$ to the correct height. This gluing function needs to have small second derivatives in order to not destroy the supersolution property, which is where the Lipschitz property of the percolation cluster is necessary.

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