

Numerical Computation of Stress Induced Microstructure

Zhiping Li (李治平)

LMAM & School of Mathematical Sciences, Peking University, Beijing 100871, P.R.China
(email: zpli@math.pku.edu.cn)

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Abstract: The mesh transformation method is applied on a two dimensional elastic crystal model to study the formation of laminated microstructure in austenite-martensite phase transition when certain external loads are applied. Numerical experiments show that simple laminated microstructures with various volume fractions and twin width can be obtained by varying the loads. Numerical experiments also show that second order laminated microstructure with branched needle-like laminates can also be obtained by certain loads.

Keywords: nonconvex energy minimization, mesh transformation, stress induced phase transition, laminated microstructure.

1 Introduction

It is well known that many elastic crystals undergo austenitic-martensitic phase transitions across the transformation temperature. It is also observed that the phase transition does not usually take place automatically unless the temperature drops well below the transformation temperature, it somehow needs to be "triggered". An external load can be applied to induce the phase transition.

For the static problem of austenitic-martensitic phase transitions, the well known geometrically nonlinear theory given by Ball and James [1, 2] leads to the consideration of minimizing the elastic energy

$$F(u; \Omega) = \int_{\Omega} f(\nabla u(x), \theta(x)) dx \quad (1.1)$$

in a set of admissible deformations

$$\mathbb{U}(u_0; \Omega) = \{u \in W^{1,p}(\Omega; R^m) : u = u_0, \text{ on } \partial\Omega_0\}, \quad (1.2)$$

where $\Omega \subset R^n$ is a bounded open set with a Lipschitz continuous boundary $\partial\Omega$, $\partial\Omega_0$ is a subset of $\partial\Omega$, θ is a given temperature field and $n < p < \infty$, and where the

elastic energy density $f(\cdot, \theta)$ is such that there is a unique potential well above the transformation temperature ($\theta > \theta_T$) and there are several symmetry related potential wells below the transformation temperature ($\theta < \theta_T$) [1, 2].

In the present paper, we consider a two dimensional model ($n = m = 2$)

$$f(\nabla u, \theta) = \Phi(C, \theta), \quad (1.3)$$

where $C = (\nabla u)^T \nabla u \in \mathbb{S}^n = \{A \in R^{n \times n} : A^T = A\}$ is the right Cauchy-Green strain tensor and

$$\begin{aligned} \Phi(C, \theta) = & \frac{b(\theta)}{4}(C_{11} - C_{22})^2 - \frac{c(\theta)}{8}(C_{11} - C_{22})^2 |C_{11} - C_{22}| \\ & + \frac{d(\theta)}{16}(C_{11} - C_{22})^4 + e C_{12}^2 + g(\text{tr } C - 2)^2, \end{aligned} \quad (1.4)$$

where

$$b(\theta) = (1 + \alpha \arctan \mu(\theta - \theta_T)) d_0 \varepsilon^2, \quad (1.5)$$

$$c(\theta) = 2(1 + \frac{1 + 2\gamma}{3} \alpha \arctan \mu(\theta - \theta_T)) d_0 \varepsilon, \quad (1.6)$$

$$d(\theta) = (1 + \gamma \alpha \arctan \mu(\theta - \theta_T)) d_0, \quad (1.7)$$

and where $d_0 > 0$, $e > 0$ and $g > 0$ are the elastic moduli, ε is the transformation strain, θ_T is the transformation temperature,

$$\alpha \approx \frac{2}{\pi}, \quad \mu > 0, \quad \text{and } \gamma < 1 \quad (1.8)$$

are the material constants used to reflect the change of elastic moduli and the energy barriers as the temperature varies.

For properly given boundary data u_0 , if $\theta < \theta_T$, the minimizing sequences of the elastic energy $F(\cdot; \Omega)$ in $\mathbb{U}(u_0; \Omega)$ will be essentially consist of finely laminated twins which are in the energy wells [1, 2]. Many numerical methods have been developed to compute the laminated microstructure (see [3, 4, 5, 6, 7, 8] among many others). The mesh transformation method is chosen for our purpose, since it minimized the mesh dependence which can be a serious problem in the computation of microstructures [9, 10].

To induce the phase transition, a load term is introduced into the total potential energy

$$F_t(u; \Omega) = \int_{\Omega} f(\nabla u(x), \theta(x)) dx - \int_{\partial\Omega_1} t \cdot u ds, \quad (1.9)$$

where t is a surface tension applied on $\partial\Omega_1$, and the minimizing procedure is performed with certain load t which is initially non-zero and vanishes later on at properly chosen "time".

In section 2, the mesh transformation method is described. In section 3, numerical experiments and results are given and discussed, and we see that the numerical computations produce laminated microstructures which are qualitatively in agreement with the physical experiments [11, 12].

2 The mesh transformation method

Consider the problem of minimizing the functional $F(u; \Omega) = \int_{\Omega} f(\nabla u(x)) dx$ in $\mathbb{U}(u_0; \Omega)$. Let $\mathfrak{T}_h(\Omega)$ be a family of regular triangulations of Ω [13]. Let

$$T(\Omega) = \{\text{bijections } g : \bar{\Omega} \rightarrow \bar{\Omega} \mid g \in (W^{1,\infty}(\Omega))^n, g^{-1} \in (W^{1,\infty}(\Omega))^n, \\ g(\partial\Omega_0) = \partial\Omega_0, \text{ and } \det \nabla g > 0, a.e. \text{ in } \Omega\} \quad (2.1)$$

and

$$T_h(\Omega) = \{g \in T(\Omega) : g|_K \text{ is affine } \forall K \in \mathfrak{T}_h(\Omega)\}. \quad (2.2)$$

Define the functional $F(\cdot, \cdot; \Omega)$ by

$$F(\bar{u}, g; \Omega) = \int_{\Omega} f(\nabla \bar{u}(\bar{x})(\nabla g(\bar{x}))^{-1}) \det \nabla g(\bar{x}) d\bar{x}. \quad (2.3)$$

By changing the variables

$$x = g(\bar{x}), \quad u(x) = \bar{u}(g^{-1}(x)), \quad (2.4)$$

we are lead to the following discrete problem

$$(MTM) \begin{cases} \text{find } (\bar{u}_h, g_h) \in \mathbb{U}_h(u_0 \circ g_h; \Omega) \times T_h(\Omega) \text{ such that} \\ F(\bar{u}_h, g_h; \Omega) = \inf_{(\bar{u}, g) \in \mathbb{U}_h(u_0 \circ g; \Omega) \times T_h(\Omega)} F(\bar{u}, g; \Omega). \end{cases} \quad (2.5)$$

This is the so called mesh transformation method (for the convergence analysis and other applications of the mesh transformation method, see [6, 7, 14]), which is equivalent to minimizing the elastic energy $F(\cdot; \Omega)$ among all finite element function spaces introduced by $\mathfrak{T}_h(D)$ and $T_h(D)$, in particular on those whose mesh are aligned with the twin boundaries, and thus is capable of producing much better numerical results than working on a fixed finite element function space, especially when the volume fractions are changing and twin boundaries are bending.

3 Numerical experiments and results

Consider the problem of minimizing the total potential energy

$$F_t(u; \Omega) = \int_{\Omega} f(\nabla u(x), \theta(x)) dx - t(u), \quad (3.1)$$

in the set of admissible deformations

$$\begin{aligned} \mathbb{U}_0(\Omega) = \{u \in W^{1,8}(\Omega; R^m) : (u(x) - x)|_{\partial\Omega_-} \cdot \mathbf{n}(\pi/4) = 0, \\ (u(x) - x)|_{\eta} \cdot \mathbf{n}(-\pi/4) = 0 \}, \end{aligned} \quad (3.2)$$

where the reference configuration $\Omega = R(\pi/4)D$ with $D = (-2, 2) \times (-1, 1)$, $\partial\Omega_- = R(\pi/4)\{x : x_1 = -2, |x_2| \leq 1\}$, $\eta = R(\pi/4)\{x : x_1 = 0, x_2 = 2\}$, and where $R(\alpha)$ is the rotational matrix corresponding to anticlockwise rotation α and $\mathbf{n}(\alpha) = (\cos(\alpha), \sin(\alpha))^T$ (see figure 1), and where the elastic energy density $f(\nabla u(x), \theta(x))$ is defined by (1.3)-(1.7) with the elastic constants $\alpha = 2.02/\pi$, $\mu = 0.25$, $\gamma = 0$, $\varepsilon = 0.05$, $d_0 = 500$, $e = 3.5$ and $g = 15$, the transformation temperature $\theta_T = 70^\circ\text{C}$. In our numerical experiments, we take $\theta(x) \equiv 60^\circ\text{C}$, and we consider bending and shear loads of which the corresponding potentials $t(u)$ are given by

$$t(u) \equiv t_b(u) = 2 t_b \left(\frac{3\pi}{4} - \arctan \left(\frac{u_2(\zeta) - u_2(\xi)}{u_1(\zeta) - u_1(\xi)} \right) \right) \quad (3.3)$$

and

$$t(u) \equiv t_s(u) = t_s \int_{\partial\Omega_+} \left(\frac{u(\zeta) - u(\xi)}{|u(\zeta) - u(\xi)|} \right) \cdot u \, ds \quad (3.4)$$

respectively, where $\xi = R(\pi/4)\{x : x_1 = 2, x_2 = -1\}$, $\zeta = R(\pi/4)\{x : x_1 = 2, x_2 = 1\}$ and $\partial\Omega_+ = R(\pi/4)\{x : x_1 = 2, |x_2| \leq 1\}$ (see figure 1).

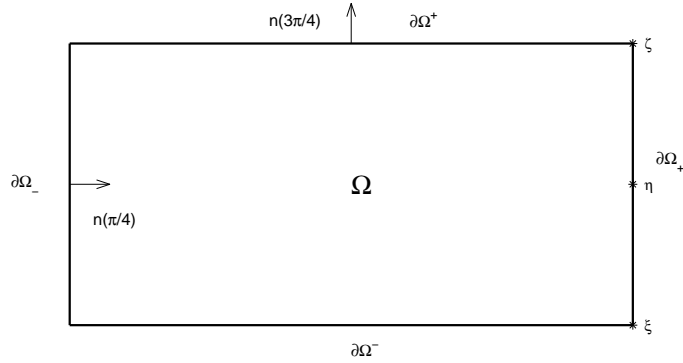


Figure 1: The reference configuration of the problem.

Let $\mathfrak{T}_{N,M}(\Omega) = \mathfrak{T}_h(\Omega)$ be a family of regular triangulations defined by

$$\mathfrak{T}_{N,M}(\Omega) = \mathfrak{T}_h(\Omega) = \mathfrak{T}_h(R(\pi/4)D) = \{R(\pi/4)K : \forall K \in \mathfrak{T}_h(D)\}, \quad (3.5)$$

where $\mathfrak{T}_h(D) = \mathfrak{T}_{N,M}(D)$, for $h = h_{N,M} = \frac{2}{N \cdot M} \sqrt{4M^2 + N^2}$ with $N \geq 2$ and $M \geq 2$, is a family of regular triangulations of D introduced by the lines

$$\begin{cases} y = -1 + \frac{2}{M}i, & 0 \leq i \leq M; \\ x = -2 + \frac{4}{N}j, & 0 \leq j \leq N; \\ y = \frac{N}{2M}(x+2) + 1 - \frac{4}{M}k, & 0 < k < \frac{M+N}{2}; \\ y = \frac{-N}{2M}(x-2) - 1 + \frac{4}{M}k, & 0 < k < \frac{M+N}{2}. \end{cases} \quad (3.6)$$

The mesh transformation method described in section 2 is applied to discretize the problem, and the conjugate gradient method is used in the minimizing process. To avoid the elements being deformed too much and too fast where the initial deformation gradient is well away from the wells, the mesh transformation map g is kept fixed in the beginning of the minimizing process until the drop of the elastic energy is getting lost of its initial momentum. To guarantee that the condition $\det \nabla g(x) > 0$ is satisfied in the minimization process, it is checked on each element in the linear search along the direction given by the conjugate gradient method and the step length is reduced whenever necessary. Remember that our purpose is not to find a minimizer of $F_t(\cdot; \Omega)$ in $\mathbb{U}_0(\Omega)$, the external load is only used to induce the phase transition. So the external load is subjected to change during the minimizing process and will be removed after a certain number of iterations when the phase transition is complete and certain microstructure has formed. Then the minimizing process will be continued on a refined mesh for the problem with respect to $t(u) \equiv 0$ until convergence is achieved, *i.e.* when certain convergence criteria (say $\|\nabla F\|_2 < 10^{-6}$) is satisfied.

Example 1. Let the initial deformation $u_0(x) = x$, for all $x \in \Omega$, that is the material is initially in the austenite phase. Take $N = 16$ and $M = 8$. A bending load with $t_b = 2.0 \times 10^{-2}$ is applied. The phase transition is complete in a few hundred iterations, and a relatively stable simple laminated microstructure is formed in 6000 iterations. Then, we set $t_b = 0$, and the convergence is achieved ($\|\nabla F\|_2 < 4 \times 10^{-7}$) in 8374 iterations, and we end up with a simple laminated microstructure with volume fraction $\lambda \approx 0.5$. The numerical result is shown in figure 2.

If after the bending load is removed, we apply a shear load with $t_s = 2.0 \times 10^{-2}$, then the volume fraction of the laminates will change in the minimizing process. In 6000 iterations, the volume fraction changes to $\lambda \approx 0.65$. Then, we set $t_s = 0$, and continue the minimizing process until the convergence is achieved ($\|\nabla F\|_2 < 4 \times 10^{-7}$ in 29281 iterations). The numerical result is shown in figure 3, where we can see that the ratio of the volume fractions of the two martensite variants is about 2 : 1.

In our numerical experiments, we found that, at 60°C , a bending load with strength $t_b \leq 1.25 \times 10^{-4}$ is not strong enough to induce the austenite-martensite phase transition, while a bending load with strength $t_b \geq 0.25$ is too strong to produce a

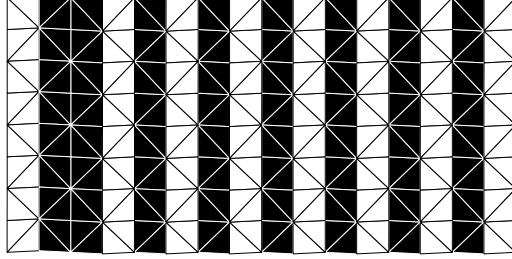


Figure 2: A simple laminated microstructure obtained by bending.

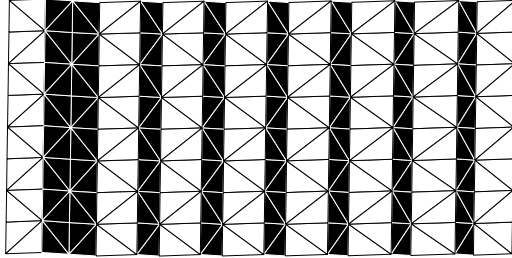


Figure 3: A simple laminated microstructure obtained by bending and shear.

well ordered microstructure. For the bending load of strength $t_b \in (2.0 \times 10^{-4}, 0.1)$, different patterns of microstructures can be produced. Typically, for sufficiently large and sufficiently small t_b , second order laminated microstructures can be produced, while for t_b around 2.0×10^{-2} if there are sufficiently many iterations before the load is removed, a simple laminated microstructure is produced. We also found in our numerical experiments that the application of the mesh transformation method is essential to obtain a well formed second order laminated microstructure.

Example 2. As in example 1, let the initial deformation $u_0(x) = x$, for all $x \in \Omega$. Take $N = 32$ and $M = 16$. A bending load with $t_b = 1.5 \times 10^{-2}$ is applied. The phase transition is complete in a few hundred iterations, and a second order laminated microstructure is formed in 4500 iterations (see figure 4).

Then, we set $t_b = 0$ and refined the mesh to $N = 128$ and $M = 64$, and continue the minimizing process. After 5500 iterations, we obtain a well formed second order laminated microstructure as shown in figure 5. In further 185000 iterations ($\|\nabla F\|_2 < 2 \times 10^{-5}$), branched needles are formed near the interface of the two laminates (see figure 6).

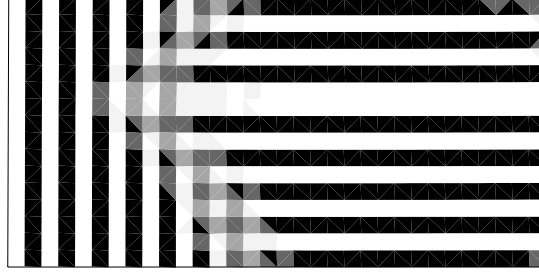


Figure 4: A second order laminated microstructure obtained by applying bending load with $t_b = 1.5 \times 10^{-2}$ in 4500 iterations.

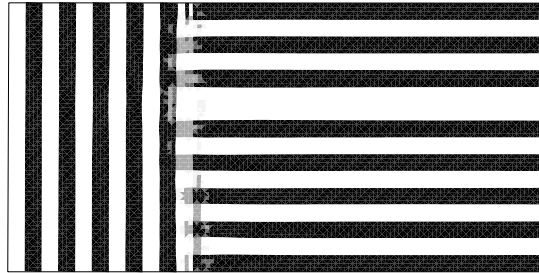


Figure 5: A second order laminated microstructure obtained after the bending load $t_b = 1.5 \times 10^{-2}$ is removed (in 5500 iterations).

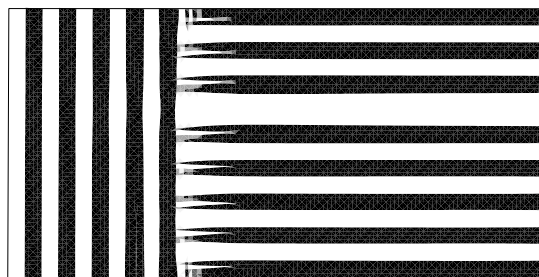


Figure 6: A second order laminated microstructure with branched needles obtained for example 2 (in further 185000 iterations).

Example 3. As in the above examples, let the initial deformation $u_0(x) = x$, for all $x \in \Omega$. Take $N = 32$ and $M = 16$. A bending load with $t_b = 2.75 \times 10^{-2}$ is applied. A second order laminated microstructure is formed in 500 iterations (see figure 7). Then, we set $t_b = 0$ and refined the mesh to $N = 128$ and $M = 64$, and continue the minimizing process. After 2300 iterations, we obtain a well formed second order laminated microstructure as shown in figure 8. In further 145000 iterations ($\|\nabla F\|_2 < 2 \times 10^{-5}$), branched needles are formed near the interfaces of the adjacent laminates (see figure 9).

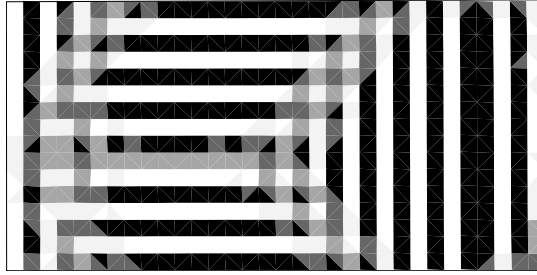


Figure 7: A second order laminated microstructure obtained by applying bending load with $t_b = 2.75 \times 10^{-2}$ in 500 iterations.

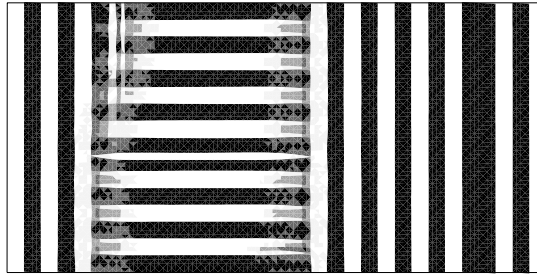


Figure 8: A second order laminated microstructure obtained after the bending load $t_b = 2.75 \times 10^{-2}$ is removed (in 2300 iterations).

4 Discussions

Since the surface energy, or strain gradient, is not considered in the elastic energy model used above, we face the fact that the energy minimizing sequences lead to finer

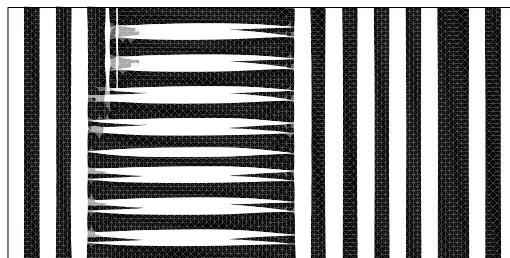


Figure 9: A second order laminated microstructure with branched needles obtained for example 3 (in further 145000 iterations).

and finer oscillations (microstructures) [1, 2], and thus what we obtain in computations are local minimizers in which the laminates' width scale is decided by the initial mesh size h (generally of order $O(h^{1/2})$ [8]). As a special case, when the mesh is aligned with the laminates, the laminates' width scale is of the same order as that of the initial mesh size h . By considering the surface energy, we can compute the size of laminated microstructures [14].

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