Numerical Simulation in 2-D martensitic phase transition and microstructure

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1. Introduction

Crystal is the solid whose atomic structures are determined by lattices, e.g.

$$L(e_{\cdot}, e_2, e_3) = \left\{ \sum_{i=1}^{3} m_i e_i : m_i \in Z, i = 1,2,3 \right\}$$

One type of special crystal is Martensitic crystal, which can undergo reversible, diffusionless, structural phase transformations. We call this kind of transformations are martensitic transformations. It is observed in various metals, alloys, ceramics and even biological systems. For instance, it has the role in strengthening steel. The martensitic microstructure is the fine-scale mixtures of coherent phases of martensitic crystals. A very good example of martensitic crystal is some shape -memory alloys.

I am interested in the martensitic microstructure produced in the typical continuum transformation, in which the high temperature austenite phase transforms to the low-temperature martensite phase. Specifically I will investigate the 2-D vectorial problem with surface energy, in which the situation along the interface will be considered. Therefore, I can foresee that more complicated structure will appear more than the lamination, for instance, needle structure and branch structure.

The martensitic phase transformations can be induced by temperature or stress. In my project, I will concentrate on the temperature induced transformations.

2. Mathematical Model

We know that materials are seeking the possible lowest energy to maintain stability. The numerical way to determine these microstructures is to construct an energy density which models the properties of a crystalline solid and then to numerically compute approximate energy minimizing deformations.

Say, we have a reference domain: $\Omega \subset R^n$ (undeformed austenite)

Let's define Energy Density $f(F)$, where $F = \nabla y \in R^{n\times n}$, deformation: $y : \Omega \to R^n$

- $f(F) \ge 0$ with $f(U_0) = f(U_1) = 0$.

  $f(F) = 0 \Leftrightarrow F \in SO(3)U_1 \cup \cdots \cup SO(3)U_N$ (energy minimizer)

  $SO(3)$ is the set of all proper rotations; $SO(3)U_i (i = 1, \cdots, N)$: energy well

- $f(RF) = f(F)$, for all rotation R. (Frame indifference)

- Minimizing gradients RU_i = variants of martensite.

- $f(F) \ge a \|F - \Pi F\|^p$, $p > 1$, Π projects onto variants.

- $f(F) \ge 0$ with $f(U_0) = f(U_1) = 0$.

Based on the nonconvex energy density function, we may consider the energy minimizing deformations. (The case of convex energy density function is trivial)

The energy-minimizing sequences can model fine-scale martensitic microstructure.

Problem: Find $y \in A$ which minimizes

$$e(y) = \int_\Omega f(\nabla y(x))dx$$

where

$$A = \{y \in \Omega \to R^3 : y(x) = y_0(x), x \in \partial\Omega\}.$$

3. The problems I will work on, the steps I will take

1) The simple test problem I will get started

   1-D problem with simple energy density function (without surface energy)

   e.g. $e(y) = \int_0^1 (y' - 1)^2 (y' + 1)^2 + y^2 dx$

   There are analytical results available for this 1-D problem. I can use them to compare my numerical solutions.

   Then I can move to 2-D scalar problem.

e.g. $\Omega = [0,1]^2, y : \Omega \to R^{2\times 2}$, $y = 0$ on $\partial\Omega$,

$$e(y) = \int_{\Omega} \left[((\partial_1 y)^2 - 1)^2 + (\partial_2 y)^2 \right] dx$$

2) 2-D vectorial problem without surface energy (Laminates)

In this case, there are complicated vectorial operations in the energy density function. I will study the two-dimensionaltwo-well problem, which is associated to the phenomena known as Twinning. My job is to investigate all possible microstructures constructable from gradients from these two wells.

I am also interested in solving other multi-well problems which correspond to the "Laminates within Laminates" structure.

3) Challenging problems, 2-D vectorial problem with surface energy

This kind of problem is realistic physical problem. Microstructure near the interface may be much more complicated, because of the abnormal energy consumption on the interface, for instance, the laminate-single variant interfaces.

In this case, the energy density function may have the high order gradients of deformation. In the presence of surface energy, the high order gradient of deformation could be very large.

4. Project goals

My goal is to obtain the numerical simulation of 2-D temperature/stress induced high order martensitic microstructure. My project will be based on several given energy density functions. The functional routine will be open. My program should be adaptive to all possible energy density functions. I will take the reasonable, realistic surface energy into my consideration. Visualization of the final result could be kind of the twinning, laminates within laminates structure. The experimental photomicrograph could be the comparison of my numerical result. My program can help people to obtain the simulation of some materials' microstructure when they want to analyze their physical characteristics.

5. Numerical Method to the minimization problem

1) Finite element deformations

We can take a finite-element approximation of the space of admissible deformations, and minimize the energy over this finite dimensional space using proper method. I will use piecewise bilinear element.

For $\Omega = [0,1]^2$, we take *h=1/N* be the mesh size. We get the uniform square mesh with elements $\Omega_{ij} = [ih,(i+1)h]\times[jh,(j+1)h]$

Using bilinear finite elements:

$$W_h = \{y \in C^0(\Omega) : y|_{\Omega_{ij}} \text{ is bilinear in each component for each i, j}\}.$$

A_h : finite element approximation to A with mesh size h.

$$A_h = \{y \in W_h : y_h(x_{ij}) = y_0(x_{ij}), x_{ij} \in \partial\Omega\}.$$

Job is to minimize $J_{l,h}(\hat{y}) := \int_\Omega f(\nabla y_h(x))dx, y_h \leftrightarrow \hat{y}$

2) Iterative Descent / Conjugate Gradient method in optimization problem

The variation of Polak-Kibière conjugate gradient algorithm is a very good method. The initial guess can be simple laminates & homogeneous deformation.

Other choices are Quasi-Newton method and probability method.

I can apply the precondition to the methods above.

3) Parallelism

I am thinking of using parallel computing to do the minimization in each element. The detailed method could depend on the final nonlinear problem coming from the optimization.

4) PDE scheme

Another idea about the numerical solver of this problem is the PDE scheme.

Say, we need to minimize an energy function $E(y) = \int_\Omega f(\nabla y)dx$

The equivalent problem is: $\left.\frac{d}{de}\right|_{e=0} \int f(\nabla y + e\nabla v)dx = \frac{\partial E}{\partial y}\cdot v = 0$, for arbitrary v

e.g. for $f(\nabla y) = y'^2 - fy$,

we may have the equivalent PDE problem $2y'' = f$.

I will solve the problems in this way by using the finite element method. I'll take this as the comparison to the optimization scheme.

6. Visualization

I am planning write my own visualization tools for this problem. The basic idea is to set up the gray-scale corresponding to different values of deformation gradients, then plot all the values of gradients in the domain.

Another option is to send output data to Matlab, use its graphic tools to do the visualization.

7. Tools

Programs will be written in C++

LAPACK++: Linear Algebra Package in C++, a software library for numerical linear algebra that solves systems of linear equations and eigenvalue problems on high performance computer architectures.

IML++: Iterative Methods Library, a C++ templated library of modern iterative methods for solving both symmetric and nonsymmetric linear systems of equations.

CVS: Concurrent Versions System, the dominant open-source network-transparent version control system.

MPI: The Message Passing Interface standard.

I will do the computation on IBM SP/2 machine at CSCAMM. It is a distributed-memory parallel system consisting of one frame of total 8 wide IBM SP nodes.

8. Validation

The numerical results should compare with analog data. Visualization of the results should compare with experimental photomicrographs.

9. Supporting materials:

My webpage for this project: http://www.math.umd.edu/~wzhong/asc.htm

I put a link to this page on my home page: http://www.math.umd.edu/~wzhong

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