# Non-uniform (zig-zag) microstructures mixing two variants of martensite

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# Talk plan

Zig-zag microstructures (alternatively: tilted twin boundaries) as a consequence of elastic energy minimization in the presence of stress. Two distinct stories, sharing certain features:

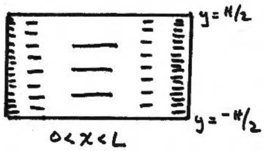
(1) A scalar model – work with Alex Misiats and Stefan Müller
   - Stress-free twins must be parallel. What if applied fields or bdry conds require vol fraction to vary?
   - Energy scaling laws are nice, but we would like to understand the pattern itself.

(2) A linear elastic model – work with Alex Misiats
   - Motivated by experiments of Chopra, Bailly, Wuttig (1996)
   - Cleaner than (1) wrt link to experiments; but “just” the energy scaling law.

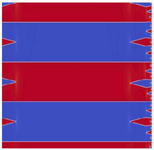
# A scalar model

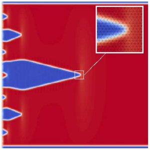
Recall K-M problem from the early 90's:

$$\min_{\substack{u=0 \text{ at } x=0,L \\ u_y=\pm 1}} \int_{\substack{0<x<L \\ -H/2<y<H/2}} u_x^2 + \varepsilon |u_{yy}|$$




- min value $\sim \varepsilon^{2/3} L^{1/3} H$
- energy in $0 < x < \rho$ is $\varepsilon^{2/3} \rho^{1/3} H$
- Conti (2000): refinement at edges is (roughly speaking) self-similar
- Dondl, Heeren, Rumpf (2016): careful numerics using $u_x^2 + (u_y^2 - 1)^2 + \varepsilon^2 u_{yy}^2$.

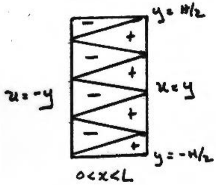




# Zig-zag microstructure

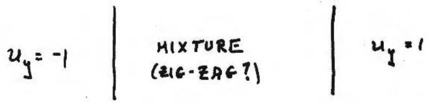
By changing the left and right boundary conditions, we can make the volume fraction of each phase vary with $x$

$$\min_{\substack{u=-y \text{ at } x=0 \\ u=y \text{ at } x=L \\ u_y=\pm 1}} \int_{\substack{0<x<L \\ -H/2<y<H/2}} u_x^2 + \varepsilon |u_{yy}|$$




Physical interpretation: stress may favor one phase over the other, eg

$$\min_{u_y=\pm 1} \int u_x^2 - (x - x_0) u_y + \varepsilon |u_{yy}|$$



# Not limited to martensite

Essential character: energy minimization requires laminated microstructure, but vol fractions must vary along the layers.

Classic example from optimal design: arrange two conducting materials in $\Omega \subset R^2$ (fixed area fractions). Heat uniformly, holding temp=0 at boundary. What arrangement minimizes the avg temp?

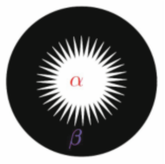
Mathematically: Let $-\nabla \cdot (A(x)\nabla u) = 1$ in $\Omega$, where $A(x) = \alpha$ or $\beta$, with $\alpha < \beta$. What arrangement solves

$$\min_{\text{arrangements}} \int_\Omega u(x)\,dx + \ell\,(\text{Area where } A(x) = \beta)\ ?$$

$0 < r < R_0$: material $\alpha$,

$R_1 < r < 1$: material $\beta$, with $R_1 = 2\beta\sqrt{\dfrac{l}{\beta - \alpha}}$

$R_0 < r < R_1$: fine mixture of $\alpha$ and $\beta$

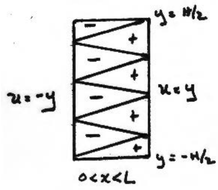



(Figure credit: F. Jouve, Structural shape and topology optimization, in a 2014 CISM volume ed by Rozvany and Lewinski).

# Returning to martensite

The scalar model of twinning is perhaps the simplest problem of this type. So let's focus on it.

$$\min_{\substack{u=-y \text{ at } x=0 \\ u=y \text{ at } x=L \\ u_y=\pm 1}} \int_{\substack{0<x<L \\ -H/2<y<H/2}} u_x^2 + \varepsilon |u_{yy}|$$



# Easy results

(1) As $\varepsilon \to 0$, minimizer $u_\varepsilon$ tends to soln of relaxed problem

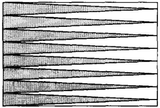
$$\min_{\substack{u=-y \text{ at } x=0 \\ u=y \text{ at } x=L \\ |u_y|\leq 1}} \int u_x^2$$

Its solution $u_*$ is the linear interpolant $u_*(x,y) = \left(\frac{2x}{L} - 1\right) y$. So the limiting energy as $\varepsilon \to 0$ is

$$E_0 = \int (u_*)_x^2 = H^3/3L.$$

(2) Scaling law for the excess energy due to positive $\varepsilon$:

$$E_\varepsilon = \min_{\substack{u=-y \text{ at } x=0 \\ u=y \text{ at } x=L \\ u_y=\pm 1}} \int_{\substack{0<x<L \\ -H/2<y<H/2}} u_x^2 + \varepsilon |u_{yy}|$$



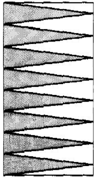
$$E_0 + C_1 \varepsilon^{2/3} L^{1/3} H \leq E_\varepsilon \leq E_0 + C_2 \varepsilon^{2/3} L^{1/3} H$$

# We would like to say more

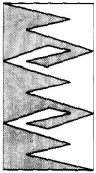
Energy scaling laws are known for many problems with microstructure.

Often the analysis stops there. Describing the minimizing pattern requires a different type of analysis.

Geometric character of the K-M model makes it a good place to start.



- Is the zig-zag pattern optimal, for some top/bottom bdry conds? (Open)
- Does the energy scaling law imply similarity to zig-zag? No.



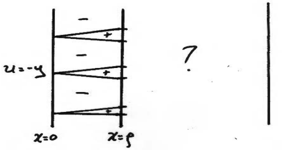
# We would like to say more

- Natural goal: show that estimates valid for zig-zag test function are also satisfied by the optimal $u_\varepsilon$. Example: for zig-zag test function,

$$\int_{-H/2}^{H/2}\int_0^\rho (u-u_*)_x^2 + \varepsilon|u_{yy}| \leq CL^{-2/3}\varepsilon^{2/3}H\rho$$

  Actual result: for minimizer $u_\varepsilon$ we get a similar estimate – with RHS larger by factor $|\log(\rho/L)|$.

- Natural tool: minimizer does better than anything we can do by hand

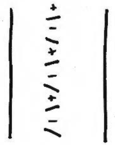


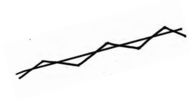
# Hints abt the math (i): the energy scaling law

$$E_0 + C_1\varepsilon^{2/3}L^{1/3}H \le E_\varepsilon \le E_0 + C_2\varepsilon^{2/3}L^{1/3}H$$

Upper bound: use the zig-zag test function ($u$ is piecewise linear!) Optimization indicates period wrt $y$ is of order $\varepsilon^{1/3}L^{2/3}$.

Lower bound (assuming $u - u_*$ is periodic in $y$): for any $x_0$, consider $y \mapsto u(x_0, y)$: avg slope is same as $(u_*)_y = \frac{2x_0}{L} - 1$, but $u_y = \pm 1$.





| | | |
|---|---|---|
| Few interfaces at some $x_0$ | $\Rightarrow$ | large $(u - u_*)(x_0, y)$ (in $L^2$ wrt $y$) |
| | $\Rightarrow$ | excess relaxed energy $\int u_x^2$ (convexity!) |
| Many interfaces at all $x_0$ | $\Rightarrow$ | large surface energy |
| Optimize tradeoff | $\Rightarrow$ | lower bound |

# Hints about the math (ii): the local estimate

The result: assume $u - u_*$ is periodic in $y$, and take $L = H = 1$ for simplicity. Then the minimizer satisifes

$$\int_{-1/2}^{1/2} \int_0^{\rho} (u - u_*)_x^2 + \varepsilon |u_{yy}| \leq C\varepsilon^{2/3} \rho |\ln \rho|$$

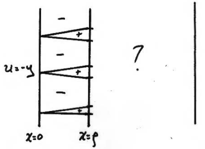
Idea: Note that

$$\iint_{0<x<\rho} u_x^2 + \varepsilon|u_{yy}| = \iint_{0<x<\rho} (u_\rho^{\mathrm{lin}})_x^2 + \iint_{0<x<\rho} (u - u_\rho^{\mathrm{lin}})_x^2 + \varepsilon|u_{yy}|$$

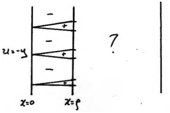
where $u_\rho^{\mathrm{lin}}$ is the linear (wrt $x$) interpolant btwn $u(0, y) = -y$ and $u(\rho, y)$. So the minimizer of $E_\varepsilon$ also minimizes

$$\iint_{0<x<\rho} (u - u_\rho^{\mathrm{lin}})_x^2 + \varepsilon|u_{yy}|.$$

Call the value $F(\rho)$. We get an estimate on $F(\rho)$ by using the comparison function sketched in the figure.



# Hints about the math (ii): the local estimate




Outcome (after some work): for a minimizer,

$$F(\rho) = \iint_{0<x<\rho} (u - u_\rho^{\mathrm{lin}})_x^2 + \varepsilon|u_{yy}|$$

satisfies

$$F(\rho) \le \rho F'(\rho) + C\int_{-1/2}^{1/2} (u - u_*)^2(\rho, y)\, dy.$$

The local estimate follows using "only" calculus and the global bound.

Some other results:

- With natural bc at top and bottom boundaries things change a bit. Our local lower bound is no longer almost linear in $\rho$ (RHS is $C\varepsilon^{2/3}\rho^{1/2}$).
- With natural bc at top and bottom, relaxed energy is unchanged but $E_\varepsilon$ is smaller, so (global) excess energy is smaller than when $u - u_*$ is periodic in $y$. But not much smaller: difference $\le C\varepsilon^\delta$ with $\delta > \frac{2}{3}$.

# Outline

(1) A scalar model – work with Alex Misiats and Stefan Müller

- Stress-free twins must be parallel. What if applied fields or bdry conds require vol fraction to vary?
- Energy scaling laws are nice, but we would like to understand the pattern itself.

(2) A linear elastic model – work with Alex Misiats

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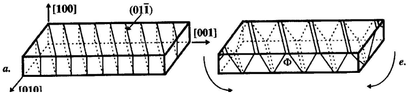
# The experiment

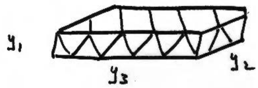
Chopra, Bailly, Wuttig: *Domain structures in bent InTl polydomain crystals*, Acta Mater 1996




- start with twinned plate (two variants, stress-free, not periodic)
- bend, by wrapping around a cylinder
- observation: zig-zag microstructure (periodic)
- release bending: parallel twins again, but periodic

Variants prefer strains

$$e(u) = \pm \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$




Bending favors $e_{33} > 0$ at top, $e_{33} < 0$ at bottom

# Elastic + surface energy

More convenient to work in a rotated frame, $(x_2, x_3) = R_{\pi/4}(y_2, y_3)$. Then

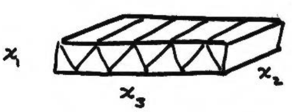
$$\text{preferred strains are } e(u) = \pm \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

and (choosing a particular Hooke's law) elastic + surface energy is

$$\int_{\text{plate}} e_{11}^2 + e_{22}^2 + e_{33}^2 + e_{12}^2 + e_{13}^2 + \varepsilon |\nabla e_{23}|$$

constrained by $e_{23} = \pm 1$ (and of course $e = e(u)$).

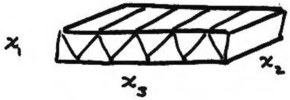
To keep things simple, assume plate thickness variable $x_1 \in [-1, 1]$ and bending is such that top and bottom are single-variant.



# Relaxed energy, and top/bottom bdry conds

As $\varepsilon \to 0$ we expect zigzag microstructure – for which vol fraction varies linearly wrt $x_1$. Weak limit of strain is then

$$e^* = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & x_1 \\ 0 & x_1 & 0 \end{pmatrix}$$



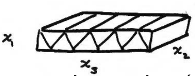

which suggests the relaxed solution

$$\begin{aligned} u_1^* &= -x_2 x_3 \\ u_2^* &= x_1 x_3 \\ u_3^* &= x_1 x_2 \end{aligned}$$

and the top/bottom bndry conds that $u = u^*$ at $x_1 = \pm 1$. Notes:

- Since $u_1$ is the out-of-plane displacement of plate, the bent plate is saddle-shaped.
- In this setting the relaxed energy vanishes! Indeed: relaxed elastic energy is $\int e_{11}^2 + e_{22}^2 + e_{33}^2 + e_{12}^2 + e_{13}^2$ and it vanishes for $e = e^* = e(u^*)$.

# The energy scaling law




For simplicity take the cross-section to be $(x_2, x_3) \in [-1, 1]^2$:

$$E_\varepsilon = \min_{\substack{u=u^* \text{ at } x_1=\pm 1 \\ e_{23}(u)=\pm 1}} \int_{[-1,1]^3} e_{11}^2 + e_{22}^2 + e_{33}^2 + e_{12}^2 + e_{13}^2 + \varepsilon|\nabla e_{23}|$$

Upper Bound: The zigzag structure shows $E_\varepsilon \leq C_1 \varepsilon^{2/3}$

Lower Bound: Restricting to deformations "invariant wrt $x_2$"

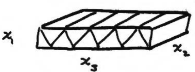
$$u_1 = u_1(x_1, x_2, x_3), \quad u_2 = u_2(x_1, x_3), \quad u_3 = x_2 \varphi(x_1, x_3)$$

we have $E_\varepsilon \geq C_2 \varepsilon^{2/3}$.

Upper bound sketch: use zig-zag, with $u_1 = u_1^*$, $u_3 = u_3^*$, and $u_2$ chosen st $\partial_3 u_2 = 2 - x_1$ in one phase and $-2 - x_1$ in the other (so $e_{23} = \pm 1$). Geometry assures that avg $e_{23}$ is $x_1$.

Microstructural scale is $\varepsilon^{1/3}$ (walls are almost vertical). In fact, if period wrt $x_3$ is $\ell$, then elastic energy $\sim \ell^2$ and surface energy $\sim \varepsilon/\ell$.

# The energy scaling law

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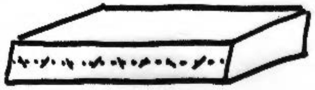
# Sketch of lower bound

Strategy: similar to scalar case. If surface energy is small then typical slice has few interfaces. Show this implies large elastic energy, by using convexity of the relaxed elastic energy.



Problem: in scalar case we could use elementary arguments, since "relaxed elastic energy" was $\int u_x^2$. Here, instead, it is linear elasticity with a degenerate Hooke's law.

Solution: use convex duality (separately, for relaxed energy above and below the slice, using restriction of $u$ to the slice as a boundary condition). With good choice of dual trial fields, get lower bound roughly analogous to that of scalar case.

Similar use of convex duality: recent papers with B. Wirth on composites optimizing elastic energy + small surface energy.

# Stepping back

- When elastic energy minimization requires microstructure, surface energy is the natural regularization, determining the pattern as well as the length scale.
- There are as yet few examples where we know more than the min energy scaling law.
- Our scalar zig-zag problem addresses a simple case where the microstructure is approximately layered, but the volume fractions are not uniform. New results and methods, but much is still open.
- Our elastic zig-zag problem is close to the Chopra-Bailly-Wuttig experiments – obtaining the energy scaling law in a new (physically relevant) example. However we have not explained the observed periodicity.
- Might zig-zag geometries be optimal for some versions of these problems?

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