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THE NATURE OF STRESS AND STRAIN FIELDS IN SHAPE MEMORY POLYCRYSTALS

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Summary A central open problem in the study of shape memory polycrystals is the prediction of their recoverable strains. Solving this problem requires an understanding of the possible stress and strain fields that arise in such polycrystals. For polycrystals made of materials undergoing cubic-tetragonal transformations, we show that the strains fields associated with macroscopic recoverable strains are related to the solutions of hyperbolic partial differential equations. We explore consequences of this relationship and connections to previous conjectures characterizing polycrystals with non-trivial recoverable strains. We also show that stress fields in shape memory polycrystals could be concentrated on lower-dimensional surfaces (planes and lines). We do this by proving a dual variational characterization of recoverable strains and presenting several examples. Implications of this characterization for effective properties and the development of numerical methods are discussed.

THE SHAPE MEMORY EFFECT IN POLYCRYSTALS

Shape memory (SM) effect is the ability of a solid to recover on heating apparently plastic deformation sustained below a critical temperature. Many alloys (e.g. NiAl, FeNiC) exhibit good SM behavior as single crystals but little or none as polycrystals while others (e.g. CuAlNi, NiTi) are good SM materials both as single crystals and as polycrystals. Since the utility of SM alloys critically depends on their polycrystalline behavior, this issue is of both scientific interest and technological importance. Thus we desire (a) to know the reason for this difference in the behavior of SM polycrystals; (b) to predict which materials generically exhibit good polycrystalline SM behavior; and (c) to characterize, for a given material, those polycrystals which exhibit good SM behavior.
This paper provides insight into these difficult problems by presenting results on the nature of stress and strain fields that arise in shape memory polycrystals.

STRAIN FIELDS IN CUBIC-TETRAGONAL POLYCRYSTALS

A model for the SM effect in single crystals and polycrystals [2, §1]

A SM single crystal has a multi-well microscopic energy, each well corresponding to a variant of Martensite. An undeformed single crystal consists of self accommodated mixtures of Martensitic variants. A deformation is recoverable precisely when the variants can accommodate it by reorganizing themselves: the recoverable strains of a single crystal are precisely those that lie in the zero-set of its mesoscopic energy. Likewise, the recoverable strains of a polycrystal are the macroscopic averages of strain fields which locally lie in the zero-set of the mesoscopic energy of each grain.

Connections with hyperbolic partial differential equations

For a material that undergoes the cubic-tetragonal transformation, the zero-set of the mesoscopic energy of an unoriented crystal is contained in the subspace

$$\left\{\epsilon \in \mathbb{R}^{3\times 3}_{\text{sym}} \mid \epsilon_{12} = \epsilon_{13} = \epsilon_{23} = 0\right\}.$$

Using the strain compatibility equation, we deduce that strain fields constrained to lie in this subspace are of the form

$$\begin{aligned}\epsilon_{11} &= f_2(x_1,x_3) - f_3(x_1,x_2) + c_1,\\ \epsilon_{22} &= f_3(x_1,x_2) - f_1(x_2,x_3) + c_2,\\ \epsilon_{33} &= f_1(x_2,x_3) - f_2(x_1,x_3) + c_3,\end{aligned}$$

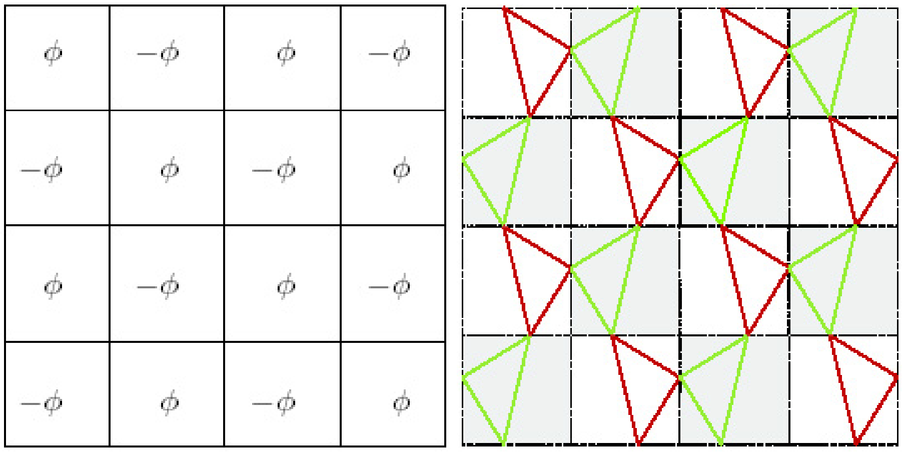
where $f_1, f_2, f_3 \in L^\infty(\mathbb{R}^2,\mathbb{R})$ satisfy

$$\begin{aligned}\left(\frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2}\right) f_1(x_2,x_3) &= 0,\\ \left(\frac{\partial^2}{\partial x_3^2} - \frac{\partial^2}{\partial x_1^2}\right) f_2(x_1,x_3) &= 0,\\ \left(\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2}\right) f_3(x_1,x_2) &= 0.\end{aligned}$$

Associated with these three hyperbolic partial differential equations are three pairs of characteristic planes.

Implication: characterizing polycrytals with non-trivial recoverable strain

Thus associated with each grain are three pairs of characteristic planes. Imposing strain compatibility at the grain boundaries is related to requiring that these characteristic planes percolate across grain boundaries. This formalizes analogies



(a) A checkerboard with grains oriented at ϕ and $-\phi$. Four periodic cells are shown.

(b) A stress field in this checkerboard as a response to loading (beyond a threashold) in the $\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ direction.

to percolation theory observed earlier in such problems [2, 3]. Polycrystals that exhibit good SM behavior are precisely those whose texture is such that at least some characteristics percolate.

The preceeding analysis is strong evidence in support of the conjecture [1, 2] that cubic-tetragonal SM polycrystals are essentially those polycrystals whose texture is either (a) a rank-I laminate or (b) bamboo like—i.e. the orientation of all grains share the same axis of rotation. It is hoped that this and similar methods will lead to the characterization of the recoverable strains of polycrystals.

STRESS FIELDS

Dual variational characterization of recoverable strains

Let $\widehat{\mathcal{S}} \subset \mathbb{R}^{n\times n}_{\text{sym}}$ be the zero-set of the mesoscopic energy of an unoriented crystal. Then $\overline{\mathcal{S}} \subset \mathbb{R}^{n\times n}_{\text{sym}}$, the zero-set of the macroscopic energy of a polycrystal has the characterization

$$\delta_{\overline{\mathcal{S}}}(\bar{\epsilon}) = \sup_{\sigma \in \mathcal{S}_{\text{ad}}} \frac{1}{|\Omega|} \int_\Omega \sigma(x) \cdot \bar{\epsilon} - \delta^\star_{\widehat{\mathcal{S}}}(R^T(x)\sigma(x)R(x))\, \mathrm{d}x.$$

Here $\delta_{(\cdot)} \colon \mathbb{R}^{n\times n}_{\text{sym}} \to \{0, \infty\}$ and $\delta^\star_{(\cdot)} \colon \mathbb{R}^{n\times n}_{\text{sym}} \to \mathbb{R}$ are the indicator and support functions of the set $\cdot$ respectively; $R\colon \Omega \to SO(n)$ is the texture of the polycrystal; and $\mathcal{S}_{\text{ad}}$ is the set of all signed radon measures with finite mass.

Implication: stress localization

This implies, in particular, that stress fields could localize to lower dimensional surfaces (plane and lines in three-dimensions). As an example, consider the two-dimensional checkerboard polycrystal shown in Figure (a). A stress field corresponding to a macroscopic strain of the form $s\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, $|s| > \tan\phi$, is shown in Figure (b). The stress localizes to the diagonal lines shown (everywhere else the polycrystal is unstressed).

This behavior is analogous and dual to the appearance of strain localization (slip planes and lines) in rigid perfectly-plastic materials. Prager in 1957 raised the question of the existance of such materials [5, 6]; our work provides an affirmative answer.

It follows that any attempt to compute the recoverable strains of a polycrystal numerically will, in general, fail unless the numerical method is able to handle stress localization. Since most current algorithms cannot do so, this calls for the development of new numerical methods.

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