

Transformation Yield Surface of Shape-Memory Alloys

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Abstract. Shape-memory alloys transform under stress, and this stress-induced transformation is useful for various practical applications. The stress at which the alloy transforms depends on the orientation of the stress relative to the specimen, and may be described using a transformation yield surface. This paper provides early results of a theoretical treatment of the transformation yield surface of shape-memory polycrystals with particular emphasis on the influence of texture.

1 Introduction

Shape-memory alloys derive their interesting properties as a result of a martensitic phase transformation between a high-temperature austenite and a low-temperature martensite phase. This transformation can also be induced by stress above the transformation temperature. This stress-induced transformation leads to practically useful properties like pseudoelasticity. The stress required to induce transformation is highly anisotropic and is often described using a so-called transformation yield surface. This paper discusses some early results on the transformation yield surface using a framework of energy minimization. Of particular interest is polycrystals and the dependence of the yield surface on texture.

The transformation yield surface of shape-memory alloys has been the topic of much recent research. There is a large literature on the experimental study of stress-induced transformations in single crystals (see for example [18, 20]). In polycrystals, where the issue is complicated by the interaction between grains, uniaxial loading experiments have been reported in NiTi, e.g. in [8, 9, 16, 22]. Systematic experimental studies of the transformation yield surface under multiaxial loading in polycrystals of copper-based shape-memory alloys (CuZnAl and CuAlBe) has been performed by Bouvet, LExcellent and their collaborators [5, 13]. More recently there are experimental studies of stress-induced transformation in NiTi polycrystals under multiaxial loading, e.g. Thamburaja

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and Anand [23]. The issue of transformation yield surface has been addressed theoretically and computationally using a variety of techniques (e.g. so-called thermodynamic approaches [10, 15, 17], ansatzes from plasticity theory [6] and so-called micro-macro modelling [1, 13, 14, 15, 19]).

We study the transformation yield surface in the framework of energy minimization with particular attention to crystallography in the spirit of [4, 21]. We largely confine ourselves to a geometrically linear theory. We first summarize some formulae for the transformation yield stress in single crystals in Section 2, mainly to fix the notation and to outline the strategy. In Section 3 we turn to polycrystalline shape-memory alloys, present several possible definitions for the transformation yield surface and methods for bounding it, and discuss the influence of texture in Section 4.

2 Yield surface in single crystal shape-memory alloys

Let $u : \Omega \rightarrow \mathbb{R}^3$ describe the displacement of a specimen $\Omega \subset \mathbb{R}^3$ and $e = e(u) = \frac{1}{2}(\nabla u + \nabla u^T)$ be the strain. The energy density of the austenite is denoted by $W_a(e)$, and that of the martensite by $W_m(e)$ so that the energy density is

$$W(e) = \min\{W_a(e), W_m(e)\}.$$

Suppose the crystal is subjected to a dead-load corresponding to a macroscopic stress $\sigma \Sigma_0$ where $\Sigma_0, |\Sigma_0| = 1$, is the ‘direction’ and $\sigma > 0$ is the magnitude. We postulate, following James [11], that the behavior of the crystal is governed by the solution of the following minimization problem

$$\min_{u=e \cdot x \text{ at } \partial\Omega} \int_{\Omega} (W(e) - \sigma \Sigma_0 \cdot e) \, dx,$$

where $\int_{\Omega} f \, dx := \frac{1}{\text{vol}(\Omega)} \int_{\Omega} f \, dx$. Since the integrand does not depend on x , it is sufficient to minimize the integrand, i.e. we consider $\min_e (W(e) - \sigma \Sigma_0 \cdot e)$. The yield stress is defined to be that stress σ_Y for which holds

$$\min_e (W(e) - \sigma \Sigma_0 \cdot e) = \begin{cases} \min_e (W_a(e) - \sigma \Sigma_0 \cdot e), & \sigma < \sigma_Y \\ \min_e (W_m(e) - \sigma \Sigma_0 \cdot e), & \sigma > \sigma_Y \end{cases}. \quad (1)$$

In the constrained theory where we assume that the elastic moduli are infinitely large (see e.g. Forclaz [7]) the energies are given by

$$W_a(e) = \begin{cases} 0 & \text{if } e = 0 \\ \infty & \text{else} \end{cases} \quad \text{and} \quad W_m(e) = \begin{cases} w & \text{if } e = e_i, \, i = 1, \dots, \nu \\ \infty & \text{else} \end{cases},$$

where $e_i, i = 1, \dots, \nu$ denote the stress-free strains of the martensitic phase and $w > 0$. Then, it is easy to verify that

$$\begin{aligned} \min_e (W_a(e) - \sigma \Sigma_0 \cdot e) &= 0 \\ \min_e (W_m(e) - \sigma \Sigma_0 \cdot e) &= \min_e (w - \sigma \Sigma_0 \cdot e_i) = w - \sigma \max_i \Sigma_0 \cdot e_i. \end{aligned} \quad (2)$$

Therefore, from (1), it follows that the yield stress σ_Y is given by

$$\sigma_Y = \frac{w}{\max_i \Sigma_0 \cdot e_i} =: \sigma_{Y1}. \quad (3)$$

This definition may be described as the *yield stress with correspondence variants*. Note for future use that

$$\sigma_{Y1} = w \left(\max_{e \in \text{co}\{e_i\}} \Sigma_0 \cdot e \right)^{-1}$$

since the e_i are the extreme points of their convex hull $\text{co}\{e_i\}$.

This definition above depends only on the relative stability of the austenite and martensite under the applied load, and does not consider the transformation pathway or the compatibility of the austenite and martensite. Two states are compatible if their strains e and e' satisfy

$$e - e' = \frac{1}{2}(a \otimes n + n \otimes a)$$

for some vectors a, n . Unfortunately a single variant of martensite is usually not compatible with the austenite. So our definition σ_{Y1} above might give us an under-estimate of the actual yield stress. Instead the austenite is compatible with a microstructure of martensite, and indeed one sees in experiments (e.g. [18, 20]) that the austenite loses stability to a microstructure of martensite.

To define yield stress in a manner that is sensitive to compatibility, we consider the set \mathcal{S} of average strains of all possible compatible microstructures of martensite. We call this set the *set of recoverable strains in a single crystal* following [4] since this is the set of all strains that a single crystal can recover in the shape-memory effect. For future use, we note that $\mathcal{S} = \{e : W_m^{qc}(e) = w\}$ where W_m^{qc} is the quasiconvex envelope of W_m (physically, this is the average energy in a single crystal of martensite after it has formed microstructure).

It turns out that if the variants of martensite are pairwise compatible, then the set of recoverable strains is simply their convex hull $\text{co}\{e_i\}$ [2]. This condition holds for transformations of interest including cubic to tetragonal and cubic to orthorhombic, but unfortunately not for cubic to monoclinic transformations.

The classical austenite-martensite interface or habit plane is an interface between the austenite and fine twins of two variants of martensite. If we consider the loss of stability of the austenite under applied stress through this habit plane, i.e. to fine twins that are compatible with the austenite, then we obtain our second definition of yield stress,

$$\sigma_{Y2} = w \left(\max_{\substack{e \in \text{co}\{e_i\} \\ e = \frac{1}{2}(a \otimes b + b \otimes a)}} \Sigma_0 \cdot e \right)^{-1}.$$

We may describe this as the *yield stress with habit planes*.

Finally, we can consider the loss of stability with any microstructure of martensite that is compatible with the austenite. We obtain our third definition of yield stress,

$$\sigma_{Y3} = w \left(\max_{\substack{e \in \text{co}\{e_i\} \\ e = \lambda e_i + (1-\lambda)e_j \\ e = \frac{1}{2}(a \otimes b + b \otimes a)}} \Sigma_0 \cdot e \right)^{-1}.$$

The three definitions of the yield stress in single crystal shape-memory alloys are related to each other by

$$\sigma_{Y1} \leq \sigma_{Y2} \leq \sigma_{Y3}.$$

We conclude this section noting that these definitions may easily be generalized to the geometrically non-linear theory. Unfortunately however, the evaluation of the analog of σ_{Y3} would be open given our lack of knowledge of the set of recoverable strains in this theory.

3 Yield surface in polycrystalline shape-memory alloys

A polycrystal is an agglomeration of crystallites or grains with identical crystal structure that are oriented differently with respect to each other. The orientations and size of the grains is known as *texture* and may be described by a rotation-valued function

$$R : \Omega \rightarrow \text{SO}(3) = \{R \in M^{3 \times 3} : R^T R = R R^T = \mathbb{1}, \det R = 1\}$$

which is constant on each grain and gives the crystalline orientation relative to a fixed reference crystal.

Hence, if e_1, \dots, e_ν are the stress-free strains of the reference crystal, then a grain with orientation R has stress-free strains $R e_1 R^T, \dots, R e_\nu R^T$. The energy of the crystal is now dependent of the position:

$$W(x, e) = \min\{W_a(x, e), W_m(x, e)\}$$

with

$$W_a(x, e) = W_a(R^T(x)eR(x)), \quad W_m(x, e) = W_m(R^T(x)eR(x)).$$

In the constrained model, or in a model with isotropic austenite, $W_a(x, e) = W_a(e)$. We assume this in what follows, though one can proceed without it.

To understand the behavior of the polycrystal under an applied load, we study the minimization problem

$$m(\sigma) := \min_e \int_{\Omega} (W(x, e) - \sigma \Sigma_0 \cdot e) dx$$

and again assume that Σ_0 , $|\Sigma_0| = 1$ is given. The x -dependence of W causes mathematical difficulties since one cannot simply determine the minimum of the integrand in order to get the minimum of the integral. This also means that the transformation yield stress can be defined in various ways.

1. We call the stress at which the first grain of the polycrystal starts to transform the *initial yield stress* σ_{Yi} . This is the stress for which the following holds

$$\begin{aligned} m(\sigma) &= \min_e (W_a(e) - \sigma \Sigma_0 \cdot e) & \text{if } 0 \leq \sigma \leq \sigma_{Yi} \\ m(\sigma) &< \min_e (W_a(e) - \sigma \Sigma_0 \cdot e) & \text{if } \sigma_{Yi} < \sigma. \end{aligned}$$

2. We refer to the stress at which all grains have started to transform as the *plateau yield stress* σ_{Yp} . This is the stress for which the following holds

$$\begin{aligned} m(\sigma) &< \min_e \int_{\Omega} (W_m(x, e) - \sigma \Sigma_0 \cdot e) dx & \text{if } 0 \leq \sigma < \sigma_{Yp} \\ m(\sigma) &= \min_e \int_{\Omega} (W_m(x, e) - \sigma \Sigma_0 \cdot e) dx & \text{if } \sigma_{Yp} \leq \sigma. \end{aligned}$$

It remains an open problem to calculate these quantities. To discuss this further, let us introduce the *effective energy* or the homogenized energy of the polycrystal¹

$$\bar{W}(e) := \min_{\int_{\Omega} e(u) dx = e} \int_{\Omega} W(x, e(u)) dx = \min_{\int_{\Omega} e(u) dx = e} \int_{\Omega} W^{qc}(x, e(u)) dx.$$

One can also define the effective energy of the martensite alone

$$\bar{W}_m(e) := \min_{\int_{\Omega} e(u) dx = e} \int_{\Omega} W_m(x, e(u)) dx = \min_{\int_{\Omega} e(u) dx = e} \int_{\Omega} W_m^{qc}(x, e(u)) dx$$

We can prove that

$$\bar{W}(e) \leq (\min\{W_a(e), \bar{W}_m(e)\})^{qc},$$

though the exact relation between them remains unclear. We say that the *set of recoverable strains in a polycrystal*, \mathcal{P} is the average strains that the polycrystal can attain by making microstructures of martensite in each grain. It follows that $\mathcal{P} = \{e : \bar{W}_m(e) = w\}$.

¹See [4] for a discussion about this definition.

We can now introduce a third notion of yield stress.

3. We refer to the *recoverable strain yield stress* σ_{Yr} as the stress at which W_a loses stability to $\bar{W}_m(e)$

$$\begin{aligned} \min_e (W_a(e) - \sigma \Sigma_0 \cdot e) &< \min_e (\bar{W}_m(e) - \sigma \Sigma_0 \cdot e) && \text{if } 0 \leq \sigma < \sigma_{Yr} \\ \min_e (\bar{W}_m(e) - \sigma \Sigma_0 \cdot e) &< \min_e (W_a(e) - \sigma \Sigma_0 \cdot e) && \text{if } \sigma > \sigma_{Yr}. \end{aligned}$$

We can show for the constrained model that

$$\sigma_{Yr} = w \left(\max_{e \in \mathcal{P}} \Sigma_0 \cdot e \right)^{-1}.$$

The term in the parenthesis above is in fact the recoverable strain of the polycrystal under applied load in the direction Σ_0 .

These three definitions of the yield stress are related to each other as follows,

$$\sigma_{Yi} \leq \sigma_{Yr} \leq \sigma_{Yp}.$$

It is as difficult to calculate \bar{W}_m and \mathcal{P} as the original problem of calculating \bar{W} , and is thus open. We can however estimate \bar{W}_m from above by using a constant strain test field (the Taylor bound), and from below by using a constant stress test field (the Sachs bound). These provide bounds on the set \mathcal{P} from inside and outside. It follows [21] that

$$\max_{e \in \mathcal{T}} \Sigma_0 \cdot e \leq \max_{e \in \mathcal{P}} \Sigma_0 \cdot e \leq \max_{x \in \Omega, e \in \mathcal{S}} \Sigma_0 \cdot R(x)^T e R(x), \quad (4)$$

where

$$\mathcal{T} := \bigcap_{x \in \Omega} R(x) \mathcal{S} R^T(x).$$

The first inequality in (4) is the lower or Taylor bound on the recoverable strain of a polycrystal under applied load in the direction Σ_0 , while the latter is the upper or the Sachs bound on the same.

We are now in a position to introduce two other, and readily accessible, definitions of yield stress.

4. We define the *Sachs yield stress* σ_{YS} to be the yield stress based on the Sachs bound on the recoverable strain,

$$\sigma_{YS} = w \left(\max_{x \in \Omega, e \in \mathcal{S}} \Sigma_0 \cdot R(x)^T e R(x) \right)^{-1}.$$

This definition is similar to that used in [14].

5. We define the *Taylor yield stress* σ_{YT} to be the yield stress based on the Taylor bound on the recoverable strain,

$$\sigma_{YT} = w \left(\max_{e \in \mathcal{T}} \Sigma_0 \cdot e \right)^{-1}. \quad (5)$$

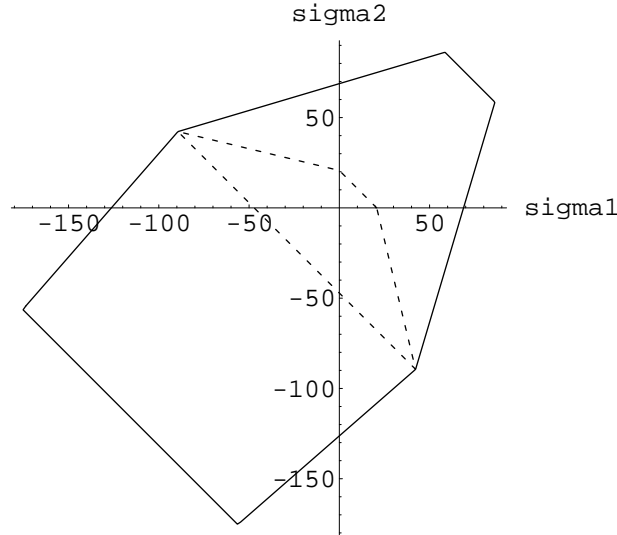


Figure 1: The Taylor transformation yield surface in arbitrary units under biaxial loading for a material undergoing cubic to orthorhombic transformation with isotropic (solid line) and uniaxial (dashed line) texture.

It follows from (4) that

$$\sigma_{YS} \leq \sigma_{Yr} \leq \sigma_{YT}.$$

We have in fact proven that

$$\sigma_{YS} \leq \sigma_{Yi} \leq \sigma_{Yr} \leq \sigma_{YT}.$$

Bhattacharya and Kohn [4] have discussed the accuracy of using the Taylor bound for recoverable strains, and Shu and Bhattacharya [21] have used it to understand the effect of texture. Kohn and Niethammer [12] have discussed the geometrically nonlinear theory for recoverable strains.

4 Yield surface and texture

We discuss the application of the Taylor yield surface to a cubic to orthorhombic phase transformation. This transformation is observed in copper-based alloys like CuAlNi. There are six variants of martensite with the transformation strain of the first variant

$$e_1 = \begin{pmatrix} \alpha & \delta & 0 \\ \delta & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

with the rest given by symmetry. These strains are pairwise compatible and \mathcal{S} is equal to their convex hull, and one has [3]

$$\mathcal{S} = \left\{ e : e_{11} + e_{22} + e_{33} = 2\alpha + \beta, \min\{\alpha, \beta\} \leq e_{11}, e_{22}, e_{33} \leq \max\{\alpha, \beta\}, \right. \\ \left. -\frac{e_{ii} - \alpha}{\beta - \alpha} \delta \leq e_{jk} \leq \frac{e_{ii} - \alpha}{\beta - \alpha} \delta \text{ for all } \{ijk\} = \text{permutation of } \{123\} \right\}.$$

For isotropic or equiaxed texture one has [3]

$$\mathcal{T}_{\text{iso}} = \left\{ e : e \text{ has eigenvalues } \lambda_1, \lambda_2, \lambda_3 \text{ which satisfy } \lambda_1 + \lambda_2 + \lambda_3 = 2\alpha + \beta, \right. \\ \min\{\alpha, \beta\} \leq \lambda_1, \lambda_2, \lambda_3 \leq \max\{\alpha, \beta\}, \\ \left. \frac{\lambda_i - \lambda_j}{2} \leq \frac{\lambda_k - \alpha}{\beta - \alpha} \delta \text{ for all } \{ijk\} = \text{permutation of } \{123\} \right\}.$$

We consider a biaxial applied stress $\Sigma_0 = \text{Diag}[\sigma_1, \sigma_2, 0]$, and use (5) to evaluate the yield stress. The results are displayed in Figure 1 (for $\alpha = 0.0483, \beta = -0.0907, \delta = 0.0249$) as the solid line (in arbitrary units).

We now contrast this with a specimen with a uniaxial texture where the $\langle 001 \rangle_{\text{cubic}}$ axis is parallel in each grain of the polycrystal. We begin by determining the set \mathcal{T}_{uni} :

$$\mathcal{T}_{\text{uni}} = \left\{ e : e = \begin{pmatrix} a & 0 & x \\ 0 & b & y \\ x & y & e_{33} \end{pmatrix}, R_\theta^T e R_\theta \in \mathcal{S} \text{ for all } \theta \right\}$$

where

$$R_\theta = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and a and b satisfy

$$a + b + e_{33} = 2\alpha + \beta, \quad \min\{\alpha, \beta\} \leq a, b, e_{33} \leq \max\{\alpha, \beta\}, \quad |a - b| \leq \frac{e_{33} - \alpha}{\beta - \alpha} 2\delta.$$

We use this to calculate the Taylor yield stress for a biaxial applied stress $\Sigma_0 = \text{Diag}[\sigma_1, \sigma_2, 0]$. The results are displayed in Figure 1 as the dashed line.

The difference between the yield surface for the equiaxed and uniaxial texture is quite striking. It should be emphasized that this reflects the Taylor yield surface which is only a bound. It remains an open question whether such a difference is also observed in the actual yield surface. Yet this result is quite provocative in terms of the importance of texture.

5 Concluding remarks

This paper presented some early results of a theoretical investigation of the transformation yield surface and its dependence on texture. We discussed various notions of yield surface for single and polycrystals. We noted the importance of texture through an example of a material undergoing cubic to orthorhombic transformation. In future work, we will present a systematic study of the yield surface in various materials with diverse textures, along with a comparison with experiment. We will also present a detailed mathematical analysis of the relationship between the various definitions.

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