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On the energy-minimizing strains in martensitic microstructures—Part 1: Geometrically nonlinear theory

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ABSTRACT

This paper addresses the theoretical prediction of the quasiconvex hull of energy-minimizing strains that can be realized by martensitic microstructures. Polyconvexification and related notions are used to derive some upper bounds (in the sense of inclusion) on the quasiconvex hull. Lower bounds are constructed by lamination techniques. The geometrically nonlinear theory (finite strains) is considered in the present Part 1. Analytical expressions are obtained for a three-well problem which encompasses the cubic to tetragonal transformation as a special case. Twelve-well problems related to cubic to monoclinic transformations are also studied. In that case, sufficient conditions are derived for the microstructure to be restricted to only two of the 12 wells.

1. Introduction

Some metallic alloys exhibit a solid/solid phase transformation between different crystallographic structures, known as austenite (stable at high temperature) and martensite (stable at low temperature). That phase transformation can be triggered both by thermal and mechanical loading. In terms of crystallographic structure, the austenite has a higher symmetry than the martensite. This leads one to distinguish several symmetry-related martensitic variants. Those variants correspond to different orientations of the martensitic lattice with respect to the austenitic lattice. Accordingly, to each martensitic variant is attached a transformation strain, describing the deformation between the crystallographic structures of the austenite and the martensite. The number of martensitic variants as well as the corresponding transformation strains depends on the alloy considered, through the structure of the austenite and martensite lattices. Some common examples include the cubic to tetragonal transformation (MnCu, MnNi), the cubic to orthorombic transformation (β_1'CuAlNi) and the cubic to monoclinic transformations (NiTi, γ_1'CuAlNi), corresponding respectively to 3, 6 and 12 martensitic variants.

The phase transformation between austenite and martensite gives rise to the shape memory effect displayed by alloys such as NiTi or CuAlNi: cooling down a stress-free sample below a critical temperature transforms the homogeneous austenite to a martensitic microstructure, in which the martensitic variants arrange themselves so as to produce a stress-free state with no macroscopic deformation. This phenomenon is classically referred to as *self-accommodation*. Deforming the sample entails a *reorientation* of the variants, i.e. a phase transformation of some martensitic variants to others. After unloading the sample, a residual stress-free strain is observed at the macroscopic level. That residual strain results from the cooperative effect of the microscopic transformation strains in each variant. Heating the sample transforms the martensite back in austenite, thus restoring the initial configuration.

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The shape memory effect is obviously limited: if for instance the strain imposed in the cooled state is too large, plastic deformations will occur and the material will no longer be able to recover its initial shape after heating. This motivates the definition of *recoverable* strains as macroscopic strains that can be restored by the shape memory effect. As explained by Bhattacharya and Kohn (1997), recoverable strains can be interpreted as minimizers of the macroscopic energy at low temperature. That macroscopic energy is itself obtained as the relaxation of a multi-well energy function Ψ that models the behavior of the material at a microscopic level. The relaxation procedure is notoriously difficult to perform and essentially consists in finding the austenite/martensite microstructures which minimize the global energy. This paper is essentially concerned with the theoretical prediction of the set of strains that minimize the macroscopic (or effective) energy, using the framework of nonlinear elasticity.

The problem can be formulated either in the geometrically nonlinear setting or in the geometrically linear setting. The geometrically nonlinear setting is more accurate and therefore to be preferred, especially as uniaxial measurements show that recoverable strains may be of the order of 10%. It turns out, however, that the problem is significantly more tractable in the geometrically linear setting, which in turn allows the analysis to be pushed further. For three-dimensional problems, exact solutions are available only in few cases. In the geometrically nonlinear theory, Ball and James (1992) solved the case of two compatible variants with the same determinant. Bhattacharya and Dolzmann (2001) extended that solution to a special case of the four-well problem, which remains two-dimensional in nature. In the geometrically linear theory, the solution of the two-well problem has been obtained by Kohn (1991). Smyshlyaev and Willis (1998) developed the approach of Kohn (1991) and adapted it to the three-well problem, deriving a lower bound on the relaxed energy and giving a sufficient condition for that lower bound to be realizable.

This paper aims at complementing existing results on that problem, essentially through the use of bounds on the set of energy-minimizing strains. Part 1 is devoted to the geometrically nonlinear theory, whereas the geometrically linear theory is considered in Part 2 (Peigney, in press). In Part 1 we are particularly interested in studying the three-well problem, in the geometrically nonlinear theory. The outline of the present Part 1 is as follows. In Section 2 is derived a general upper bound based on distinctive properties of Young measures (Kinderlehrer and Pedregal, 1991; Ball and James, 1992; Müller, 1999). Lower bounds are obtained using sequential lamination techniques (Kohn, 1991; Ball and James, 1992; Dolzmann, 1999; Stupkiewicz and Petryk, 2002). To that purpose, the solution of the two-well problem plays an essential role and therefore is recalled in Section 3. Most of the results in Section 3 are already known, but for the sake of comprehensiveness they are reported explicitly and stated as theorems for latter reference. The two-well problem also serves as a first illustrative example of the methodology introduced in Section 2. Building on the results of Sections 2 and 3, a three-well problem is studied in detail in Section 4. Much emphasis is put on the cubic to tetragonal transformation, which is a special case of the three-well problem considered. Closed-form expressions of upper and lower bounds on the set of energy-minimizing strains are obtained and compared. Section 5 focuses on cubic to monoclinic transformations: using results of Section 2, we give sufficient conditions on the macroscopic deformation for the microstructure to involve only two of the 12 variants, extending similar studies carried out by Ball and James (1992) and Bhattacharya et al. (1999) for the cubic to tetragonal and cubic to orthorombic transformations, respectively.

2. Upper bounds on $\boldsymbol{Q}\mathcal{K}$

At the microscopic level, the free energy density Ψ of martensitic crystals is classically modeled as a multi-well function of the form $\min_{1\le r\le n+1}\Psi_r$ where Ψ_r is the free energy of phase r and n is the number of martensitic variants. We label the phases so that $r=n+1$ corresponds to the austenite, and $1\le r\le n$ corresponds to the martensite variants. Each free energy Ψ_r is a function of the deformation gradient $\boldsymbol{F}$ and is frame indifferent, i.e. satisfies $\Psi_r(\boldsymbol{RF})=\Psi_r(\boldsymbol{F})$ for all $\boldsymbol{R}\in \mathrm{SO}(3)$ and for all $\boldsymbol{F}$. Moreover, the free energies Ψ_r of the martensite variants are symmetry related, i.e. for each $1\le r\le n$ there exists a rotation $\boldsymbol{R}_r$ such that

$$\Psi_r(\boldsymbol{F})=\Psi_1(\boldsymbol{R}_r\boldsymbol{F}\boldsymbol{R}_r^T) \quad \text{for all } \boldsymbol{F}. \tag{2.1}$$

Let us denote by $\mathcal{K}$ the set of deformation gradients $\boldsymbol{F}$ that minimize the function Ψ. The property (2.1) immediately shows that $\min\Psi_r=\min\Psi_1$ for all $r\le n$, so that $\min\Psi=\min\{\min\Psi_1,\min\Psi_{n+1}\}$. At a temperature below the transformation temperature, martensite achieves the minimum energy, i.e. $\min\Psi_{n+1}>\min\Psi_1$. In such case, the set $\mathcal{K}$ is given by

$$\mathcal{K}=\bigcup_{r=1}^{n}\mathcal{K}_r, \tag{2.2}$$

where $\mathcal{K}_r=\{\boldsymbol{F}\,|\,\Psi_r(\boldsymbol{F})=\min\Psi_r\}$. The frame indifference of Ψ_r implies that $\mathcal{K}_r$ can be written as $\mathcal{K}_r=\mathrm{SO}(3)\mathcal{U}_r$ where $\mathcal{U}_r$ is a set of symmetric definite positive tensors. More specifically, for martensitic crystals, the set $\mathcal{K}_r$ assumes the form

$$\mathcal{K}_r=\mathrm{SO}(3)\boldsymbol{U}_r, \tag{2.3}$$

where the distinct symmetric positive definite tensors $\{\boldsymbol{U}_r\}_{1\le r\le n}$ are the transformation strains of the different variants. Note from (2.1) that the strains $\{\boldsymbol{U}_r\}$ are symmetry related, i.e. $\boldsymbol{U}_r$ can be written as $\boldsymbol{U}_r=\boldsymbol{R}_r\boldsymbol{U}_1\boldsymbol{R}_r^T$, where $\boldsymbol{R}_r$ is the rotation appearing in (2.1).

Consider now a martensitic single crystal occupying a domain Ω in the reference configuration. We denote by $\boldsymbol{x}\mapsto\boldsymbol{u}(\boldsymbol{x})$ the mapping between the reference configuration and a deformed configuration at equilibrium. The crystal is subjected to