



A non-convex lower bound on the effective energy of polycrystalline shape memory alloys

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ABSTRACT

This paper addresses the estimation of the effective free energy of polycrystalline shape memory alloys, in the framework of nonlinear elasticity and infinitesimal strains. The translation method is combined with a Hashin–Shtrikman type variational formulation to provide rigorous lower bounds on the effective free energy. Those bounds incorporate both intra-grain compatibility conditions (resulting in a non-convex bound) and inter-grain constraints (by taking one- and two-point statistics into account). Some examples are given to compare the results obtained with other bounds from the literature.

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1. Introduction

The peculiar properties of shape memory alloys (SMAs) are associated with a diffusionless solid/solid phase transformation between different crystallographic structures (austenite and martensite). In a polycrystalline specimen (which is the common form of commercially produced SMAs), one typically observes the formation of martensitic microstructures in each grain. The selection of those microstructures is notably dependent on the *texture*, i.e. the distribution, shapes and orientations of the grains. Polycrystalline SMAs thus involve three different length scales, assumed in the following to be well separated. The finest scale is the *microscopic* scale of microstructures formed in each grain. The *mesoscopic* scale is the scale of individual grains, whereas the *macroscopic* scale is the scale of a polycrystalline material, consisting in numerous grains.

To account for the phase transformation between austenite and martensite, the microscopic free energy is generally modelled as a piecewise quadratic function, with multiple wells. The mesoscopic free energy is then obtained by relaxation (or quasiconvexification) of the microscopic free energy. This is a difficult problem, which still remains largely open. It essentially amounts to solve an optimal design problem, consisting in finding the geometric arrangement of austenite and martensite that minimizes the total energy (Kohn, 1991). Except in few special cases, the exact solution remains elusive. However, bounds on the relaxed energy can be derived, notably using lamination techniques for upper bounds (Avallaneda and Milton, 1989; Tartar, 1990; Kohn, 1991) or the translation method for lower bounds (Milton, 1990; Pipkin, 1991; Firoozye, 1991). Such bounds are formulated as optimization problems, which, although simpler than the original relaxation problem, may still be difficult to solve in a closed form.

At the macroscopic scale, polycrystalline SMAs can be considered as composite materials, viewing groups of grains with the same orientation as individual homogeneous materials, governed by mesoscopic free energy functions. The general problem of estimating the macroscopic (or effective) free energy of a nonlinear composite has been extensively studied

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(see e.g. the review by [Ponte Castañeda and Suquet \(1998\)](#)). General methods have notably been developed to obtain rigorous bounds in terms of the free energies of the constituent materials and of the texture. However, applying such methods to polycrystalline SMAs is not straightforward because of the complicated mathematical structure of the mesoscopic free energy, which arises from relaxation.

So far, Taylor- and Sachs-type of bounds have been the approach of choice for studying polycrystalline SMAs: making the assumption of constant strain, [Bhattacharya and Kohn \(1997\)](#) have proposed a lower bound on the set of recoverable strains. That bound only takes limited information on the texture into account, because it only depends on the list of orientations that are present. Making the assumption of constant stress leads to the convexification lower bound on the macroscopic free energy, as notably considered by [Hackl et al. \(2007\)](#). The result is a convex function, whereas the free energy of SMAs is not necessarily so. Recently, [Hackl and Heinen \(2008\)](#) have proposed an elaborate upper bound for polycrystalline SMAs, combining lamination techniques with the ‘non-local’ variational approach of [Smyshlyaev and Willis \(1998a\)](#). Their results account for the possible non-convexity of the free energy and depend on two-point statistics of the texture. In the present paper, a rigorous lower bound with the same properties is proposed. We first apply the translation method to derive a lower bound on the free energy of single crystals (Section 2). Taking the special structure of the bound obtained into account, a generalization to polycrystals is presented in Section 4. In particular, this allows one to derive a non-convex polycrystalline bound depending on one-point statistics (Section 5). Next, using a Hashin–Shtrikman type of variational formulation, a bound depending on two-point statistics is proposed (Section 6). The corresponding results are compared with other bounds from the literature.

2. Single crystal

Let us first consider a reference single crystal of SMA. To account for the solid/solid phase transformation between austenite and martensite, the microscopic free energy Ψ^0 is generally modelled as a multiwell function of the form

$$\Psi^0(\mathbf{e}) = \min_{1 \leq i \leq k} \Psi_i^0(\mathbf{e}) \quad (1)$$

where

$$\Psi_i^0(\mathbf{e}) = \frac{1}{2}(\mathbf{e} - \mathbf{e}_i^0) : \mathbf{L}^0 : (\mathbf{e} - \mathbf{e}_i^0) + w_i^0 \quad (2)$$

represents the free energy of phase i . The total number k of phases as well as the reference transformation strains $\mathbf{e}_1^0, \dots, \mathbf{e}_k^0$ is obtained from the crystallographic structure of the alloy considered (see e.g. [Bhattacharya, 2003](#)). The number k is equal to $nv + 1$ where nv is the number of martensitic variants. The coefficients w_i^0 depend on the temperature and are usually given the same value for all martensitic variants. In (2) we implicitly make the assumption that all the individual phases have the same elastic moduli \mathbf{L}^0 . This assumption is frequently used in the literature as it considerably simplifies the analysis, but its validity remains questionable. The more relevant bounds from the literature have been obtained under that particular assumption (see e.g. [Smyshlyaev and Willis, 1998a](#); [Hackl and Heinen, 2008](#)). At the present stage, the extension of those bounds to a more general context is unclear and remains to be investigated. The same remark also applies to the methodology presented in this paper.

The mesoscopic free energy of the reference single crystal is the relaxation of Ψ^0 , defined by

$$Q\Psi^0(\bar{\mathbf{e}}) = \inf_{\mathbf{e} \in \mathcal{X}(\bar{\mathbf{e}})} \frac{1}{|\Omega|} \int_{\Omega} \Psi^0(\mathbf{e}) \, d\mathbf{x} \quad (3)$$

where

$$\mathcal{X}(\bar{\mathbf{e}}) = \{\mathbf{e} | \exists \mathbf{u}(\mathbf{x}) \text{ such that } \mathbf{e} = (\nabla \mathbf{u} + \nabla^T \mathbf{u})/2 \text{ in } \Omega; \mathbf{u}(\mathbf{x}) = \bar{\mathbf{e}} \cdot \mathbf{x} \text{ on } \partial\Omega\} \quad (4)$$

The result is known to be independent on the domain Ω considered (see [Dacorogna, 2008](#) and references therein). Following [Kohn \(1991\)](#), we have

$$Q\Psi^0(\bar{\mathbf{e}}) = \inf_{\theta \in \mathcal{F}} Q\Psi^0(\bar{\mathbf{e}}, \theta) \quad (5)$$

where $\mathcal{F} = \{\theta = (\theta_1, \dots, \theta_k) \in \mathbb{R}_k | \theta_i \geq 0; \sum_{i=1}^k \theta_i = 1\}$ and $Q\Psi^0(\bar{\mathbf{e}}, \theta)$ is the so-called relaxation at fixed volume fractions, defined by

$$Q\Psi^0(\bar{\mathbf{e}}, \theta) = \inf_{\chi_i} \inf_{\mathbf{e} \in \mathcal{X}(\bar{\mathbf{e}})} \frac{1}{|\Omega|} \int_{\Omega} \sum_{i=1}^k \chi_i(\mathbf{x}) \Psi_i^0(\mathbf{e}) \, d\mathbf{x}$$

In this expression, the first infimum is taken over characteristic functions χ_i compatible with volume fractions θ . Such functions satisfy

$$\chi_i(\mathbf{x}) \in \{0, 1\}; 1 = \sum_{i=1}^k \chi_i(\mathbf{x}); \theta_i = \frac{1}{|\Omega|} \int_{\Omega} \chi_i(\mathbf{x}) \, d\mathbf{x} \quad (6)$$

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