PERGAMON

Journal of the Mechanics and Physics of Solids
49 (2001) 899–925

JOURNAL OF THE
MECHANICS AND
PHYSICS OF SOLIDS

www.elsevier.com/locate/jmps

The effective energy and laminated microstructures in martensitic phase transformations

Guillermo H. Goldsztein *

Applied Mathematics, Caltech, Pasadena, CA 91125, USA

Received 2 November 1999; received in revised form 13 July 2000; accepted 14 July 2000

Abstract

We study the behavior of crystals that undergo *martensitic transformations*. On cooling, the high-temperature phase (*austenite*) transforms to the *martensite* phase changing its crystalline symmetry. The lower crystalline symmetry of the martensite gives rise to several *variants* of martensite. Each variant has an associated *transformation strain*. These variants accommodate themselves (according to the boundary conditions) forming a *microstructure* that minimizes the *elastic energy*. This minimum value of the energy is called the *effective energy*. We assume that all the material is in the martensite phase (i.e. the material is at low temperatures). We show that, assuming the geometrically linear approximation, the maximum of the effective energy restricted to applied strains in the convex hull of the transformation strains is attained by an applied strain that is a convex combination of only two transformation strains. We derive a recurrence relation to compute the energy corresponding to *laminated microstructures* of arbitrary rank, under the assumption that the variants of martensite are *linearly elastic* and their elastic moduli are isotropic. We use this recurrence relation to develop an algorithm that minimizes the energy over microstructures that belong to the class of rank-r laminates. We apply our methods to the case in which the transformation is cubic to monoclinic (corresponding to TiNi). We conclude with some comments on the possible implications of our calculations on the behavior of this shape-memory alloy. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: A. Microstructures; A. Phase transformation; B. Layered material; C. Numerical algorithms; C. Optimization

---

1. Introduction

In this paper we study the behavior of single crystals that undergo *martensitic transformations*. These transformations are stress or temperature induced solid-to-solid

---

* Present address: School of Mathematics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA. Tel.: +1-404-894-2286; fax: +1-404-894-4409.
E-mail address: ggold@math.gatech.edu (G.H. Goldsztein).

PII: S0022-5096(00)00057-0

phase transitions. On cooling, the high-temperature phase (*austenite*) transforms to the *martensite* phase changing its crystalline symmetry. The lower crystalline symmetry of the martensite gives rise to several *variants*. Each variant has an associated *stress-free* or *transformation strain*. The mathematical model adopted in this paper assumes that the variants accommodate themselves forming a *microstructure* that minimizes the *elastic energy*. This minimum value of the energy is usually called the *effective* or *relaxed energy*.

Given homogeneous boundary conditions, the problem of computing the effective energy and the optimal microstructures has been extensively studied. In the presence of only two stress-free strains and when the corresponding phases (variants in our context) are linearly elastic with the same elastic moduli, this problem has been solved assuming the geometrically linear approximation. In particular, it has been shown that optimal microstructures are not unique, there always exist optimal microstructures among the class of layered mixtures (or *laminates*), and formulae for the effective energy were given (see Khachaturyan, 1966; Kohn, 1991; Pipkin, 1991; Lurie and Cherkaev, 1988). Another case in which the effective energy has been successfully computed (also assuming the geometrically linear approximation) is when the variants are linearly elastic with the same elastic moduli and the transformation strains are *pairwise compatible*. More precisely, it has been shown that, under these conditions, the effective energy is the *convexification* of the minimum of the microscopic energies of each variant (see Bhattacharya, 1993). Although there has also been substantial progress in the more general case in which more than two variants are involved but they are not pairwise compatible (see Smyshlyaev and Willis, 1999; Firoozye and Kohn, 1993), no closed formula or method for the computation of the effective energy has been obtained. We should also mention that much progress has also been accomplished when the geometrically linear approximation is not assumed (see for example Ball and James, 1987; Bhattacharya et al., 1994) and that the list of references given here is by no means complete.

In this paper we assume the geometrically linear approximation, that all the material is in its martensite phase (i.e. the material is at low temperatures), that the variants are linearly elastic and that their elastic moduli are isotropic. This mathematical model has been widely used in the literature and it is reviewed in Section 2.

In Section 3 we obtain our first result, namely, we show that the maximum of the effective energy restricted to applied strains in the convex hull of the transformation strains is attained by an applied strain that is a convex combination of only two transformation strains. This result is also valid if the elastic moduli of the variants are not isotropic. In that same section, we also bound the difference between the effective energy and its convexification for any applied strain.

In Section 4 we make use of the fact that the variants have the same density to simplify the existing formulae (Khachaturyan, 1966; Kohn, 1991; Pipkin, 1991) for the energy corresponding to rank-one laminates, and to derive a recurrence relation to compute the energy associated with laminates of higher rank. These formulae allow us to develop a *global* minimization algorithm that computes optimal rank-r laminated microstructures and the corresponding energies. This algorithm is presented in Section 5.

In Section 6 we argue that approximating the effective energy by the result of restricting the minimization of the energy to microstructures in the class of low-rank laminates works best when the applied strain is a convex combination of only two transformation strains. Thus, the results of Section 3 complement nicely with the numerical method of Section 5. We can compute an upper bound for the effective energy restricted to applied strains that are a convex combination of two transformation strains with our numerical method, and we can use this computation and the results of Section 3 to obtain an upper bound for the effective energy for any applied strain. In Section 6 we apply our methods to the case in which the austenite phase has cubic symmetry and martensite phase has monoclinic symmetry (with the transformation strains corresponding to TiNi). We conclude with some comments on the possible implications of our calculations on the behavior of this shape memory alloy.

One of the motivations for the present study lies in a recently introduced numerical method for the simulation of martensitic transformations in polycrystals (see Bruno et al., 1996; Bruno and Goldsztein, 1999, 2000). This method makes use of the effective energy for single crystals. While previous implementations were done for materials in which the effective energy for single crystals was known (such as two-dimensional examples and three-dimensional cubic to orthorhombic transformations), future studies (such as cubic to monoclinic transformations) will make use of the results presented here. This paper can also be regarded as a contribution in the characterization of the set of strains that can be attained with small energies. The relevance of this set lies in its critical role in some models of shape-memory materials (see Bhattacharya and Kohn, 1996, 1997; Shu and Bhattacharya, 1998 for example).

2. The mathematical model

In this section we describe the mathematical model that we adopt in this paper. Since this model is well established and has been extensively used in the literature to study martensitic phase transitions, we will keep our description brief.

We consider a material that, on cooling, transforms from the austenite phase to the martensite phase changing its crystalline symmetry. Due to this change in the relative distance of the atoms, the stress-free strains of both phases are different from each other. For convenience, we will choose our coordinate system so that the stress-free strain of the austenite is 0. The lower crystalline symmetry of the martensite gives rise to several stress-free strains (usually called transformation strains). Each transformation strain is associated with a variant of martensite. The transformation strain associated with the ith variant will be denoted by $\varepsilon^{T(i)}$. The number of variants N depends on the crystalline symmetry of the material. More precisely, for any pair of transformation strains $\varepsilon^{T(i)}$ and $\varepsilon^{T(j)}$, there is at least one rotation R, among the rotations that form the group symmetries associated with the atomic lattice of the austenite, such that $\varepsilon^{T(i)} = R\varepsilon^{T(j)}R^{-1}$.

We assume that all the material is in the martensite phase, that the variants of martensite are linearly elastic and that their elastic moduli are isotropic. Thus, the elastic moduli of all the variants are equal (they will be denoted by C) and they are determined by the Poison ratio v and the shear modulus μ

$$C_{ijk\ell} = \mu\left(\frac{2v}{1-2v}\delta_{ij}\delta_{k\ell} + \delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}\right). \tag{1}$$

The displacement will be denoted by $u = u(x)$ and its associated linear strain by $\varepsilon = \varepsilon(x)$

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = \frac{1}{2}(u_{i,j} + u_{j,i}). \tag{2}$$

The energy density $W = W(\varepsilon, \varepsilon^T) = W(\varepsilon(x), \varepsilon^T(x))$ at a point x is given by

$$W = \frac{1}{2}(\varepsilon - \varepsilon^T)C(\varepsilon - \varepsilon^T) = \frac{1}{2}C_{ijk\ell}(\varepsilon_{ij} - \varepsilon^T_{ij})(\varepsilon_{k\ell} - \varepsilon^T_{k\ell}), \tag{3}$$

where $\varepsilon^T = \varepsilon^T(x) = \varepsilon^{T(m)}$ if the material is in the mth variant at the position x. The displacement u satisfies the equilibrium equations

$$\sigma_{ij,j} = 0, \tag{4}$$

where σ denotes the stress

$$\sigma_{ij} = C_{ijk\ell}(\varepsilon_{k\ell} - \varepsilon^T_{k\ell}). \tag{5}$$

If the domain of the material Ω (we assume that the interior of Ω is not empty) is subject to homogeneous Dirichlet boundary conditions

$$u_i(x) = \varepsilon^{\mathrm{a}}_{ij}x_j \quad x \in \partial\Omega \tag{6}$$

(ε^{a} is a constant tensor) we assume that the material *attempts* to form a microstructure that minimizes the energy. This infimum value of the energy is usually called the effective, macroscopic or relaxed energy

$$E(\varepsilon^{\mathrm{a}}) = \inf_{\varepsilon^T} \frac{1}{|\Omega|}\int_\Omega W(\varepsilon(x), \varepsilon^T(x))\,\mathrm{d}x. \tag{7}$$

The infimum in this last equation is taken over all possible microstructures (i.e. $\varepsilon^T(x) \in \{\varepsilon^{T(1)}, \varepsilon^{T(2)}, \ldots, \varepsilon^{T(N)}\}$, the strain $\varepsilon(x)$ is given by Eq. (2) and displacement $u(x)$ satisfies the boundary conditions (6) and the equilibrium equations (4)). It is known that the effective energy E depends only on the *applied strain* ε^{a} and not on the domain Ω. We said that the material attempts to minimize its energy because in general minimizers of Eq. (7) do not exist. Thus, sequences or families of microstructures for which their associated energies have a limit are usually considered. When this limiting value is the effective energy, the associated family of microstructures is usually called a *minimizing sequence*. For future reference, we remind the reader that the effective energy E is quasiconvex (see Bhattacharya and Kohn, 1997 for example) and thus, it satisfies

$$E(\varepsilon^{\mathrm{a}}) = \inf\left\{\frac{1}{|\Omega|}\int_\Omega E(\varepsilon(x))\,\mathrm{d}x\text{: } u \text{ is continuous and satisfies (6)}\right\}, \tag{8}$$

where ε is given by Eq. (2) (see Dacorogna, 1989 for example).

3. Upper bound for the effective energy

In this section we will prove the following proposition:

Proposition 1. *The maximum of the effective energy restricted to applied strains in the convex hull of the transformation strains is attained by an applied strain that is a convex combination of only two transformation strains.*

We will also bound the difference between the effective energy and its convexification for any applied strain.

We stress here that the validity of the results of this section relies on the fact that the transformation strains have the same hydrostatic component. We mention that Proposition 1 is also valid if the elastic moduli of the variants are not isotropic and that this proposition can be regarded as a generalization of the analysis of Bhattacharya (1993) to show that the effective energy restricted to applied strains in the convex hull of the transformation strains is 0 if the transformation strains are pairwise compatible.

3.1. Compatible strains and laminates

The analysis of this section requires that we first review the notion of compatible strains and laminated microstructures (see for example Ball and James, 1987; Bhattacharya, 1993 or Wechsler et al., 1953). Two constant linear strains $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ are compatible if there is a displacement u whose associated linear strain ε is of the form

$$\varepsilon(x) = \begin{cases} \varepsilon^{(\gamma)} & \text{if } x \in V, \\ \varepsilon^{(\beta)} & \text{if } x \in R^3 - V, \end{cases} \tag{9}$$

where V is neither empty nor equal to R^3.

Let us denote by $y_1 \leq y_2 \leq y_3$ the eigenvalues of $\varepsilon^{(\gamma)} - \varepsilon^{(\beta)}$. It is well known that $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ are compatible if and only if $y_2 = 0$. If in addition $\varepsilon^{(\gamma)} \neq \varepsilon^{(\beta)}$, the boundary of V is the union of parallel planes whose normal $\hat{n}$ depends on the strains $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$. In particular, let us choose the set V to be the union of parallel layers of the same thickness with the property that the distances between two neighboring layers are equal. More precisely, for any $0 \leq \lambda \leq 1$, and any $\delta > 0$, let us define

$$V = V(\delta) = V(\lambda, \delta) = \left\{ x \colon \sum_{i=1}^{3} x_i \hat{n}_i \in \bigcup_{k \in Z} [k\delta, (k+\lambda)\delta] \right\}. \tag{10}$$

Assume that λ is fixed. We now have a family of displacements u parameterized by δ, $u = u(x, \delta)$ whose linear strains are given by Eqs. (9)–(10). To avoid arbitrary translations and infinitesimal rotations, we require that u satisfies

$$u_i(x) = u_i(x, \delta) = \varepsilon_{ij}^{(\gamma)} x_j \quad \text{if } \sum_{i=1}^{3} x_i \hat{n}_i \in [0, \lambda\delta]. \tag{11}$$

The microstructure described above is usually called laminate. Note that, for any x, we have

$$\lim_{\delta\to 0} u_i(x,\delta) = \lambda\varepsilon^{(\gamma)}_{ij}x_j + (1-\lambda)\varepsilon^{(\beta)}_{ij}x_j. \tag{12}$$

Thus, we say that $\lambda\varepsilon^{(\gamma)} + (1-\lambda)\varepsilon^{(\beta)}$ is the macroscopic strain of the laminate and that $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ are its microscopic strains.

3.2. Proof of Proposition 1

The proof of Proposition 1 results from the following observations:

Observation 1. *Let $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ be two constant strains. Assume that both strains have the same hydrostatic component (i.e. both matrices have the same trace* $\mathrm{tr}(\varepsilon^{(\gamma)}) = \mathrm{tr}(\varepsilon^{(\beta)})$*). Then, $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ are compatible if and only if the determinant of their difference is* 0.

This observation follows from the fact that the sum of the eigenvalues of $\varepsilon^{(\gamma)} - \varepsilon^{(\beta)}$ is equal to 0 (because the trace of $\varepsilon^{(\gamma)} - \varepsilon^{(\beta)}$ is 0) and the fact that two strains are compatible if and only if the middle eigenvalue of their difference is 0.

Observation 2. *Let S be a linear subspace of the space of* 3×3 *real matrices. If the dimension of S is greater than* 1, *there exists a matrix $M \in S$ different from* 0 *such that its determinant is* 0.

To prove this observation, let M_1 and M_2 be two linearly independent matrices that belong to S. If the determinant of any of these matrices is 0 there is nothing to prove. On the other hand, if the determinants of both matrices are different from 0, consider the function

$$p(x) = \det(xM_1 + M_2), \tag{13}$$

where x is a real number and $\det(A)$ denotes the determinant of the matrix A. Since the matrices M_i are 3×3 (and real) and $\det(M_1) \neq 0$, $p(x)$ is a real polynomial of degree 3. Thus, it has a real root x_0. Since M_1 and M_2 are linearly independent, we have that $M = x_0M_1 + M_2$ is different from 0, it belongs to S, and its determinant is 0, which proves observation 2.

Observation 3. *Let $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ be two compatible constant strains. Then, for any* $\lambda \in [0,1]$ *the following holds*:

$$E(\lambda\varepsilon^{(\gamma)} + (1-\lambda)\varepsilon^{(\beta)}) \leq \lambda E(\varepsilon^{(\gamma)}) + (1-\lambda)E(\varepsilon^{(\beta)}). \tag{14}$$

This is a well-known observation. It can be proven as follows. Let $u^\star$ denote the family of displacements corresponding to the laminate whose microscopic strains are $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ and the volume fraction occupied by $\varepsilon^{(\gamma)}$ is λ (see Eqs. (9)–(11)). This family of displacements is parameterized by the thickness of the layers δ. Let $\varepsilon^\star$ be the associated family of strains (i.e. $\varepsilon^{\star}$ is given by Eqs. (9)–(10)). Let $\varepsilon^{\mathrm{a}} = \lambda\varepsilon^{(\gamma)} + (1-\lambda)\varepsilon^{(\beta)}$. Given Eq. (12), the boundary conditions (6) are satisfied in the thin layer limit $\delta \to 0$. Thus, from Eq. (8) we conclude

$$E(\lambda\varepsilon^{(\gamma)} + (1-\lambda)\varepsilon^{(\beta)}) \le \lim_{\delta\to 0} \frac{1}{|\Omega|}\int_{\Omega} E(\varepsilon^{\star})\,\mathrm{d}x = \lambda E(\varepsilon^{(\gamma)}) + (1-\lambda)E(\varepsilon^{(\beta)}).$$

Observation 4. *Suppose that the applied strain ε^{a} is a convex combination of k transformation strains $\varepsilon^{T(1)}, \varepsilon^{T(2)}, \ldots, \varepsilon^{T(k)}$. Then*

$$E(\varepsilon^{\mathrm{a}}) \le \max_{0\le\lambda\le 1}\ \max_{1\le i<j\le k} E(\lambda\varepsilon^{T(i)} + (1-\lambda)\varepsilon^{T(j)}). \tag{15}$$

To prove this observation we proceed by induction on k. First note that we can assume that ε^{a} is not a convex combination of $k-1$ of these k transformation strains. If k is equal to 1 or 2, the inequality (15) is trivially true. Now, let k be greater than 2. Consider the linear subspace S, generated by $\{\varepsilon^{T(1)} - \varepsilon^{\mathrm{a}}, \varepsilon^{T(2)} - \varepsilon^{\mathrm{a}}, \ldots, \varepsilon^{T(k)} - \varepsilon^{\mathrm{a}}\}$. Since ε^{a} cannot be written as a convex combination of 2 of these transformation strains, we have that the dimension of S is greater than 1. Thus, from observation 2, we can select $\varepsilon \in S$ such that its determinant is 0, $\det(\varepsilon) = 0$. Consider the semi-line $\varepsilon^{\mathrm{a}} + y\varepsilon$ with $y \ge 0$. It is easy to see that there exists a strain $\varepsilon^{(\gamma)}$ in this semi-line that is a convex combination of $k-1$ of these transformation strains. Analogously, let $\varepsilon^{(\beta)}$ be a strain of the form of $\varepsilon^{\mathrm{a}} + y\varepsilon$, $y \le 0$, that is a convex combination of $k-1$ of these transformation strains. Since $\det(\varepsilon) = 0$, we have $\det(\varepsilon^{(\gamma)} - \varepsilon^{(\beta)}) = 0$. Given that all the transformation strains have the same hydrostatic component, we have that $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ also have the same hydrostatic component. Thus, $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ are compatible. Now note that ε^{a} is a convex combination of $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$. Thus, from observation 3 it follows that:

$$E(\varepsilon^{\mathrm{a}}) \le \max\{E(\varepsilon^{(\gamma)}), E(\varepsilon^{(\beta)})\}. \tag{16}$$

Finally, since both $\varepsilon^{(\gamma)}$ and $\varepsilon^{(\beta)}$ are convex combinations of $k-1$ transformation strains, we can apply our inductive hypothesis to conclude the proof of this observation.

Obviously, this last observation implies Proposition 1 (just take $k = N$).

3.3. Applied strains outside the convex hull of the transformation strains

We now turn to the derivation of our upper bound for the effective energy valid for applied strains ε^{a} outside the convex hull of the transformation strains. We first note that (under the present conditions) the convexification of the effective energy is given by

$$E^{(\mathrm{c})}(\varepsilon^{\mathrm{a}}) = \min_{\varepsilon\in H} \frac{1}{2}(\varepsilon^{\mathrm{a}} - \varepsilon)C(\varepsilon^{\mathrm{a}} - \varepsilon), \tag{17}$$

where H denotes the convex hull of the transformation strains

$$H = \left\{\varepsilon\colon\ \varepsilon = \sum_{i=1}^{N} \lambda_i \varepsilon^{T(i)} \text{ where } \lambda_i \ge 0 \text{ and } \sum_{i=1}^{N} \lambda_i = 1\right\}.$$

Let ε^{c} be the minimizer of Eq. (17). For any arbitrary field of transformation strains $\varepsilon^T = \varepsilon^T(x)$, we certainly have

$$\frac{1}{2}(\varepsilon^{\mathrm{a}}-\varepsilon^T)C(\varepsilon^{\mathrm{a}}-\varepsilon^T)=E^{(\mathrm{c})}(\varepsilon^{\mathrm{a}})+(\varepsilon^{\mathrm{a}}-\varepsilon^{\mathrm{c}})C(\varepsilon^{\mathrm{c}}-\varepsilon^T)+\frac{1}{2}(\varepsilon^{\mathrm{c}}-\varepsilon^T)C(\varepsilon^{\mathrm{c}}-\varepsilon^T). \tag{18}$$

Let T be a set of transformation strains $T = \{\varepsilon^{T(i_1)}, \varepsilon^{T(i_2)}, \dots, \varepsilon^{T(i_k)}\}$ such that ε^{c} is in the convex hull of T, but ε^{c} is not a convex combination of $k-1$ elements of T. Since ε^{c} is the minimizer of Eq. (17), we have that for any transformation strain $\varepsilon^{T(i_\ell)}$ in T,

$$(\varepsilon^{\mathrm{a}} - \varepsilon^{\mathrm{c}})C(\varepsilon^{\mathrm{c}} - \varepsilon^{T(i_\ell)}) = 0. \tag{19}$$

Let us now denote by $E^{(\mathrm{s})}(\varepsilon^{\mathrm{a}}, T)$ the effective energy associated with the material that can only transform to variants whose associated transformation strains are in T. In other words, $E^{(\mathrm{s})}(\varepsilon^{\mathrm{a}}, T)$ is the result of restricting the minimization (7) to fields of transformation strains $\varepsilon^T(x)$ that satisfy $\varepsilon^T(x) \in T$ for all x. Given these remarks and Eqs. (7), (18) and (19), we obtain

$$E(\varepsilon^{\mathrm{a}}) \le E^{(\mathrm{c})}(\varepsilon^{\mathrm{a}}) + E^{(\mathrm{s})}(\varepsilon^{\mathrm{c}}, T).$$

On the other hand, the observation 4 implies

$$E^{(\mathrm{s})}(\varepsilon^{\mathrm{c}}, T) \le \max\{E^{(\mathrm{s})}(\lambda\varepsilon^{T(i)} + (1-\lambda)\varepsilon^{T(j)}, T)\colon \varepsilon^{T(i)}, \varepsilon^{T(j)} \in T \text{ and } 0 \le \lambda \le 1\}.$$

We now note that, for any ε, $E^{(\mathrm{s})}(\varepsilon, T_1) \le E^{(\mathrm{s})}(\varepsilon, T_2)$ whenever $T_2 \subseteq T_1$. Thus, if we denote by T_{ij} the set of the two transformation strains $\varepsilon^{T(i)}$ and $\varepsilon^{T(j)}$ ($T_{ij}=\{\varepsilon^{T(i)}, \varepsilon^{T(j)}\}$), it follows that:

$$E^{(\mathrm{s})}(\lambda\varepsilon^{T(i)} + (1-\lambda)\varepsilon^{T(j)}, T) \le E^{(\mathrm{s})}(\lambda\varepsilon^{T(i)} + (1-\lambda)\varepsilon^{T(j)}, T_{ij})$$

for any $0 \le \lambda \le 1$ and any pair of transformation strains $\varepsilon^{T(i)}$ and $\varepsilon^{T(j)}$ that belong to T. From these last three equations, it immediately follows:

$$E(\varepsilon^{\mathrm{a}}) \le E^{(\mathrm{c})}(\varepsilon^{\mathrm{a}}) + \max_{1\le i<j\le N}\{E^{(\mathrm{s})}(\lambda\varepsilon^{T(i)} + (1-\lambda)\varepsilon^{T(j)}, T_{ij})\colon 0 \le \lambda \le 1\}.$$

Finally, from the analysis of the next section, it can be easily inferred that the right-hand side is maximized at $\lambda = \frac{1}{2}$ and that the following equation is valid:

$$E(\varepsilon^{\mathrm{a}}) \le E^{(\mathrm{c})}(\varepsilon^{\mathrm{a}}) + \frac{(1+\nu)}{4}\mu \max_{1\le i<j\le N}\{\min\{z^2\colon z \text{ eigenvalue of } \varepsilon^{T(i)} - \varepsilon^{T(j)}\}\} \tag{20}$$

which gives us a bound on the difference between the effective energy and its convexification valid for any applied strain.

4. Laminates and their associated energies

In this section we review the notion of laminates in more detail and we simplify the existing formulae (Khachaturyan, 1966; Kohn, 1991; Pipkin, 1991) for the energy corresponding to this class of microstructures. This analysis is not new (see Khachaturyan, 1966; Kohn, 1991; Pipkin, 1991), but since in our context all the transformation strains have the same hydrostatic component, we can go a step further than previous work. We will first consider rank-one laminates and then laminates of higher rank.

4.1. Rank-one laminates

Consider the following family of microstructures:

$$\varepsilon^T(x) = \varepsilon^T(x,\delta) = \varepsilon^T(x,\lambda,\delta) = \begin{cases} \varepsilon^{T(\gamma)} & \text{if } x \in V, \\ \varepsilon^{T(\beta)} & \text{otherwise,} \end{cases} \tag{21}$$

where $\varepsilon^{T(\gamma)}$ and $\varepsilon^{T(\beta)}$ are a pair of transformation strains, the set $V = V(\lambda,\delta,\hat{n})$ is given by Eq. (10) and $\hat{n}$ is a given unit vector.

Let $u = u(x) = u(x,\delta)$ be the family of displacements given by Eqs. (9)–(11). The strains ε^γ and ε^β are completely determined (as functions of $\varepsilon^{T(\gamma)}$, $\varepsilon^{T(\beta)}$, $\hat{n}$, λ and ε^{a}) once we require that (for each δ) u satisfies the equilibrium equations (4) and

$$\varepsilon^{\mathrm{a}} = \lambda\varepsilon^\gamma + (1-\lambda)\varepsilon^\beta. \tag{22}$$

More precisely, the strains ε^γ and ε^β are found as follows: The continuity of the displacement u imposes a compatibility condition, namely, there exist a vector b such that

$$\varepsilon^\gamma = \varepsilon^{\mathrm{a}} + (1-\lambda)(b \otimes \hat{n} + \hat{n} \otimes b) \tag{23}$$

and

$$\varepsilon^\beta = \varepsilon^{\mathrm{a}} - \lambda(b \otimes \hat{n} + \hat{n} \otimes b). \tag{24}$$

In these last two equations, we have used the notation $x \otimes y$ (where x and y are vectors) to denote the matrix whose components are $(x \otimes y)_{ij} = x_i y_j$. The equilibrium equations (4) imply

$$[C(b \otimes \hat{n} + \hat{n} \otimes b)]\hat{n} = [C(\varepsilon^{T(\gamma)} - \varepsilon^{T(\beta)})]\hat{n}. \tag{25}$$

This last equation determines b as a function of $\hat{n}$ and the transformation strains $\varepsilon^{T(\gamma)}$ and $\varepsilon^{T(\beta)}$ (this calculation is done in the appendix).

Note that, for every x, Eq. (12) is valid. This fact and Eq. (22) imply that the boundary conditions (6) are satisfied in the thin layer limit $\delta \to 0$. Thus, the limiting value of the energies corresponding to the family of microstructures (21) can be computed by assuming that the corresponding displacements are given by $u = u(x) = u(x,\delta)$, the family of displacements described above. This can be easily done

$$\lim_{\delta\to 0} \frac{1}{|\Omega|} \int_\Omega W(\varepsilon(x), \varepsilon^T(x))\,\mathrm{d}x = \lambda W(\varepsilon^\gamma, \varepsilon^{T(\gamma)}) + (1-\lambda) W(\varepsilon^\beta, \varepsilon^{T(\beta)}). \tag{26}$$

So far no restriction has been made on the normal to the layers $\hat{n}$. But according to our assumptions, low-energy microstructures are preferred over high-energy ones. Thus, we will restrict our attention to orientations that minimize the energy. In other words, we will assume $\hat{n}$ is a minimizer of Eq. (26).

The family of microstructures we have described above, which we denote by L, is called a rank-one laminate. The energy associated with this laminate (i.e. the minimum of Eq. (26) with respect to the layer orientation $\hat{n}$), which we denote by $E^{(\ell)}(\varepsilon^{\mathrm{a}}, L)$, is computed in the appendix. There we obtain

$$E^{(\ell)}(\varepsilon^{\mathrm{a}}, L) = \frac{1}{2}(\varepsilon^{\mathrm{a}} - \varepsilon^{T(L)}) C (\varepsilon^{\mathrm{a}} - \varepsilon^{T(L)}) + P(L). \tag{27}$$

In this last equation we have introduced the following notation:

$$\varepsilon^{T(L)} = \lambda\varepsilon^{T(\gamma)} + (1-\lambda)\varepsilon^{T(\beta)} \tag{28}$$

and

$$P(L) = \mu\lambda(1-\lambda)(1+v)\min\{z^2\colon z \text{ eigenvalue of } \varepsilon^{T(\gamma)} - \varepsilon^{T(\beta)}\}. \tag{29}$$

We say that $\varepsilon^{T(L)}$ is the macroscopic transformation strain of the laminate L and that $\varepsilon^{T(\gamma)}$ and $\varepsilon^{T(\beta)}$ are its microscopic transformation strains. We also say that $P(L)$ is the *penalty* energy or the *cost* to form the laminate L. This energy $P(L)$ is due to the incompatibility of the microscopic transformation strains of the laminate. In the rest of this paper, we will identify any rank-one laminate L with a single *effective* phase whose properties are determined by its macroscopic transformation strain $\varepsilon^{T(L)}$ and its cost of formation $P(L)$.

Before considering higher rank laminates we make a few remarks. There is more than one optimal orientation (see the appendix). Nevertheless, since we are interested only in the energy, we will make reference to the optimal orientations as if there were only one. The optimal orientation $\hat{n}$ does not depend on the applied strain ε^{a}. For convenience, we will identify the different transformation strains $\varepsilon^{T(k)}$ with rank-zero laminates. Thus, if L is a rank-zero laminate, there exists k $(1 \le k \le N)$ such that $\varepsilon^{T(L)} = \varepsilon^{T(k)}$ and $P(L) = 0$.

4.2. Rank-*r* laminates

We will identify any rank-r laminate L with a single effective phase. Roughly speaking, L is a laminate whose material layers are two lower rank laminates ℓ_1 and ℓ_2 (the rank of one of these laminates is $r-1$). More precisely, if λ is the volume fraction of ℓ_1, we can give the following description of rank-r laminates (we only consider rank-r laminates whose layer orientation is optimal):

A rank-r laminate L can be identified with a single effective phase whose properties are determined by its macroscopic transformation strain $\varepsilon^{T(L)}$ and its cost of formation $P(L)$. The macroscopic transformation strain $\varepsilon^{T(L)}$ is given by

$$\varepsilon^{T(L)} = \lambda\varepsilon^{T(\ell_1)} + (1-\lambda)\varepsilon^{T(\ell_2)}, \tag{30}$$

where $\varepsilon^{T(\ell_1)}$ and $\varepsilon^{T(\ell_2)}$ are the macroscopic transformation strains of the lower rank laminates ℓ_1 and ℓ_2, respectively (we also say that $\varepsilon^{T(\ell_1)}$ and $\varepsilon^{T(\ell_2)}$ are the microscopic transformation strains of L). The penalty energy $P(L)$ is given by

$$\begin{aligned} P(L) = {} & \mu\lambda(1-\lambda)(1+v)\min\{z^2\colon z \text{ eigenvalue of } \varepsilon^{T(\ell_1)} - \varepsilon^{T(\ell_2)}\} \\ & + \lambda P(\ell_1) + (1-\lambda)P(\ell_2). \end{aligned} \tag{31}$$

Given the notation introduced above, and following the analysis of rank-one laminates, it can be easily shown that Eq. (27) is valid for laminates of arbitrary rank.

5. Optimal laminates and their associated energies

In this section we develop a *global* minimization algorithm that computes optimal rank-r laminated microstructures and the corresponding energies. More precisely, we will describe a method to evaluate $E_r(\varepsilon^{\mathrm{a}})$, where

$$E_r(\varepsilon^{\mathrm{a}}) = \min\{E^{(\ell)}(\varepsilon^{\mathrm{a}}, L)\colon \text{ rank of } L \le r\} \tag{32}$$

and to find the optimal laminates (i.e. the minimizers of Eq. (32)).

The limiting value of $E_r(\varepsilon^{\mathrm{a}})$ as $r \to \infty$, which we denote by $E_\infty(\varepsilon^{\mathrm{a}})$, is the rank-one convexification of $\varphi(\varepsilon^{\mathrm{a}}) = \min_{1 \le i \le N} W(\varepsilon^{\mathrm{a}}, \varepsilon^{T(i)})$ (see Eq. (3)). On the other hand, $E(\varepsilon^{\mathrm{a}})$ is the quasiconvexification of $\varphi(\varepsilon^{\mathrm{a}})$. Although the example given in Šverák (1990) shows that rank-one convexity does not imply quasiconvexity, it is not known in our particular context if $E_\infty(\varepsilon^{\mathrm{a}}) = E(\varepsilon^{\mathrm{a}})$.

The numerical minimization of energies over laminated microstructures has been previously considered in Ortiz and Repetto (1999), Ortiz et al. (2000) and Dolzmann (1999). The method developed in Ortiz and Repetto (1999), and Ortiz et al. (2000) was used in their theory of dislocation structures. A particular feature of this method is the use of an optimal rank-r laminate as an initial guess to find an optimal rank-$r+1$ laminate. In our context, this approach could run the risk of finding a local minimum instead of the global minimum. On the other hand, the method introduced in Dolzmann (1999) computes the rank-one convexification of any given function. This method is very general but as a consequence, it is prohibitively slow and it requires too much memory if used for our problem in hand. Here we will make use of the fact that we have at our disposal the formulae (27), (30) and (31) to develop an algorithm that always finds the global minimum, it is reasonably fast and does not present memory problems. In the example presented in Section 6, our method cannot go beyond rank-two laminates. The reason for this limitation is that in that example (in which we have 12 transformation strains) there are *too many* rank-three laminates and our algorithm explores many of them to guarantee that the minimum found is global. We now proceed with the description of our method.

5.1. Representation of laminates by trees

Our first step is to represent laminates by binary trees. For our purposes, a binary tree can be described as a set of nodes and edges that satisfy the following: Each node is either single or a parent. Each parent has exactly two children, its left child and its right child (these children are also nodes). Each single does not have any children. Every node except one (called root) has exactly one parent. The root does not have any parents. Nodes are connected by edges. Each node is connected only to its children (if the node is a parent) and to its parent (if the node is not the root). Fig. 1 shows an example of a binary tree.

It is now convenient to introduce the following notation: If a node n is a parent, we will denote by left(n) its left child and by right(n) its right child. The parent of any node n that is not the root will be denoted by parent(n). The root of a tree G will be denoted by root(G). The set of singles of a tree G will be denoted by $\mathscr{S}(G)$

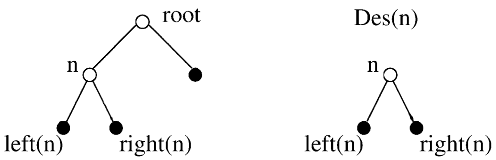

Fig. 1. The left figure shows an example of a binary tree. The black nodes are single and the white nodes are parents. The height of this tree is 2. The right figure shows Des(n), the tree formed by the node n and its descendents.

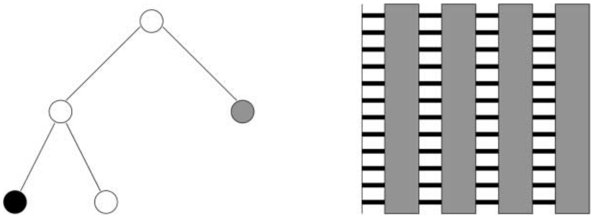

Fig. 2. Illustration of a laminate (right figure) and its associated tree (left figure). The transformation strains of the single nodes, as well as the spatial distribution of transformation strains in the laminate are represented by colors. Same colors represent the same transformation strain.

and the set of parents by $\mathscr{P}(G)$. The height of a tree G, which we will be denoted by Height(G), is the number of elements -1 of the largest sequence of nodes $\{n_i\}$ with the property that parent$(n_i)=n_{i-1}$. Note that any node n, its descendents and the edges connecting them form a tree. We will denote this tree by Des(n) (see Fig. 1).

Each node n will have an associated strain that will be refered to as the transformation strain of the node n and it will be denoted by $\varepsilon^{T(n)}$. In addition, each node p that is a parent will have an associated scalar variable $\lambda(p) \in [0,1]$. We now proceed with the description of the representation of laminates by binary trees by induction on the rank of the laminate. If L_0 is a rank-zero laminate, its corresponding tree $G(L_0)$ consists of a single node n whose transformation strain is equal to the transformation strain of L_0, $\varepsilon^{T(n)} = \varepsilon^{T(L_0)}$. Let us now consider a rank-r laminate L, where $r > 0$. Let ℓ_1 and ℓ_2 be the lower rank laminates that form the material layers of L, $G(\ell_1)$ and $G(\ell_2)$ their corresponding trees, and λ the volume fraction of ℓ_1. The tree G that represents L is the tree that satisfies Des(left(root(G)))$=G(\ell_1)$ and Des(right(root(G)))$=G(\ell_2)$. The transformation strain of root(G) is equal to the macroscopic transformation strain of the laminate L, $\varepsilon^{T(\text{root}(G))} = \varepsilon^{T(L)}$, and $\lambda(\text{root}(G))$ is equal to the volume fraction of ℓ_1, $\lambda(\text{root}(G)) = \lambda$. The transformation strain of any other node n of G ($n \neq \text{root}(G)$) is the same transformation strain n has associated as a node of $G(\ell_1)$ or $G(\ell_2)$, and analogously, the value of $\lambda(p)$, for any parent p (that is not the root), does not change if we consider p to be a node of G instead of being a node of $G(\ell_1)$ or $G(\ell_2)$. In the rest of this paper we will denote by $G(L)$ the tree that represents the laminate L. In Fig. 2 we illustrate this correspondence between laminates and binary trees with an example. Note that the rank of a laminate is equal to the height of its corresponding tree.

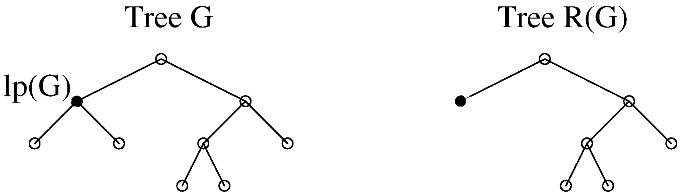

Fig. 3. The black node of the tree G (left figure) is lp(G). The right tree R(G) is the result of removing the children of lp(G) from the tree G.

5.2. *Recurrence relation to evaluate the energy*

We will now use the tree representation of laminates to derive a recurrence relation to evaluate the energy. To that end, we first need to define a few operations on binary trees. Let G be a binary tree (as described above). We will denote by lp(G) the most left parent that is not a grandparent. In other words, lp(G) is the parent that satisfies the following property: the children of lp(G) are single and if n is another parent whose children are single, there exist an ancestor a (of both lp(G) and n) such that $\mathrm{lp}(G) \in \mathrm{Des}(\mathrm{left}(a))$ and $n \in \mathrm{Des}(\mathrm{right}(a))$. We will denote by R($G$) the tree that results from removing the children of lp(G) (and the corresponding edges) from the tree G. In Fig. 3 we illustrate these definitions with an example.

We next introduce a number of tensors. Let ε be a constant linear strain that is a linear combination of the transformation strains

$$\varepsilon = \sum_{i=1}^{N} z_i \varepsilon^{T(i)}. \tag{33}$$

Let p_2, p_1 and p_0 be the coefficients of its characteristic polynomial

$$\det(\beta I - \varepsilon) = \beta^3 + p_2\beta^2 + p_1\beta + p_0, \tag{34}$$

where I denotes the identity matrix and $\det(M)$ denotes the determinant of the matrix M. We define f_{ijk} and g_{ij} ($1 \le i,\ j,\ k \le N$) as the symmetric tensors that satisfy

$$p_0 = f_{ijk} z_i z_j z_k \quad \text{and} \quad p_1 = g_{ij} z_i z_j \ \text{ for all } \varepsilon \text{ of the form (33).}$$

We also introduce the tensors a_{ij} and b_i

$$a_{ij} = \frac{1}{2}\varepsilon^{T(i)} C \varepsilon^{T(j)} \quad \text{and} \quad b_i = -\frac{1}{2}\varepsilon^{T(i)} C \varepsilon^{\mathrm{a}}, \ \ 1 \le i,\ j \le N,$$

where ε^{a} is the applied strain.

We are now ready to describe a recurrence relation to evaluate the energy. Let L be the laminate under consideration and $G = G(L)$ its corresponding tree. Let N_{p} be the number of parents of the tree G. We define the sequence of trees

$$G_0 = G, \quad G_{q+1} = R(G_q) \quad 0 \le q \le N_{\mathrm{p}} - 1.$$

For convenience, we introduce the functions

$$h_1(a,b,x) = ax + b(1-x), \quad h_2(a,b,c,x) = ax^2 + 2bx(1-x) + c(1-x)^2$$
$$\text{and} \quad h_3(a,b,c,b,x) = ax^3 + 3bx^2(1-x) + 3cx(1-x)^2 + d(1-x)^3. \tag{35}$$

We define

$$a^{(0)}_{st} = a_{ij}, \quad b^{(0)}_{s} = b_i, \quad f^{(0)}_{stu} = f_{ijk} \quad \text{and} \quad g^{(0)}_{st} = g_{ij} \qquad \forall s,t,u \in \mathscr{S}(G_0),$$

where $i = i(s)$, $j = j(t)$ and $k = k(u)$ are the integers that satisfy

$$\varepsilon^{T(s)} = \varepsilon^{T(i)}, \quad \varepsilon^{T(t)} = \varepsilon^{T(j)} \quad \text{and} \quad \varepsilon^{T(\mathrm{u})} = \varepsilon^{T(k)}.$$

To simplify the notation in the formulae that will follow, let

$$p = p(q) = \mathrm{lp}(G_q), \quad \ell = \mathrm{left}(p) \quad \text{and} \quad r = \mathrm{right}(p). \tag{36}$$

We now define the family of tensors $f^{(q+1)}$ $(0 \le q \le N_\mathrm{p} - 1)$

$$f^{(q+1)}_{ppp} = h_3(f^{(q)}_{\ell\ell\ell}, f^{(q)}_{\ell\ell r}, f^{(q)}_{\ell rr}, f^{(q)}_{rrr}, \lambda(p)), \quad f^{(q+1)}_{pps} = h_2(f^{(q)}_{\ell\ell s}, f^{(q)}_{\ell rs}, f^{(q)}_{rrs}, \lambda(p)),$$

$$f^{(q+1)}_{pst} = h_1(f^{(q)}_{\ell st}, f^{(q)}_{rst}, \lambda(p)) \quad \text{and} \quad f^{(q+1)}_{stu} = f^{(q)}_{stu} \ \forall s,t,u \in \mathscr{S}(G_{q+1}) - \{p\}$$

and we complete the definition of $f^{(q+1)}$ by requiring these tensors to be symmetric, i.e. $f^{(q+1)}_{pst} = f^{(q+1)}_{pts}$, etc. Similarly, we define

$$g^{(q+1)}_{pp} = h_2(g^{(q)}_{\ell\ell}, g^{(q)}_{\ell r}, g^{(q)}_{rr}, \lambda(p)), \quad g^{(q+1)}_{ps} = h_1(g^{(q)}_{\ell s}, g^{(q)}_{rs}, \lambda(p)), \quad g^{(q+1)}_{st} = g^{(q)}_{st}$$

(the tensors $g^{(q+1)}$ are also symmetric, i.e. $g^{(q+1)}_{ps} = g^{(q+1)}_{sp}$) and

$$a^{(q+1)}_{pp} = h_2(a^{(q)}_{\ell\ell}, a^{(q)}_{\ell r}, a^{(q)}_{rr}, \lambda(p)), \quad a^{(q+1)}_{ps} = h_1(a^{(q)}_{\ell s}, a^{(q)}_{rs}, \lambda(p)), \quad a^{(q+1)}_{st} = a^{(q)}_{st}$$

(we also have $a^{(q+1)}_{ps} = a^{(q+1)}_{sp}$), $\forall s,t \in \mathscr{S}(G_{q+1}) - \{p\}$. Let β_p be the middle root of the polynomial

$$\beta^3 + p_1(p)\beta + p_0(p), \tag{37}$$

(for reasons to be discussed later, all the roots of this polynomial are real) whose coefficients $p_0(p)$ and $p_1(p)$ are given by

$$p_0(p) = \sum_{0 \le i,j,k \le 1} (-1)^{i+j+k} f^{(q)}_{c(i)c(j)c(k)} \quad \text{and} \quad p_1(p) = \sum_{0 \le i,j \le 1} (-1)^{i+j} g^{(q)}_{c(i)c(j)}, \tag{38}$$

where $c(0) = \ell$ and $c(1) = r$. We can now define the tensors $b^{(q+1)}$ as

$$b^{(q+1)}_{\mathrm{p}} = h_1(b^{(q)}_{\ell}, b^{(q)}_{r}, \lambda(p)) + \mu\frac{(1+v)}{2}\lambda(p)(1-\lambda(p))\beta^2_\mathrm{p}, \quad b^{(q+1)}_{s} = b^{(q)}_{s},$$

$\forall s \in \mathscr{S}(G_{q+1}) - \{p\}$. The above formulae allows us to evaluate the energy. More precisely, we have the following proposition:

Proposition 2. *The energy associated with the laminate L is given by*

$$E^{(\ell)}(\varepsilon^\mathrm{a}, L) = a^{(N_\mathrm{p})}_{mm} + 2b^{(N_\mathrm{p})}_{m} + \frac{1}{2}\varepsilon^\mathrm{a} C \varepsilon^\mathrm{a}, \quad \text{where } m = root(G)$$

and N_p is the number of parents of the tree G.

The validity of the above formula follows from a series of observations.

Observation 5. $a^{(q)}_{st} = \frac{1}{2}\varepsilon^{T(s)} C \varepsilon^{T(t)}$, $\forall s,t \in \mathrm{S}(G_q)$ $(0 \le q \le N_\mathrm{p})$.

Observation 6. *Let ε be a linear combination of the transformation strains associated with the singles of the tree G_q*

$$\varepsilon = \sum_{s\in S(G_q)} z_s \varepsilon^{T(s)}.$$

The coefficients p_0 and p_1 of the characteristic polynomial of ε (see Eq. (34)) *are given by*

$$p_0 = f^{(q)}_{stu} z_s z_t z_u \quad \text{and} \quad p_1 = g^{(q)}_{st} z_s z_t.$$

Observation 7. *The eigenvalue of minimum absolute value of $\varepsilon^{T(\ell)} - \varepsilon^{T(r)}$ is $\beta_{\rm p}$ the middle root of the polynomial* (37) (*see also Eqs.* (36) *and* (38)).

In fact, the polynomial (37) is the characteristic polynomial of $\varepsilon^{T(\ell)} - \varepsilon^{T(r)}$. Thus, since $\varepsilon^{T(\ell)} - \varepsilon^{T(r)}$ is symmetric, all the roots of the polynomial (37) are real.

Observation 8. *For any node $s \in \mathscr{S}(G_q)$ $(0 \le q \le N_{\rm p})$ we have*:

$$b^{(q)}_s = -\frac{1}{2}\varepsilon^{T(s)} C \varepsilon^{\rm a} + \frac{P(L_s)}{2},$$

where L_s is the laminate that is represented by Des(s) (s being regarded as a node of G) and $P(L_s)$ is the cost of formation of L_s (see Eq. (31)).

The proofs of the above observations can be obtained by induction on q. They are very simple and thus we will omit them. Given these observations, the validity of Proposition 2 follows immediately.

5.3. Numerical method to minimize the energy over laminates

To evaluate $E_r(\varepsilon^{\rm a})$ (see Eq. (32)), we will proceed as follows. For a given tree G that satisfies Height(G) $\le r$, and a given assignment of transformation strains to its singles, we will minimize the energy with respect to the variables $\{\lambda(p)\colon p \in \mathscr{P}(G)\}$. We will then minimize over all possible assignments of transformation strains to the singles and all trees G, under the restriction Height(G) $\le r$. More precisely, introducing the notation

$$\begin{aligned}\mathscr{G}(r) = \{&G \text{ tree}: \ \text{Height}(\text{Des}(\text{left}(n))) = \text{Height}(\text{Des}(n)) - 1 \text{ and } \forall n \in \mathscr{P}(G)\\ &\text{and Height}(G) \le r\},\end{aligned} \tag{39}$$

$$\begin{aligned}\mathscr{I}(G) = \{&I : \mathscr{S}(G) \to \{1,2,\dots,N\} : s = \text{left}(p) \in \mathscr{S}(G) \text{ and } t = \text{right}(p) \in \mathscr{S}(G)\\ &\text{for some } p \in \mathscr{P}(G) \Rightarrow I(s) < I(t)\}\end{aligned} \tag{40}$$

and

$$\mathscr{L}(G,I) = \{L \text{ laminate}: G(L) = G \text{ and } \varepsilon^{T(s)} = \varepsilon^{T(I(s))}\ \forall s \in \mathscr{S}(G)\}$$

we will compute $E_r(\varepsilon^{\rm a})$ as indicated in the following formula

$$E_r(\varepsilon^{\rm a}) = \min_{G\in\mathscr{G}(r)} \min_{I\in\mathscr{I}(G)} \min_{L\in\mathscr{L}(G,I)} E^{(\ell)}(\varepsilon^{\rm a}, L).$$

The choice of the sets $\mathscr{G}$ and $\mathscr{I}$ is to avoid some unnecessary calculations due to the fact that laminates can be represented by more that one tree.

Note that any laminate $L \in \mathscr{L}(G,I)$ is determined by the variables $\{\lambda(p)\colon\ p \in \mathscr{P}(G)\}$ once G and I are fixed. Let N_{p} be the number of parents of the tree G and let us label these parents in some arbitrary way with integer indexes from 1 to N_{p}, $\mathscr{P}(G)=\{p_i\colon\ 1 \le i \le N_{\mathrm{p}}\}$. We denote by $\boldsymbol{\lambda}$ the vector whose components are $\lambda_i=\lambda(p_i)$ $(1 \le i \le N_{\mathrm{p}})$. Thus, the minimization over $\mathscr{L}(G,I)$ can be written as

$$\min_{\boldsymbol{\lambda}\in[0,1]^{N_{\mathrm{p}}}} E^{(\ell)}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda}) = \min_{L\in\mathscr{L}(G,I)} E^{(\ell)}(\varepsilon^{\mathrm{a}},L) \quad \text{where } E^{(\ell)}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda}) = E^{(\ell)}(\varepsilon^{\mathrm{a}},L), \tag{41}$$

(for convenience, we do not explicitly display the dependence of $E^{(\ell)}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda})$ on G and I). Let $\boldsymbol{\lambda}^{\min}$ be a minimizer of the above equation. If one of the components of $\boldsymbol{\lambda}^{\min}$ is equal to 0 or 1, the corresponding laminate can be represented by another tree with fewer nodes. It is not difficult to see from formulae of Section 5.2 that $E^{(\ell)}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda})$ is a continuous function of $\boldsymbol{\lambda}$ but its derivatives might have discontinuities. Thus, any minimizer of (41) $\boldsymbol{\lambda}_{\min}$ whose components are different from 0 or 1, $0 < \lambda_i^{\min} < 1$, belongs to the set of critical points Λ given by

$$\Lambda = \left\{ \overset{\circ}{\boldsymbol{\lambda}}\colon\ \inf \lim_{\boldsymbol{\lambda}\to\overset{\circ}{\boldsymbol{\lambda}}} \frac{\partial E^{(\ell)}}{\partial \lambda_i}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda}) \le 0 \le \sup \lim_{\boldsymbol{\lambda}\to\overset{\circ}{\boldsymbol{\lambda}}} \frac{\partial E^{(\ell)}}{\partial \lambda_i}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda})\ \forall i \right\}.$$

Consequently, we have

$$E_r(\varepsilon^{\mathrm{a}}) = \min_{G\in\mathscr{G}(r)} \min_{I\in\mathscr{I}(G)} E^{(G,I)}(\varepsilon^{\mathrm{a}}),$$

where

$$E^{(G,I)}(\varepsilon^{\mathrm{a}}) = \min\{E^{(\ell)}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda})\colon\ \boldsymbol{\lambda} \in \Lambda \cap [0,1]^{N_{\mathrm{p}}}\}. \tag{42}$$

In the above formula, we take $E^{(G,I)}(\varepsilon^{\mathrm{a}}) = \infty$ if the set $\Lambda \cap [0,1]^{N_{\mathrm{p}}}$ is empty.

Given prescribed errors of tolerance $\delta_{\mathrm{e}} > 0$ and $\delta_\lambda > 0$, our algorithm provide us with a tree $G^\star \in \mathscr{G}(r)$, a function $I^\star \in \mathscr{I}(G)$, and a vector $\boldsymbol{\lambda}^\star$ (each component of $\boldsymbol{\lambda}^\star$ is given with an error bounded by δ_λ) that represent an optimal laminate $L^\star$ (i.e. a minimizer of Eq. (32)), as well as the value of $E_r(\varepsilon^{\mathrm{a}})$ (with an error bounded by δ_{e}). If there exists more than one minimizer, a minor modification on the algorithm that we will describe would provide us with all the minimizers.

Suppose that we have an upper bound U of $E_r(\varepsilon^{\mathrm{a}})$ and the tree representation, G^{u}, I^{u} and $\boldsymbol{\lambda}^{\mathrm{u}}$, of a laminate whose associated energy is U. For given G and I our algorithm tells us if $E^{(G,I)}(\varepsilon^{\mathrm{a}}) < U$. If this is the case, our algorithm gives us $\boldsymbol{\lambda}^{\min}$, a minimizer of Eq. (42), it updates the value of the upper bound U to $U := E^{(G,I)}(\varepsilon^{\mathrm{a}})$ and it also updates the laminate whose energy is equal to the upper bound by setting $G^{\mathrm{u}} := G$, $I^{\mathrm{u}} := I$ and $\boldsymbol{\lambda}^{\mathrm{u}} := \boldsymbol{\lambda}^{\min}$. After all functions $I \in \mathscr{I}(G)$ and all trees $G \in \mathscr{G}(r)$ are considered, we achieve our goal, i.e. $E_r(\varepsilon^{\mathrm{a}}) = U$ and an optimal laminate is represented by $G^\star = G^{\mathrm{u}}$, $I^\star = I^{\mathrm{u}}$ and $\boldsymbol{\lambda}^\star = \boldsymbol{\lambda}^{\mathrm{u}}$.

To locate the minimizers of Eq. (42), our algorithm refines the domain $[0,1]^{N_{\mathrm{p}}}$ a number of times. If a region Q is the result of having refined $[0,1]^{N_{\mathrm{p}}}$ i times, we say that its level is i. The set of regions whose level is i is denoted by $Q^{(i)}$

$$Q^{(i)} = \{Q_j^{(i)}\}_{1\le j\le \#(Q^{(i)})}.$$

The variable lev (which is dynamic), indicates the highest level of the regions being explored at the time. These regions are denoted by $Q^{(i)}_{\mathrm{cur}(i)}$ $(0 \le i \le \mathrm{lev})$. Regions with the same level are disjoint and satisfy

$$\bigcup_{1\le j\le \#(Q^{(i)})} Q^{(i)}_j \subseteq Q^{(i-1)}_{\mathrm{cur}(i-1)} \quad (1 \le i \le \mathrm{lev}).$$

To decide whether $E^{(G,I)}(\varepsilon^{\mathrm{a}}) < U$, and if this is the case to also evaluate $E^{(G,I)}(\varepsilon^{\mathrm{a}})$ and find a minimizer $\boldsymbol{\lambda}^{\min}$, our algorithm follows the next sequence of steps:

Step 1: *It sets* $Q^{(0)}_1 := [0,1]^{N_{\mathrm{p}}}$, $Q^{(0)} := \{Q^{(0)}_1\}$, $\mathrm{lev} := 0$ *and* $\mathrm{cur}(0) := 1$.

Step 1 is the initialization step.

Step 2: *While* $\mathrm{cur}(\mathrm{lev}) > \#(Q^{(\mathrm{lev})})$ *and* $\mathrm{lev} \ge 0$, *the algorithm sets* $\mathrm{cur}(\mathrm{lev}-1) := \mathrm{cur}(\mathrm{lev}-1) + 1$ *and* $\mathrm{lev} := \mathrm{lev} - 1$.

Step 2 simply says that after having explored all the sets whose level is lev, the algorithm moves on to explore the sets whose level is lev − 1 and have not been previously explored.

Step 3: *If* $\mathrm{lev} = -1$, *the algorithm stops* (*it moves on to a new pair* (G,I)). *Otherwise*, *it obtains* $B^{(\mathrm{u})}$ *and* $B^{(\ell)}$ *upper and lower bounds of* $E^{(\ell)}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda})$ *restricted to* $\boldsymbol{\lambda} \in Q^{(\mathrm{lev})}_{\mathrm{cur}(\mathrm{lev})}$

$$B^{(\ell)} \le \min\{E^{(\ell)}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda}):\ \boldsymbol{\lambda} \in Q^{(\mathrm{lev})}_{\mathrm{cur}(\mathrm{lev})}\} \le \max\{E^{(\ell)}(\varepsilon^{\mathrm{a}},\boldsymbol{\lambda}):\ \boldsymbol{\lambda} \in Q^{(\mathrm{lev})}_{\mathrm{cur}(\mathrm{lev})}\} \le B^{(\mathrm{u})}.$$

The calculation of $B^{(\mathrm{u})}$ and $B^{(\ell)}$ and their properties will be discussed later in this paper.

Step 4: *If* $B^{(\mathrm{u})} < U$, *the algorithm updates the upper bound* U *by setting of* $U := B^{(\mathrm{u})}$ *and the minimizer* $\boldsymbol{\lambda}^{\min}$ *by setting it equal to the center of* $Q^{(\mathrm{lev})}_{\mathrm{cur}(\mathrm{lev})}$.

Step 5: *If* $B^{(\ell)} > U$, *the algorithm sets* $\mathrm{cur}(\mathrm{lev}) := \mathrm{cur}(\mathrm{lev}) + 1$ *and it goes back to step* 2. *Otherwise*, *if* $B^{(\mathrm{u})} - B^{(\ell)} < \delta_{\mathrm{e}}$ *and the length of each side of* $Q^{(\mathrm{lev})}_{\mathrm{cur}(\mathrm{lev})}$ *is bounded* $2\delta_\lambda$, *the algorithm also sets* $\mathrm{cur}(\mathrm{lev}) := \mathrm{cur}(\mathrm{lev}) + 1$ *and goes back to step* 2.

In step 5 the algorithm decides whether it will continue exploring the set $Q^{(\mathrm{lev})}_{\mathrm{cur}(\mathrm{lev})}$ (i.e. go to step 6) or not. Later in this paper we will describe a procedure that for convenience we call Refine. This procedure takes as input a region $Q \subseteq [0,1]^{N_{\mathrm{p}}}$ of the form $Q = \prod_{1\le i\le N_{\mathrm{p}}} [a_i, b_i]$ and gives as output a sequence of disjoint regions included in Q of the form $Q_\alpha = \prod_{1\le i\le N_{\mathrm{p}}} [a^{(\alpha)}_i, b^{(\alpha)}_i]$ $(1 \le \alpha \le n(Q))$ with the property

$$\Lambda \cap Q \subseteq \bigcup_{\alpha=1}^{n(Q)} Q_\alpha, \quad b^{(\alpha)}_i - a^{(\alpha)}_i \le \frac{1}{2}(b_i - a_i)\ \forall i,\alpha \quad \text{and} \quad 0 \le n(Q) \le 2^{N_{\mathrm{p}}}.$$

Step 6: *Let* $\{Q_i\}_{1\le i\le n(Q)}$ *be the output of applying Refine to* $Q = Q^{(\mathrm{lev})}_{\mathrm{cur}(\mathrm{lev})}$. *If* $n(Q) = 0$, *the algorithm sets* $\mathrm{cur}(\mathrm{lev}) := \mathrm{cur}(\mathrm{lev}) + 1$. *Otherwise*, *it sets* $Q^{(\mathrm{lev}+1)}_i := Q_i$ $(1 \le i \le n(Q))$, $Q^{(\mathrm{lev}+1)} := \{Q_i\}_{1\le i\le n(Q)}$, $\mathrm{cur}(\mathrm{lev}+1) := 1$ *and it updates* lev *to* $\mathrm{lev} := \mathrm{lev} + 1$. *In either case*, *it then goes back to step* 2.

If $E^{(G,I)}(\varepsilon^{\mathrm{a}}) \ge U$, the condition of step 4 is never satisfied before the algorithm stops considering the pair (G,I). Otherwise, the value of U is already updated by the time $\mathrm{lev} = -1$ (see step 3) and $\boldsymbol{\lambda}^{\min}$ is a minimizer.

5.4. The procedure Refine

We now turn to the description of the procedure Refine that our algorithm uses in step 6. To that end, let Q be a region of the form

$$Q = \prod_{i=1}^{N_\mathrm{p}} [\lambda_i^{(0)} - \Delta\lambda_i, \lambda_i^{(0)} + \Delta\lambda_i].$$

Given the formulae of Section 5.2, it is easy device and algorithm (that requires $O(N_\mathrm{p})$ operations) to compute $B^{(\ell)}$ and $B^{(\mathrm{u})}$, lower and upper bounds of $E^{(\ell)}(\varepsilon^\mathrm{a}, \boldsymbol{\lambda})$ restricted to $\boldsymbol{\lambda} \in Q$, with the property

$$0 \leq \min_{\boldsymbol{\lambda}\in Q} E^{(\ell)}(\varepsilon^\mathrm{a}, \boldsymbol{\lambda}) - B^{(\ell)} = \sum_{i=1}^{N_\mathrm{p}} O(\Delta\lambda_i)^2$$

and

$$0 \leq B^{(\mathrm{u})} - \max_{\boldsymbol{\lambda}\in Q} E^{(\ell)}(\varepsilon^\mathrm{a}, \boldsymbol{\lambda}) = \sum_{i=1}^{N_\mathrm{p}} O(\Delta\lambda_i)^2.$$

Analogously, taking derivatives of the formulae of Section 5.2, we can also bound the second derivatives of $E^{(\ell)}(\varepsilon^\mathrm{a}, \boldsymbol{\lambda})$

$$0 \leq \min_{\boldsymbol{\lambda}\in Q} \frac{\partial^2 E^{(\ell)}}{\partial\lambda_i \partial\lambda_j}(\varepsilon^\mathrm{a}, \boldsymbol{\lambda}) - B_{ij}^{(\ell)} = \sum_{i=1}^{N_\mathrm{p}} O(\Delta\lambda_i)^2$$

and

$$0 \leq B_{ij}^{(\mathrm{u})} - \max_{\boldsymbol{\lambda}\in Q} \frac{\partial^2 E^{(\ell)}}{\partial\lambda_i \partial\lambda_j}(\varepsilon^\mathrm{a}, \boldsymbol{\lambda}) = \sum_{i=1}^{N_\mathrm{p}} O(\Delta\lambda_i)^2.$$

Let A be the matrix whose components are

$$a_{ij} = \frac{1}{2}(B_{ij}^{(\mathrm{u})} + B_{ij}^{(\ell)}) \quad (1 \leq i,j \leq N_\mathrm{p}),$$

and ΔA the matrix with components

$$\Delta a_{ij} = \frac{1}{2}(B_{ij}^{(\mathrm{u})} - B_{ij}^{(\ell)}) \quad (1 \leq i,j \leq N_\mathrm{p}).$$

If A and $\nabla E^{(\ell)}(\varepsilon^\mathrm{a}, \boldsymbol{\lambda}^{(0)})$ are defined ($\boldsymbol{\lambda}^{(0)}$ denotes the vector whose components are $\lambda_i^{(0)}$) and A is not singular, any $\boldsymbol{\lambda} \in \Lambda \cap Q$ is of the form

$$\boldsymbol{\lambda} = \boldsymbol{\lambda}^{(\mathrm{c})} + \boldsymbol{\delta\lambda}^{(\mathrm{c})},$$

where

$$\boldsymbol{\lambda}^{(\mathrm{c})} = \boldsymbol{\lambda}^{(0)} - A^{-1}\nabla E^{(\ell)}(\varepsilon^\mathrm{a}, \boldsymbol{\lambda}^{(0)}),$$

and the components of $\delta\boldsymbol{\lambda}^{(\mathrm{c})}$ satisfy

$$|\delta\lambda_i^{(\mathrm{c})}| \leq \Delta\lambda_i^{(\mathrm{c})} = |a_{ij}^{(-1)}|\Delta a_{jk}\Delta\lambda_k$$

($a_{ij}^{(-1)}$ are the components of A^{-1}). Thus, we have

$$Q \cap \Lambda \subseteq Q^*,$$

where

$$Q^* = Q \cap \prod_{i=1}^{N_{\mathrm{p}}} [\lambda_i^{(\mathrm{c})} - \Delta\lambda_i^{(\mathrm{c})}, \lambda_i^{(\mathrm{c})} + \Delta\lambda_i^{(\mathrm{c})}].$$

If A or $\nabla E^{(\ell)}(\varepsilon^{\mathrm{a}}, \boldsymbol{\lambda}^{(0)})$ are not defined, or A is singular, we simply set $Q^* = Q$. Given the definition of Q^*, we have that Q^* is either empty or of the form

$$Q^* = \prod_{i=1}^{N_{\mathrm{p}}} [\lambda_i^* - \Delta\lambda_i^*, \lambda_i^* + \Delta\lambda_i^*].$$

We are now ready to describe the output of the procedure Refine when its input is the region Q. If Q^* is empty, the output of Refine is $n(Q) = 0$. Otherwise, let $X^{(k)}$ be the sets of regions defined inductively as follows:

$$X^{(0)} = \{Q^*\} \tag{43}$$

and

$$X^{(k)} = \begin{cases} \{Q \cap \{\lambda_k \leq \lambda_k^*\}, Q \cap \{\lambda_k \geq \lambda_k^*\} : Q \in X^{(k-1)}\} & \text{if } 2\Delta\lambda_k^* > \Delta\lambda_k, \\ X^{(k-1)}, & \text{otherwise.} \end{cases} \tag{44}$$

The output of the procedure Refine is the set of regions $X^{(N_{\mathrm{p}})}$ and $n(Q) = \#(X^{(N_{\mathrm{p}})})$.

5.5. Remarks on the numerical algorithm

The numerical algorithm described in this section is a *global* minimization algorithm. It always finds the global minimum. Most of the computational time is spent in the first few levels of refinement. Once we know that the critical point is inside a set $Q = \prod [a_i, b_i]$, where $b_i - a_i$ is small enough for all i, the method behaves like a sequentially quadratic programming algorithm (to minimize the function $E^{(\ell)}(\varepsilon^{\mathrm{a}}, \boldsymbol{\lambda})$) or a Newton–Raphson method (to find the zeros of the gradient of $E^{(\ell)}(\varepsilon^{\mathrm{a}}, \boldsymbol{\lambda})$).

If $\{Q_i\}$ is the output of applying Refine to Q, the algorithm can be sped up by reordering the set $\{Q_i\}$ in such a way that $E^{(\ell)}(\varepsilon^{\mathrm{a}}, \boldsymbol{\lambda})$ evaluated at the center of Q_1 is less or equal to $E^{(\ell)}(\varepsilon^{\mathrm{a}}, \boldsymbol{\lambda})$ evaluated at the center of Q_i for any $i \neq 1$. This requires the evaluation of $E^{(\ell)}(\varepsilon^{\mathrm{a}}, \boldsymbol{\lambda})$ at the center of Q_i (for all $1 \leq i \leq n(Q)$), but this is inexpensive. Once Q_1 is selected, the recursive formulae of Section 5.2 suggest the order of the rest of the regions Q_i to minimize the number of operations required by the algorithm.

6. Applications. Cubic to monoclinic transformations

In this section we will apply our methods to a particular example. Namely, we will assume that the austenite has cubic symmetry and the martensite has monoclinic

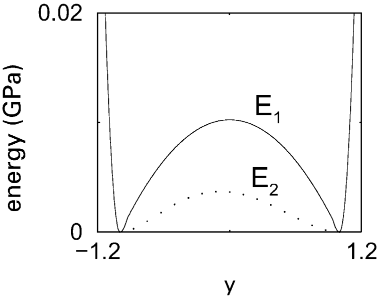

Fig. 4. Optimal energies corresponding to microstructures in the classes of rank-one and rank-two laminates for applied strains of the form (47). The solid line corresponds to $E_1(\varepsilon^{\mathrm{a}}(y))$ and the dotted line to $E_2(\varepsilon^{\mathrm{a}}(y))$ (see Eqs. (32) and (47)). When $|y| \geq 1$, both curves coincide.

symmetry. More precisely, we have chosen one of the transformation strains (say $\varepsilon^{T(1)}$) to be

$$\varepsilon^{T(1)} = \begin{bmatrix} 0.025 & 0.06 & 0.04 \\ 0.06 & 0.025 & 0.04 \\ 0.04 & 0.04 & -0.05 \end{bmatrix}. \tag{45}$$

These values are similar to the ones corresponding to the transformation strains in Ti-50.6Ni (see Knowles and Smith, 1981). The rest of the transformation strains (there are 12 of them) can be obtained by rotating $\varepsilon^{T(1)}$ with rotations in the group of symmetries of the cubic lattice.

6.1. Numerical calculations

We will use the results obtained in our numerical calculations to evaluate our upper bound. Thus, we are interested in the energy for applied strains that are a convex combination of two transformation strains. In the case under consideration, the transformation strains are not pairwise compatible. In fact, any transformation strain is incompatible with exactly three other transformation strains. For example, the transformation strain $\varepsilon^{T(1)}$ given by Eq. (45) and the transformation strain

$$\varepsilon^{T(2)} = \begin{bmatrix} -0.05 & -0.04 & -0.04 \\ -0.04 & 0.025 & 0.06 \\ -0.04 & 0.06 & 0.025 \end{bmatrix} \tag{46}$$

are incompatible. Thus, we consider applied strains of the form

$$\varepsilon^{\mathrm{a}} = \varepsilon^{\mathrm{a}}(y) = \varepsilon^{T(1)} + \frac{1+y}{2}(\varepsilon^{T(2)} - \varepsilon^{T(1)}). \tag{47}$$

In our computations we have used the following values for the Poisson ratio and shear modulus: $v = 0.25$ and $\mu = 100$ GPa. In Fig. 4 we have plotted the optimal energies corresponding to microstructures in the classes of rank-one and rank-two laminates for applied strains of the form (47) (i.e. we have plotted $E_r(\varepsilon^{\mathrm{a}}(y))$ as a function of y for

$r = 1$ and 2). As expected, these curves are not convex. They exhibit a double-well structure.

Let us consider in more detail one of these applied strains, namely

$$\varepsilon_0^{\mathrm{a}} = \varepsilon^{\mathrm{a}}(0) = \frac{1}{2}(\varepsilon^{T(1)} + \varepsilon^{T(2)}). \tag{48}$$

The optimal rank-one laminate L_1 corresponding to this applied strain (i.e. $E_1(\varepsilon_0^{\mathrm{a}}) = E^{(\ell)}(\varepsilon_0^{\mathrm{a}}, L_1)$) has as microscopic transformation strains $\varepsilon^{T(1)}$ and $\varepsilon^{T(2)}$ with volume fractions 0.5 each. Thus, the macroscopic transformation strain of this laminate $\varepsilon^{T(L_1)}$ (see Eq. (28)) is equal to the applied strain. All the energy $E_1(\varepsilon_0^{\mathrm{a}}) = 0.01024$ GPa is due to the incompatibility of $\varepsilon^{T(1)}$ and $\varepsilon^{T(2)}$. In other words, all this energy is equal to the penalty energy $P(L_1)$ (last term in Eq. (27)).

On the other hand, the optimal rank-two laminate L_2 (i.e. $E_2(\varepsilon_0^{\mathrm{a}}) = E^{(\ell)}(\varepsilon_0^{\mathrm{a}}, L_2)$) has as material layers two rank-one laminates ℓ_1 and ℓ_2 with the volume fraction of ℓ_1 being $\lambda = 0.498$. These rank-one laminates are described as follows. The microscopic transformation strains of ℓ_1 are

$$\varepsilon^{T(3)} = \begin{bmatrix} -0.05 & 0.04 & 0.04 \\ 0.04 & 0.025 & 0.06 \\ 0.04 & 0.06 & 0.025 \end{bmatrix} \tag{49}$$

and $\varepsilon^{T(2)}$ (see Eq. (46)) with the volume fraction of $\varepsilon^{T(3)}$ being $\lambda_1 = 0.344$, and the microscopic transformation strains of ℓ_2 are

$$\varepsilon^{T(4)} = \begin{bmatrix} 0.025 & -0.06 & -0.04 \\ -0.06 & 0.025 & 0.04 \\ -0.04 & 0.04 & -0.05 \end{bmatrix} \tag{50}$$

and $\varepsilon^{T(1)}$ with the volume fraction of $\varepsilon^{T(4)}$ being $\lambda_2 = 0.272$. Note that $P(\ell_i) = 0$, i.e. the microscopic transformation strains of the laminate ℓ_i are compatible, for both $i = 1$ and 2. Note also that the macroscopic transformation strain of this rank-two laminate $\varepsilon^{T(L_2)}$ is not equal to $\varepsilon_0^{\mathrm{a}}$ and thus, the first term of the right-hand side of Eq. (27) is not 0. However, it was energetically preferable to first mix $\varepsilon^{T(1)}$ and $\varepsilon^{T(2)}$ with other transformation strains ($\varepsilon^{T(4)}$ and $\varepsilon^{T(3)}$, respectively) to decrease the penalty due to incompatibility and then form the rank-two laminate L_2. The total energy is $E_2(\varepsilon_0^{\mathrm{a}}) = E^{(\ell)}(\varepsilon^{\mathrm{a}}, L_2) = 0.003655$ GPa.

Before we leave this discussion of our numerical computations, we make the following observations. While $E_1(\varepsilon^{\mathrm{a}}(y))$ is even with respect to y, $E_2(\varepsilon^{\mathrm{a}}(y))$ is not. If we replace $\varepsilon^{T(1)}$ and $\varepsilon^{T(2)}$ by any other pair of incompatible transformation strains, we would obtain the same curves or the reflection of these curves along the vertical axis $y=0$. Finally, we mention that the maximum of $E_1(\varepsilon^{\mathrm{a}}(y))$ (for $y \in [-1, 1]$) is attained at $y=0$ but the maximum of $E_2(\varepsilon^{\mathrm{a}}(y))$ is attained at $y=-0.04$. This maximum value is $E_2(\varepsilon^{\mathrm{a}}(-0.04)) = 0.003703$ GPa.

6.2. Characteristics of the upper bound

We are now ready to evaluate our upper bound. From our numerical calculations, we have a bound on the effective energy restricted to applied strains that are a convex combination of two transformation strains

$$U_i = \max_{-1\leq y\leq 1} E_2(\varepsilon^{\mathrm{a}}(y)) = 0.003703 \text{ GPa} \tag{51}$$

and we have the maximum of the energies required to form rank-one laminates (which is equal to the last term of Eq. (20))

$$U_{\mathrm{o}} = \max_{-1\leq y\leq 1} E_1(\varepsilon^{\mathrm{a}}(y)) = E_1(\varepsilon_0^{\mathrm{a}}) = 0.01024 \text{ GPa}. \tag{52}$$

Thus, our upper bound reads

$$E(\varepsilon^{\mathrm{a}}) \leq \begin{cases} U_i & \text{if } \varepsilon^{\mathrm{a}} \text{ is in the convex hull of the transformation strains,} \\ U_{\mathrm{o}} + E^{(\mathrm{c})}(\varepsilon^{\mathrm{a}}) & \text{otherwise,} \end{cases} \tag{53}$$

where $E^{(\mathrm{c})}$ is the convexification of the effective energy (see Eq. (17)). Note that the evaluation $E^{(\mathrm{c})}$ requires the solution of a simple quadratic programming problem.

At this point the following question arises. Given an applied strain ε^{a} in the convex hull of the transformation strains, why do we not make use of our numerical method and compute $E_r(\varepsilon^{\mathrm{a}})$ (the optimal energy among rank-r laminates) to bound the effective energy instead of using our upper bound (Proposition 1)? The answer to this question is: If our numerical method is able to compute $E_r(\varepsilon^{\mathrm{a}})$ with r large (probably $r \geq 5$), we expect our numerical method to be sharper than our upper bound. On the other hand, if r is small (probably $r \leq 4$), we expect our upper bound to be sharper. (We mention that even though our numerical method was developed to compute $E_r(\varepsilon^{\mathrm{a}})$ for any r, it becomes prohibitively slow in the present example if r is greater than 2).

To illustrate the above statement, consider a different example in which the transformation is cubic to orthorhombic with one of the transformation strains given by

$$\begin{bmatrix} \alpha & \beta & 0 \\ \beta & \alpha & 0 \\ 0 & 0 & -2\alpha \end{bmatrix} \tag{54}$$

for some material parameters α and β. In this case, the transformation strains are pairwise compatible. Thus, the effective energy corresponding to any applied strain in the convex hull of the transformation strains is 0. Moreover, as it was shown in [3], for any such applied strain there exists an optimal microstructure in the class of laminates of rank no higher than five. In fact, a dimensionality argument shows that laminates of rank at least four are required to attain general applied strains in the convex hull of the transformation strains with 0 energy (it is the belief of the author that for some applied strains rank-four laminates are not enough, we really need rank-five laminates). In this example we have $E_1(\varepsilon^{\mathrm{a}}) = 0$ for any applied strain ε^{a} that is a convex combination of only two transformation strains. Thus, our upper bound gives us the exact value of the effective energy, $E(\varepsilon^{\mathrm{a}}) = 0$ for applied strains in the convex hull of the transformation strains, even if we only know how to compute the energies associated with rank-one laminates (something that can be done by hand). On the other hand, to obtain the same results with our numerical code (without the use of Proposition 1), our numerical code should be able to handle at least rank-four laminates and most likely rank-five laminates.

This last example hints us a *rule* (not a rigorous statement) that we expect to be valid in most situations: Suppose that the applied strain ε^{a} can be written as a convex combination of k transformation strains. If k is low, we expect that low values of r are enough for $E_r(\varepsilon^{\mathrm{a}})$ to approximate *well* $E_\infty(\varepsilon^{\mathrm{a}})$. As k increases, we expect to need higher values of r. Another reason to believe the validity of this rule is the following observation: Let $\varepsilon^{T(\mathrm{av})}$ be the average transformation strain

$$\varepsilon^{T(\mathrm{av})} = \frac{1}{|\Omega|}\int_\Omega \varepsilon^T(x)\,\mathrm{d}x. \tag{55}$$

Let $E^{(\mathrm{av})}(\varepsilon^{T(\mathrm{av})})$ be the result of minimizing the energy over microstructures whose average transformation strain is $\varepsilon^{T(\mathrm{av})}$ when the applied strain is also $\varepsilon^{T(\mathrm{av})}$

$$E^{(\mathrm{av})}(\varepsilon^{T(\mathrm{av})}) = \inf_{\varepsilon^T}\left\{\frac{1}{|\Omega|}\int_\Omega W(\varepsilon(x),\varepsilon^T(x))\,\mathrm{d}x\colon\ \varepsilon^{\mathrm{a}} = \frac{1}{|\Omega|}\int_\Omega \varepsilon^T(x)\,\mathrm{d}x = \varepsilon^{T(\mathrm{av})}\right\} \tag{56}$$

A simple calculation shows that, for any applied strain ε^{a}, we have

$$E(\varepsilon^{\mathrm{a}}) = \min_{\varepsilon^{T(\mathrm{av})}}\left\{\frac{1}{2}(\varepsilon^{\mathrm{a}}-\varepsilon^{T(\mathrm{av})})C(\varepsilon^{\mathrm{a}}-\varepsilon^{T(\mathrm{av})}) + E^{(\mathrm{av})}(\varepsilon^{T(\mathrm{av})})\right\}. \tag{57}$$

If the applied strain ε^{a} is a convex combination of only two transformation strains, say $\varepsilon^{\mathrm{a}} = x\varepsilon^{T(i)} + (1-x)\varepsilon^{T(j)}$ (for some $0 < x < 1$, $1 \leq i,j \leq N$), we expect that the volume fraction of any other transformation strain, $\varepsilon^{T(m)}$ with $m \neq i,j$, in an optimal microstructure is *small* in order to keep the first term of Eq. (57) *small*. If this is the case, this optimal microstructure will be *close* to a rank-one laminate (whose microscopic transformation strains are $\varepsilon^{T(i)}$ and $\varepsilon^{T(j)}$). Similar arguments considering applied strains that are a convex combination of a higher number of transformation strains support the rule stated above.

To complete our discussion, let us consider another example. Going back to our cubic to monoclinic transformation (one of the transformation strains given by Eq. (45)), consider the applied strain $\varepsilon^{\mathrm{a}} = 0$. It is known that the effective energy of this applied strain is 0 (see Bhattacharya, 1992) and that this 0 value of the energy can be attained with a rank-four laminate. We computed numerically the optimal energies among the microstructures in the classes of rank-one and rank-two laminates for this applied strain. The values obtained were

$$E_1(0) = 0.45375\ \mathrm{GPa} \quad \text{and} \quad E_2(0) = 0.02667\ \mathrm{GPa}.$$

On the other hand, as already mentioned before, the values obtained from our upper bound are 0.01025 GPa if we consider only rank-one laminates and 0.003703 GPa if we consider rank-two laminates. Note that, in agreement with our previous discussion, the upper bound approximates much better the effective energy, for this applied strain $\varepsilon^{\mathrm{a}} = 0$, than the direct numerical calculation when we consider laminates of rank one and two only.

6.3. Discussion

We will now comment on the possible significance of the calculations presented in this section. Shape-memory alloys are materials that recover their original shape when heated after having undergone apparently plastic deformations. A main component in some models of shape-memory materials is the assumption that the set of recoverable strains R (i.e. the applied strains that can be recovered on heating) are the strains for which the effective energy is small (see Bhattacharya and Kohn, 1996, 1997; Shu and Bhattacharya, 1998)

$$R = \{\varepsilon\colon E(\varepsilon) \leq \delta\}. \tag{58}$$

Sometimes δ is taken to be 0, but materials can withstand coherently small elastic strains and thus, it is possible that strains for which the energy is small but not 0 may also be recoverable. In any case, δ should be very small. If the transformation strains are pairwise compatible, the effective energy restricted to the convex hull of the transformation strains is 0 and outside this set it increases quadratically, remaining *small* only for a short distance. Thus, if the transformation strains are pairwise compatible, the convex hull of the transformation strains is regarded by these models as a good approximation of the set of recoverable strains. The question that arises is: If the transformation strains are not pairwise compatible, under what conditions (i.e. for what material parameters) is the convex hull of the transformation strains a good approximation of the set of recoverable strains?

We are not attempting to completely answer this question here, just to discuss it. In this regard, we note that our upper bound for the effective energy restricted to the convex hull of the transformation strains is 0.003707 GPa. As a source of comparison, we note that $\varepsilon^{T(1)}C\varepsilon^{T(1)}/2 = 1.74$ GPa, thus, roughly speaking, an elastic strain whose energy is $\varepsilon C\varepsilon/2 = 0.003707$ GPa, is a lot smaller than the transformation strain (if $\varepsilon = x\varepsilon^{T(1)}$, we have $x = 0.046$). Thus, we can say that our upper bound is small. We remark that the fact that our upper bound is small does not mean that the set of zero energy is close to the convex hull of the transformation strains (the effective energy can be small but nonzero in a large set).

The exact evaluation of the effective energy has proven to be a very difficult problem. If the goal is to answer the above question regarding shape-memory alloys, our calculations suggest it might be worth pursuing an alternative easier approach, namely, improve upon the bound obtained here (by for example considering laminates of higher rank than two and allowing for the elastic moduli to be anisotropic since Proposition 1 is also valid in this case). Having sharper quantitative results would allow to test the existing theories, in particular, try to establish under which conditions Eq. (58) is valid and how small should δ be.

Acknowledgements

I would like to thank Professor Oscar Bruno for introducing me to the area of martensitic transformations and for helpful discussion throughout the progress of this research. This research was supported by the NSF through Contract No. DMS-9523292.

Appendix. Optimal rank-one laminates

In this appendix we present the calculations required in Section 4.1 to compute optimal rank-one laminates. We start by solving Eq. (25) for b. We first note that

$$(b \otimes \hat{n})\hat{n} = b \quad \text{and} \quad (\hat{n} \otimes b)\hat{n} = (\hat{n}.b)\hat{n}.$$

Next we introduce the notation

$$\tau = \varepsilon^{T(\gamma)} - \varepsilon^{T(\beta)} \tag{A.1}$$

and manipulate Eq. (25) to rewrite it as

$$b + \frac{(\hat{n}.b)}{1-2v}\hat{n} = \tau\hat{n} + \frac{v}{1-2v}\,\mathrm{tr}(\tau)\hat{n}. \tag{A.2}$$

where $\mathrm{tr}(\tau)$ denotes the trace of τ, $\mathrm{tr}(\tau) = \sum_{i=1}^{3} \tau_{ii}$. We now multiply (A.2) by $\hat{n}$ to get

$$\frac{2(1-v)}{1-2v}\hat{n}.b = \hat{n}\tau\hat{n} + \frac{v}{1-2v}\,\mathrm{tr}(\tau) \tag{A.3}$$

and finally conclude (from the last two equations) that

$$b = \tau\hat{n} + \frac{v\,\mathrm{tr}(\tau) - (\hat{n}\tau\hat{n})}{2(1-v)}\hat{n}. \tag{A.4}$$

We now proceed to minimize Eq. (26) over all vectors $\hat{n}$ with norm 1. Using Eqs. (3), (23) and (24), and after some algebraic manipulation, we can rewrite Eq. (26) as

$$\begin{aligned} &\lambda W(\varepsilon^{\gamma}, \varepsilon^{T(\gamma)}) + (1-\lambda)W(\varepsilon^{\beta}, \varepsilon^{T(\beta)}) \\ &\quad = \frac{1}{2}(\varepsilon^{\mathrm{a}} - \varepsilon^{T(L)})C(\varepsilon^{\mathrm{a}} - \varepsilon^{T(L)}) \\ &\quad\quad + \frac{1}{2}\lambda(1-\lambda)(b\otimes\hat{n} + \hat{n}\otimes b - \tau)C(b\otimes\hat{n} + \hat{n}\otimes b - \tau), \end{aligned}$$

where $\varepsilon^{T(L)}$ was introduced in Eq. (28). Our problem in hand now reduces to minimize

$$f = f(\hat{n}) = \frac{1}{2\mu}(b\otimes\hat{n} + \hat{n}\otimes b - \tau)C(b\otimes\hat{n} + \hat{n}\otimes b - \tau) \tag{A.5}$$

over all vectors $\hat{n}$ of norm 1, with b given by Eq. (A.4). Using the expressions for the elastic tensor C (see Eq. (1)), f can be explicitly written as a function of $\hat{n}$ and τ

$$f = \tau_{ij}\tau_{ij} + \frac{v}{1-v}\,\mathrm{tr}(\tau)^2 - \frac{2v}{1-v}\,\mathrm{tr}(\tau)(\hat{n}\tau\hat{n}) + \frac{1}{1-v}(\hat{n}\tau\hat{n})^2 - 2|\tau\hat{n}|^2. \tag{A.6}$$

We minimize this last equation using Lagrange multipliers

$$\frac{\partial f}{\partial \hat{n}_i} = 4a\hat{n}_i \quad \text{for some real number } a.$$

More explicitly we have

$$\frac{(\hat{n}\tau\hat{n}) - v\,\mathrm{tr}(\tau)}{1-v}\tau\hat{n} - \tau^2\hat{n} = a\hat{n}. \tag{A.7}$$

To compute a as function of $\hat{n}$ and τ, we multiply Eq. (A.7) by $\hat{n}$

$$a = \frac{(\hat{n}\tau\hat{n}) - v\,\mathrm{tr}(\tau)}{1-v}(\hat{n}\tau\hat{n}) - |\tau\hat{n}|^2. \tag{A.8}$$

We now argue as follows. Let v be an eigenvector of τ and let z be its eigenvalue. Multiplying Eq. (A.7) by v we obtain

$$\hat{n}.v = 0 \quad \text{or} \quad z^2 + \frac{v\,\mathrm{tr}(\tau) - (\hat{n}\tau\hat{n})}{1-v}z + a = 0. \tag{A.9}$$

If τ has 3 different eigenvalues, these equations imply that $\hat{n}.v=0$ for some eigenvector v (because if not, the second degree polynomial in z given in Eq. (A.9) would have 3 different roots). If τ does not have 3 different eigenvalues, then, it is also (trivially) true that $\hat{n}.v = 0$ for some eigenvector of τ. Thus, given also that τ is symmetric, we conclude that we can write

$$\hat{n} = y_1 v_1 + y_2 v_2 \tag{A.10}$$

for some eigenvectors v_i of τ and some numbers y_i. Let z_i be the eigenvalue of v_i. If both y_1 and y_2 are different from 0, then, from Eq. (A.9), we have

$$z_1 z_2 = a \quad \text{and} \quad z_1 + z_2 = \frac{(\hat{n}\tau\hat{n}) - v\,\mathrm{tr}(\tau)}{1-v}. \tag{A.11}$$

From Eqs. (A.6), (A.8) and (A.11) and the fact that

$$\tau_{ij}\tau_{ij} = \sum_{i=1}^{3} z_i^2,$$

after some algebraic manipulation, we obtain that

$$f = (1+v)z_3^2 \tag{A.12}$$

(z_3 being the other eigenvalue, corresponding to the eigenvector v_3 orthogonal v_1 to and v_2). If on the other hand one of the numbers y_i of Eq. (A.10) is 0, i.e. $\hat{n}$ is eigenvector of τ of eigenvalue say z_1, we can immediately compute f

$$f = \frac{v}{1-v}(z_2 + z_3)^2 + z_2^2 + z_3^2. \tag{A.13}$$

This last two equations gives us all the possible extreme values of f. Since we are interested in the minimum (and $0 < v < 1$), obviously our best choice would be Eq. (A.12) with z_3 being the eigenvalue of minimum absolute value. For this choice to be valid, we need to check that we can find numbers y_1 and y_2 so that Eqs. (A.11) are satisfied with $\hat{n}$ having norm 1 and given by Eq. (A.10). Some algebra shows that for such a solution to exist, the two eigenvalues of τ with largest absolute value (z_1 and z_2) have to have different sign (unless one is 0). This condition is certainly satisfied if the trace of τ is 0, and since this is the only case we consider, we have that for the purposes of this paper the minimum value of f is

$$f = (1+v)\min\{z^2 : z \text{ is eigenvalue of } \tau\}, \tag{A.14}$$

from where (27) and (29) immediately follows.

References

Ball, J.M., James, R.D., 1987. Fine phase mixtures as minimizers of energy. Arch. Ration. Mech. Anal. 100, 13–52.

Bhattacharya, K., 1992. Self-accommodation in martensite. Arch. Ration. Mech. Anal. 120, 201–244.

Bhattacharya, K., 1993. Comparison of the geometrically nonlinear and linear theories of martensitic transformation. Continuum Mech. Thermodyn. 5, 205–242.

Bhattacharya, K., Firoozye, N.B., James, R.D., Kohn, R.V., 1994. Restrictions on microstructure. Proc. Roy. Soc. Edinburgh A 124, 843–878.

Bhattacharya, K., Kohn, R.V., 1996. Symmetry, texture and the recoverable strain of shape-memory polycrystals. Acta Mater. 44, 529–542.

Bhattacharya, K., Kohn, R.V., 1997. Elastic energy minimization and the recoverable strain of polycrystalline shape-memory materials. Arch. Ration. Mech. Anal. 139, 99–180.

Bruno, O.P., Goldsztein, G.H., 1999. A fast algorithm for the simulation of polycrystalline misfits: martensitic transformations in two space dimensions. Proc. Roy. Soc. London A 455, 4245–4276.

Bruno, O.P., Goldsztein, G.H., 2000. Numerical simulation of martensitic transformations in two and three-dimensional polycrystals. J. Mech. Phys. Solids 48, 1175–1201.

Bruno, O.P., Reitich, F., Leo, P.H., 1996. The overall elastic energy of polycrystalline martensitic solids. J. Mech. Phys. Solids 44, 1051–1101.

Dacorogna, B., 1989. Direct Methods in the Calculus of Variations. Springer, New York.

Dolzmann, G., 1999. Numerical computation of rank-one convex envelopes. SIAM J. Numer. Anal. 36, 1621–1635.

Firoozye, N.B., Kohn, R.V., 1993. Geometric parameters and the relaxation of multiwell energies. In: Kinderlehrer, D., James, R., Luskin, M., Ericksen, J.L. (Eds.), Microstructure and Phase Transition. Springer, New York, pp. 854–109.

Khachaturyan, A.G., 1966. Some questions concerning the theory of phase transformations in solids. Sov. Phys.-Solid State 8, 2163–2168.

Knowles, K.M., Smith, D.A., 1981. The crystallography of the martensitic transformation in equiatomic nickel–titanium. Acta Metall. 29, 101–110.

Kohn, R.V., 1991. The relaxation of a double-well energy. Continuum Mech. Thermodyn. 3, 193–236.

Lurie, K.A., Cherkaev, A.V., 1988. On a certain variational problem of phase equilibrium. In: Ball, J.M. (Ed.), Material Instabilities in Continuum Mechanics, University Press, Oxford, pp. 257–268.

Ortiz, M., Repetto, E.A., 1999. Nonconvex energy minimization and dislocation structures in ductile single crystals. J. Mech. Phys. Solids 47, 397–462.

Ortiz, M., Repetto, E.A., Stainer, L., 2000. A theory of subgrain dislocation structures. J. Mech. Phys. Solids 48, 2077–2114.

Pipkin, A.C., 1991. Elastic materials with two preferred states. Q. J. Mech. Appl. Math. 44, 1–15.

Shu, Y.C., Bhattacharya, K., 1998. The influence of texture on the shape-memory effect in polycrystals. Acta Mater. 46, 5457–5473.

Smyshlyaev, V.P., Willis, J.R., 1999. On the relaxation of a three-well energy. Proc. Roy. Soc. London A 455, 779–814.

Šverák, V., 1990. Rank-one convexity does not imply quasiconvexity. Proc. Roy. Soc. Edinburgh Sect. A 120, 185–189.

Wechsler, M.S., Lieberman, D.S., Read, T.A., 1953. On the theory of the formation of martensite. J. Metals 197, 1503–1515.