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ORIGINAL ARTICLE

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Mixed analytical–numerical relaxation in finite single-slip crystal plasticity

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Abstract The modeling of the finite elastoplastic behaviour of single crystals with one active slip system leads to a nonconvex variational problem, whose minimization produces fine structures. The computation of the quasiconvex envelope of the energy density involves the solution of a nonconvex optimization problem and faces severe numerical difficulties from the presence of many local minima. In this paper, we consider a standard model problem in two dimensions and, by exploiting analytical relaxation results for limiting cases and the special structure of the problem at hand, we obtain a fast and efficient numerical relaxation algorithm. The effectiveness of our algorithm is demonstrated with numerical examples. The precision of the results is assessed by lower bounds from polyconvexity.

Keywords Relaxation · Quasiconvexity · Crystal plasticity

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1 Introduction and model problem

In this paper we develop a mixed numerical–analytical relaxation method and apply it to a variational model for finite single-slip crystal plasticity in ductile single crystals. Relaxation is a general theory which permits the study of the macroscopic behavior of materials which develop microstructures; its practical application has been up to now largely limited by the fact that it has rarely been possible to obtain efficiently the explicit relaxation of the problem at hand. Indeed, whereas only very few problems admit an analytical relaxation, a direct numerical relaxation which does not exploit any special structure is faced with huge numerical difficulties from the presence of many local minima. We address here this difficulty by providing, for one test case from crystal plasticity which has already been studied several times in the literature, a method which combines some analytical results with an efficient numerical optimization of the microstructure, within a restricted class.

We focus on two spatial dimensions and on the case that only one slip system is active, and use a variational model based on a time discrete formulation. This falls within the class of time-discrete variational models for geometrically nonlinear plasticity, which have been recently studied exploiting the analogy with problems from martensitic microstructures. This analogy, and the possibility to study each incremental problem in plasticity

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via a variational functional depending on the deformation gradient $F = D\phi$, as in nonlinear elasticity, was advanced by Ortiz and Repetto in [37]; in the same paper the variational origin of geometrical softening is discussed and comparisons to experimental observations of microstructures in plastic materials are provided.

We focus here on the model defined in [13] and simulated in [9,29]. The model of [13] permits the treatment of unloading through the study of a sequence of variational problems; we shall here however, focus on the first time-step alone. This restriction is appropriate for monotone loading, and closely related to the deformation theory of plasticity. Precisely, we consider one slip system, described by an orthonormal pair of vectors s and m, with s denoting the slip direction and m the normal to the slip plane. In a geometrically nonlinear context, we assume the multiplicative decomposition of the deformation gradient $F = F_e F_p$ with $F_p = \mathrm{Id} + \gamma s \otimes m$ and the plastic slip $\gamma \in \mathbb{R}$. Hardening is included through a single internal variable $p \in \mathbb{R}$. Within the framework of rate-independent processes [30–32], we consider one time step in an implicit time-discrete scheme. Minimizing out locally the internal variables, the incremental problem can be cast equivalently into a variational formulation expressed only in terms of the deformation gradient F and can therefore be analysed by the methods of the calculus of variations.

The constitutive behaviour of the single crystal is described in terms of two potentials: the free energy density $W_{ep}(F, \gamma, p)$ and the dissipation potential $J(\gamma, p)$. The free energy density is the sum of the elastic and the plastic contribution,

$$W_{ep}(F, \gamma, p) = W_e(F(\mathrm{Id} - \gamma s \otimes m)) + W_p(p), \tag{1.1}$$

where we used the relations $F_p = \mathrm{Id} + \gamma s \otimes m$, $F_e = F F_p^{-1} = F(\mathrm{Id} - \gamma s \otimes m)$. Here

$$W_p(p) = \frac{h}{2} p^2 \tag{1.2}$$

and $U(F) = \frac{\kappa}{4}((\det F)^2 - 1) - \frac{\kappa+2\mu}{2} \log(\det F)$,

$$W_e(F_e) = \begin{cases} U(F_e) + \dfrac{\mu}{2}(|F_e|^2 - 2) & \text{if } \det F_e > 0, \\ \infty & \text{else.} \end{cases} \tag{1.3}$$

Here and throughout, μ, $\kappa > 0$ are elastic constants and $h > 0$ is the hardening modulus. The function W_e is polyconvex, hence in the absence of plastic deformation (this is, if one prescribes $\gamma = p = 0$ everywhere) no microstructure is expected. In this case the condensed energy W (defined next) equals W_e and the condensed problem (defined next) has minimizers [5]. The functional form is chosen so that W_e is nonnegative, and vanishes on $SO(2)$ the group of orthogonal matrices of $\mathbb{R}^{2\times 2}$ with positive determinant. The dissipation potential $J(\gamma, p)$ is

$$J(\gamma, p) = \begin{cases} \tau_{cr}|\gamma| & \text{if } |\gamma| + p \le 0 \\ \infty & \text{else,} \end{cases} \tag{1.4}$$

with $\tau_{cr} > 0$ the critical shear stress. We use $|\cdot|$ for the Euclidean norm ($|F|^2 = \mathrm{Tr}\, F^T F$ for matrices) and $\cdot$ for the scalar product in $\mathbb{R}^2$.

We focus here on the first time-step of a time-incremental formulation. In this case the considered model reduces to the minimization of

$$\int_\Omega \big[W_{ep}(D\phi, \gamma, p) + J(\gamma, p)\big]\,\mathrm{d}x + \text{ external forces} \tag{1.5}$$

over deformations $\phi : \Omega \subset \mathbb{R}^2 \to \mathbb{R}^2$, with γ, $p : \Omega \to \mathbb{R}$ subject to appropriate boundary conditions. Since the internal variables (γ, p) enter locally into the energy, it is convenient to minimize them out pointwise. One immediately obtains $p = -|\gamma|$ whereas minimization in γ leads to the condensed energy [13]

$$W(F) = U(F) + \frac{\mu}{2}(|F|^2 - 2) - \frac{1}{2}\frac{(\max\{0, \mu|Fs \cdot Fm| - \tau_{cr}\})^2}{\mu|Fs|^2 + h}. \tag{1.6}$$

This is the starting point of our analysis. The variational problem (1.5) then reduces to the condensed problem of minimizing

$$\int_\Omega W(D\phi)\mathrm{d}x + \text{ external forces.}$$

At the same time, the plastic slip reads

$$\gamma(F) = \frac{\max\{0,\ \mu|Fs \cdot Fm| - \tau_{\mathrm{cr}}\}}{\mu|Fs|^2 + h}\operatorname{sign}(Fs \cdot Fm). \tag{1.7}$$

The energy density (1.6) is not rank-one convex and, hence, not quasiconvex [13]. General theory shows then that for many boundary data the functional (1.5) does not have a minimizer, and that low-energy sequences develop fine-scale oscillations in the gradient [6,7,20,22,34]. For the case under consideration, the occurrence of such microstructures has been indeed illustrated in [24] by a direct finite element simulation using representative volume elements under affine-periodic boundary conditions.

The macroscopic material behaviour is modelled by minimizing out locally the possible microstructures, which amounts to computing the quasiconvex envelope W^{qc} of W. The latter is defined as the pointwise supremum of the family of the quasiconvex functions which bound W from below; a function $V : \mathbb{R}^{m\times n} \to \mathbb{R} \cup \{\infty\}$ is called quasiconvex if, for all $F \in \mathbb{R}^{m\times n}$ and all $\varphi \in W_0^{1,\infty}((0,1)^n; \mathbb{R}^m)$ for which the integral exists,

$$V(F) \le \int\limits_{(0,1)^n} V(F + \nabla\varphi)\mathrm{d}x.$$

If W is continuous one can show that

$$W^{\mathrm{qc}}(F) = \inf\left\{ \int\limits_{(0,1)^n} W(F + \nabla\varphi)\mathrm{d}x : \varphi \in W_0^{1,\infty}((0,1)^n; \mathbb{R}^m) \right\}. \tag{1.8}$$

For additional details see, e.g., [20,34]. Knowledge of W^{qc} permits one to perform macroscopic finite-element simulations, where the energy density W is replaced by W^{qc}. Equivalently, the variational problem is replaced by its relaxation. Since optimal microstructure is in this case already accounted for in the energetics, it is not necessary to resolve it explicitly by the finite-element solution. This leads to mesh-independent results, and permits to successfully use rather coarse meshes to study realistic experimental geometries, as was done for example in [4,14,19,29]. A largely similar situation arires in the setting of shape optimization, see [2,26] and references therein. In both cases usage of the relaxation technique for mechanical problems with microstructure has been up to now mainly limited by the difficulty of determining the relaxation W^{qc}.

A closed form for the quasiconvex envelope of condensed energies of the kind of W is known only in few simplified cases [1,11,17,18,21,25,26,43]. In practical applications one usually resorts to an approximation to W^{qc} based on laminates. Equation (1.8) shows that the quasiconvex envelope can be determined by optimizing over all possible distributions of gradients $F + \nabla\varphi$; laminates constitute a large and yet simply accessible class of such distributions. Precisely, laminates are probability measures on $\mathbb{R}^{m\times n}$ which can be described as the weak limit of the distribution of special sequences of gradients. A laminate of zeroth order is a Dirac delta, i.e., it has the form $\nu = \delta_F$, and corresponds to the limit of the gradient distribution of the (constant) sequence $\varphi(x) = Fx$. A laminate of nth order is defined inductively from a laminate of order $n-1$ by replacing each of the terms $c\delta_F$ by a sum $c(\lambda\delta_{F_1} + (1-\lambda)\delta_{F_2})$, where $\lambda F_1 + (1-\lambda)F_2 = F$, $\lambda \in [0,1]$, $\operatorname{rank}(F_1 - F_2) \le 1$ and $c \in (0,1]$. One says that the matrix F has been split into F_1 and F_2. Since laminates are probability measures, the average of a function V over a laminate ν is denoted by $\langle \nu, V\rangle = \int_{\mathbb{R}^{m\times n}} V(A)d\nu(A)$. For example, first-order laminates have the form $\nu = \lambda\delta_{F_1} + (1-\lambda)\delta_{F_2}$, with $F_1 - F_2 = a \otimes n$, and are the limits of the gradient distributions of the maps

$$\varphi_\varepsilon(x) = F_1 x - a\varepsilon\chi\left(\frac{x\cdot n}{\varepsilon}\right)$$

where $\chi : \mathbb{R} \to \mathbb{R}$ is defined by $\chi(0) = 0$, $\chi'(t) = 0$ if $t \in (k, k+\lambda)$ and $\chi'(t) = 1$ if $t \in (k+\lambda, k+1)$, for $k \in \mathbb{Z}$. For small ε, the gradients $\nabla\varphi_\varepsilon$ oscillate on a fine scale between the values F_1 and F_2, with average $F = \lambda F_1 + (1-\lambda)F_2$. As $\varepsilon \to 0$, the sequence φ_ε converges weakly-$*$ in $W^{1,\infty}(\mathbb{R}^n; \mathbb{R}^m)$ to the affine function $\varphi(x) = Fx$; the function $V(\nabla\varphi_\epsilon)$ converges weakly to $\langle \nu, V\rangle = \lambda V(F_1) + (1-\lambda)V(F_2)$. Refining this argument one can show that mixtures are always possible between rank-one connected matrices, hence that all laminates as defined above are attainable as weak limits of gradients. For additional details see, e.g., [20,22,34].

Restricting the infimization in (1.8) to laminates of a given order produces an upper bound to W^{qc}, which is called the lamination envelope of order k. Precisely,

$$W^{\mathrm{qc}}(F) \le W^{\mathrm{lc},k}(F) = \inf \left\{ \int_{\mathbb{R}^{m\times n}} W(A)\mathrm{d}\nu(A) : \nu \text{ laminate of order } k, \int_{\mathbb{R}^{m\times n}} A\,\mathrm{d}\nu(A) = F \right\}. \tag{1.9}$$

In order to compute $W^{\mathrm{lc},k}$ one has to determine, for each F, the best laminate of order k, which is a finite-dimensional global nonconvex optimization problem. Practical implementation is, however, difficult, because the objective function may present an exponential (in k) number of nearby optimal local minima [12]. The method based on discretizing the function W on a regular mesh proposed by Dolzmann [23] is efficient only in low dimension, and for smooth functions W. In particular, since the structure of the mesh is relevant for the algorithm, it is difficult to extend that approach to models like the one of interest here which incorporate a strong penalization on volume changes, or even a nonlinear constraint on the determinant.

Within the techniques of global optimization, probabilistic global search procedures are the ones commonly adopted, but they remain computationally quite expensive. Since in a finite element framework this optimization must be performed at every material point (e.g. Gauss point), for real applications it is mandatory to develop fast techniques for the numerical relaxation. In the literature the computational effort related to the global search is usually reduced by fixing some of the parameters of the laminate on the basis of conjectures motivated by physical considerations [4,28,29,38].

In this paper we present a different approach to the relaxation of W over laminates. Rather than attacking the global minimization by brute-force global optimization, we exploit in an essential fashion the structure of the problem both to achieve a fundamental understanding on the optimal microstructure and, in parallel, to design an efficient numerical relaxation scheme. At variance with [4,29] we do not start from a restriction to the kinematics, but from an approximation to the energy, which is then in a second stage relaxed numerically. Specifically, we shall use analytical expressions of the quasiconvex envelope of simplified versions of the relevant energy. Inspired by results based on the global optimization [9] and on analytical relaxation [15,16,18], we determine analytically a second-order laminate which has "good" energy and furnishes an upper bound to the relaxed energy. This laminate is then used as initial guess for the local minimization. Thereby we have constructed an effective procedure to obtain, for every deformation gradient F, a locally optimal laminate ν for the relaxation of W. The resulting energy $W^{\mathrm{opt}} = \langle W, \nu\rangle$ gives an upper bound on the relaxation, $W^{\mathrm{opt}} \ge W^{\mathrm{qc}}$.

In a second stage we assess the quality of our result. To this end we seek a polyaffine function that coincides with the unrelaxed energy on the support of the laminate and verify that it is below the condensed energy W, up to a small error term. The size of this error gives us an upper bound on the size of the error done in the relaxation, i.e., on the difference $W^{\mathrm{opt}} - W^{\mathrm{qc}}$.

Since plastic deformation is isochoric, one expects the relevant macroscopic deformation gradients F to have determinant close to unity. Our heuristics is focused on the case $\det F = 1$, and in our numerical examples the macroscopic deformation gradient will obey this condition. The support of the laminate obtained by numerical optimization is however, not restricted to this set. Our results can easily be generalized to other values of F by taking the laminate corresponding to the deviatoric part of a generic F as a starting point for the local relaxation.

The layout of the paper is as follows. After this introduction, Sect. 2 is devoted to the construction of approximate (first and second) order laminates. This section consists in turn of three subsections. In the first one, we recall from [16] the analytical expression of the quasiconvex envelope in the case of rigid elasticity, linear hardening and no dissipation. In the second one, we construct a second-order laminate with fixed lamination direction, whereas in the last subsection we present an approximate first order laminate. These laminates are built so that the corresponding energy bounds from above the quasiconvex envelope of the condensed energy in the case of no dissipation. Section 3 is devoted to the numerical optimization problem and describes the algorithm employed for the local minimization and the definition of the laminate whereas, Sect. 4 focuses on the optimality check, which is obtained by computing a polyaffine function supported on the laminate at the given deformation gradient F. Numerical examples of relaxation for simple shear with different shear directions and for biaxial deformation gradient are given in Sect. 5 whereas final remarks conclude the paper in Sect. 6.

2 Partial analytical relaxation

We first consider some simplifications of the general model (1.6) which will allow either the explicit evaluation of the quasiconvex envelope (such as in Sect. 2.1) or the constructions of laminates (second order in Sect. 2.2 and first order in Sect. 2.3) with good "energetic" content.

2.1 The quasiconvex envelope for the rigid case in $2D$

This section recalls the analysis in [16] for a simplification of the model (1.6) in the case of so called geometric softening [3,37]. We assume rigid elastic behaviour, that is, $F = QF_\mathrm{p}$ with $Q \in SO(2)$, $F_\mathrm{p} = \mathrm{Id} + \gamma s \otimes m$, $p = |\gamma|$ and zero dissipation, that is, $\tau_\mathrm{cr} = 0$. Under these conditions, the condensed energy reads as follows:

$$W_1(F) = \begin{cases} \dfrac{h}{2}\gamma^2 & \text{if } F = Q(\mathrm{Id} + \gamma s \otimes m) \quad \text{for some } Q \in SO(2) \text{ and } \gamma \in \mathbb{R}, \\ \infty & \text{else.} \end{cases} \tag{2.1}$$

This energy density is not rank one convex, hence neither quasiconvex. The quasiconvex envelope can be determined analytically and reads as follows.

Proposition 2.1 (From [16]) *The quasiconvex envelope $W_1^{\mathrm{qc}}(F)$ of $W_1(F)$ reads*

$$W_1^{\mathrm{qc}}(F) = \begin{cases} \frac{h}{2}(|Fm|^2 - 1) & \text{if } \det F = 1 \text{ and } |Fs| \le 1, \\ \infty & \text{else.} \end{cases} \tag{2.2}$$

Moreover, the quasi-, poly-, and first order laminate-convex envelope coincide. The optimal laminate corresponding to a matrix F is supported on the matrices

$$F_1 = F + \upsilon_1 a \otimes b \quad \text{and} \quad F_2 = F + \upsilon_2 a \otimes b \tag{2.3}$$

where $b = s$, $a = Fm/|Fm|$, and υ_i for $i = 1, 2$ are the two real solutions of the equation

$$\upsilon^2 + 2\upsilon \frac{Fm \cdot Fs}{|Fm|} + |Fs|^2 - 1 = 0, \tag{2.4}$$

with $\upsilon_1 \upsilon_2 \le 0$.

Proof The proof of the lower bound is obtained by showing that $W_1^{\mathrm{qc}}(F)$ is polyconvex and $W_1^{\mathrm{qc}}(F) \le W_1(F)$. As a result, one obtains $W_1^{\mathrm{qc}}(F) \le W_1^{\mathrm{pc}}(F) \le W_1(F)$. For the proof of the upper bound one shows that $W_1^{\mathrm{qc}}(F)$ is obtained by considering the first lamination convex envelope, and then constructs a test function $\varphi \in W_0^{1,\infty}((0,1)^2; \mathbb{R}^2)$ using convex integration techniques from [35] by following the same arguments as in [18]. The details are included in [16] and hence omitted here. □

Remark 2.2 The two phases F_1 and F_2 have the same plastic slip γ in absolute value. This corresponds to the condition $W_1(F_1) = W_1(F_2)$ or equivalently $|F_1 m| = |F_2 m|$. Since $m \cdot s = 0$, the latter is a trivial consequence of (2.3) and the fact that $b = s$.

2.2 An approximate 2nd-order laminate

In this section we address the construction of second order laminates which have "good" energy, neglecting dissipation. The key idea is to construct an optimal first-order laminate between a purely elastic phase and the analytic relaxation W_1^{qc} obtained in Proposition 2.1. Both functions are—in appropriate domains—quadratic, hence, given a lamination direction, the relaxation can be determined analytically, by computing the convex envelope of the minimum of two parabolas.

Compared to the situation of Sect. 2.1, we only keep the assumption that $\tau_\mathrm{cr} = 0$ and consider the following energy density

$$W_2(F) = \min_{\gamma \in \mathbb{R}} W_{\mathrm{ep}}(F, \gamma), \tag{2.5}$$

where $W_{\rm ep}(F,\gamma)=W_{\rm e}(F(\mathrm{Id}+\gamma s\otimes m)^{-1})+\frac{h}{2}\gamma^2$ is obtained from (1.1) with $p=-|\gamma|$ and $F_{\rm e}=F(\mathrm{Id}+\gamma s\otimes m)^{-1}=F(\mathrm{Id}-\gamma s\otimes m)$.

Then a first result that relates the energy $W_2(F)$ with $W_1(F)$ defined by (2.1) and $W_{\rm e}$ defined by (1.3) is given in the following.

Lemma 2.3 *The following bound holds*

$$W_2(F)\le\min\{W_1(F),\ W_{\rm e}(F)\}. \tag{2.6}$$

Proof From (2.5) we have

$$W_2(F)\le W_{\rm ep}(F,0)=W_{\rm e}(F). \tag{2.7}$$

By accounting for (2.1) and (1.3) we have also

$$W_1(F)=\begin{cases} W_{\rm ep}(F,\gamma) & \text{if } F=Q(\mathrm{Id}+\gamma s\otimes m),\\ \infty & \text{else.}\end{cases} \tag{2.8}$$

Therefore,

$$W_{\rm ep}(F,\gamma)\le W_1(F)\quad\text{for every }\ \gamma\in\mathbb{R}. \tag{2.9}$$

Recalling (2.5) one obtains

$$W_2(F)\le W_1(F). \tag{2.10}$$

This and (2.7) imply (2.6). □

Equation (2.6) bounds W_2 with the minimum of the two functions W_1 and $W_{\rm e}$. For both, the quasiconvex envelope is known: of the first one from Proposition 2.1, of the second one by the fact that $W_{\rm e}$ is polyconvex, and hence $W_{\rm e}^{\rm qc}=W_{\rm e}$. The relaxation of W_2 is therefore bounded by the relaxation of $\min\{W_1^{\rm qc},W_{\rm e}\}$, and in particular by its first lamination convex envelope. The latter can be easily determined by taking the convex envelope along each rank-one direction. Since $W_1^{\rm qc}$ is infinite away from the unit-determinant surface, if $\det F=1$ the laminate is necessarily isochoric. Precisely, let S^1 denote the set of elements of $\mathbb{R}^2$ with unit norm, given a lamination direction $b\in S^1$ with $b=(\cos\beta,\ \sin\beta)$ for $\beta\in[0,\ \pi/2)$, for any $\upsilon\in\mathbb{R}$ the condition $\det(F+\upsilon\, a\otimes b)=1$ gives

$$a=\frac{Fb^\perp}{|Fb^\perp|}, \tag{2.11}$$

with $b^\perp=(-\sin\beta,\ \cos\beta)$. For each direction $b\in S^1$, consider then the function $f:\mathbb{R}\times S^1\to\mathbb{R}$

$$f(\upsilon\,;b)=\min\{W_1^{\rm qc}(F+\upsilon\, a\otimes b),\ W_{\rm e}(F+\upsilon\, a\otimes b)\}. \tag{2.12}$$

Here we work at fixed F and a is given by (2.11). The convex envelope of (2.12) with respect to its first argument $\upsilon\in\mathbb{R}$ and fixed b is denoted by

$$f^{**}(\cdot;b)=\mathrm{conv}\ f(\cdot;b). \tag{2.13}$$

Since f is the minimum of two parabolas, f^{**} can be computed analytically; for brevity we do not report the explicit formula here and denote succintly by

$$(\upsilon_1(b),\ \upsilon_2(b))=\textsc{ConEnv}(F;b)$$

the abscissa of the tangent points to $W_{\rm e}(F+\upsilon\, a\otimes b)$ and $W_1^{\rm qc}(F+\upsilon\, a\otimes b)$, respectively, and the function that defines those values.

The main result of this section then reads as follows.

Proposition 2.4 *The quasiconvex envelope $W_2^{\rm qc}$ of the energy density W_2 defined by (2.5) satisfies*

$$W_2^{\rm qc}(F)\le f^{**}(0;b)\quad\textit{for all } b \textit{ with } |b|=1. \tag{2.14}$$

Proof On matrices F with $\det F \leq 0$, all functions mentioned in the statement equal ∞, hence the result is true.

On the set of matrices F with $\det F > 0$ one has $W_2^{\mathrm{qc}} \leq W_2 < \infty$, hence on the same set W_2^{qc} is rank-one convex. Fix $F \in \mathbb{R}^{2\times 2}$ with $\det F > 0$, let $b \in S^1$, and a as in (2.11). Then rank-one convexity implies convexity of the function $g : \mathbb{R} \to \mathbb{R}$ defined by

$$g(\upsilon) = W_2^{\mathrm{qc}}(F + \upsilon a \otimes b).$$

Lemma 2.3 implies that $g \leq f$. By the convexity of g this implies $g(\upsilon) \leq f^{**}(\upsilon; b)$ for all $\upsilon \in \mathbb{R}$; in particular $W_2^{\mathrm{qc}}(F) = g(0) \leq f^{**}(0; b)$. □

Condition (2.14) states that for any given lamination direction b one can construct a second order laminate with energy higher than W_2^{qc}. We can therefore look for the laminates with the least energy. This problem consists of finding $b \in S^1$ that minimize $f^{**}(0; b)$ and their search reduces to a one-dimensional global optimization problem. Let b_{opt} be such that

$$f^{**}(0; b_{\mathrm{opt}}) = \min_{b\in S^1} f^{**}(0; b).$$

We define, for future reference, the optimal energy obtained this way as W_{f},

$$W_{\mathrm{f}}(F) = f^{**}(0; b_{\mathrm{opt}}) = \min_{b\in S^1} f^{**}(0; b). \tag{2.15}$$

Obviously $W_2^{\mathrm{qc}} \leq W_2^{\mathrm{lc},2} \leq W_{\mathrm{f}}$.

The second-order laminate corresponding to W_{f} is supported on three matrices, say, F_1, F_{21} and F_{22}. The deformation gradient F_1 is defined as

$$F_1 = F + \upsilon_1(b_{\mathrm{opt}}) \frac{F b_{\mathrm{opt}}^{\perp}}{|F b_{\mathrm{opt}}^{\perp}|} \otimes b_{\mathrm{opt}}$$

where $\upsilon_1(b_{\mathrm{opt}})$ is the abscissa of the tangent point to $W_{\mathrm{e}}(F + \upsilon \frac{F b_{\mathrm{opt}}^{\perp}}{|F b_{\mathrm{opt}}^{\perp}|} \otimes b_{\mathrm{opt}})$ in the evaluation of the convex envelope $f^{**}(\upsilon; b_{\mathrm{opt}})$, and F_{21} and F_{22} are obtained using the analytical results of Sect. 2.1 with

$$F_2 = F + \upsilon_2(b_{\mathrm{opt}}) \frac{F b_{\mathrm{opt}}^{\perp}}{|F b_{\mathrm{opt}}^{\perp}|} \otimes b_{\mathrm{opt}}$$

where $\upsilon_2(b_{\mathrm{opt}})$ is the abscissa of the tangent point to $W_1^{\mathrm{qc}}(F + \upsilon \frac{F b_{\mathrm{opt}}^{\perp}}{|F b_{\mathrm{opt}}^{\perp}|} \otimes b_{\mathrm{opt}})$. Figure 1 depicts the definition of $\upsilon_1(b)$ and $\upsilon_2(b)$, whereas Box 1 summarizes the steps for the definition of the laminate described in this section. In Box 1 the laminate is represented as $\nu_2 = \lambda_1 \delta_{F_1} + (1-\lambda_1)\lambda_{21}\delta_{F_{21}} + (1-\lambda_1)(1-\lambda_{21})\delta_{F_{22}}$ with δ_F the Dirac measure concentrated at F [34,40,41].

Remark 2.5 The laminates we consider split F into two phases: an elastic one F_1 and a plastic one F_2. The plastic phase F_2, in turn, is being splitted according to Proposition 2.1 and following remark into other two phases: F_{21} and F_{22} with $\gamma(F_{21}) = -\gamma(F_{22})$. The graph of the laminate is shown in Fig. 2.

Remark 2.6 Assuming as condensed energy

$$W_{\mathrm{CT}}(F) = \begin{cases} \tau_{\mathrm{cr}}|\gamma| & \text{if } F = Q(\mathrm{Id} + \gamma s \otimes m) \quad \text{for some } \gamma \text{ and } Q \in SO(2) \\ \infty & \text{else} \end{cases} \tag{2.16}$$

corresponding to rigid elasticity and zero free plastic energy, the following expression for the quasiconvex envelope is obtained in [18]

$$W_{\mathrm{CT}}^{\mathrm{qc}}(F) = \begin{cases} \tau_{\mathrm{cr}}\,(\lambda_2(F) - \lambda_1(F)) & \text{if } \det F = 1 \text{ and } |Fs| \leq 1, \\ \infty & \text{else,} \end{cases} \tag{2.17}$$

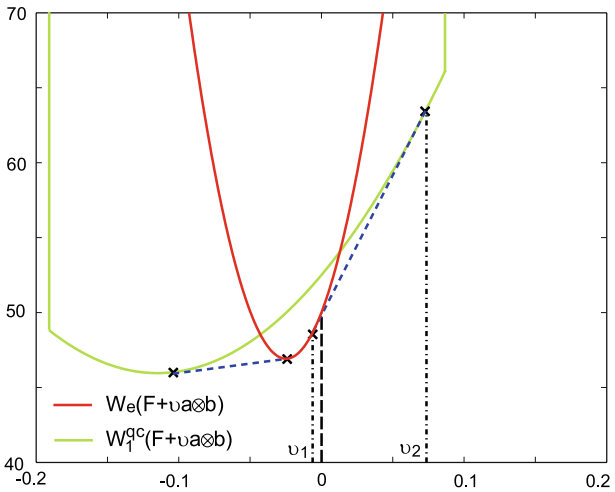


Fig. 1 Definition of $f^{**}(\upsilon; b)$ together with υ_1 and υ_2 for computing $f^{**}(0; b)$ for a given lamination direction $b \in S^1$

Box 1 Construction of a second order laminate with energy bounding from above W_2^{qc}

DATA:	$m,\ s\ \in \mathbb{R}^2$ for $F_{\mathrm{p}} = \mathrm{Id} + \gamma s \otimes m$
INPUT:	$F \in \mathbb{R}^{2\times 2}$ with $\det F = 1$
FIND:	$b_{\mathrm{opt}} = \arg\min_{b\in S^1} f^{**}(0; b)$ with $f^{**}(0; b)$ from (2.13)
	$(\upsilon_1(b_{\mathrm{opt}}),\ \upsilon_2(b_{\mathrm{opt}}) = \mathrm{CONENV}(F; b_{\mathrm{opt}})$
SOLVE:	quadratic equation $\upsilon^2 + 2\upsilon \dfrac{F_2 m \cdot F_2 s}{\lvert F_2 m\rvert} + \lvert F_2 s\rvert^2 - 1 = 0$
	with two real solutions υ_1 and υ_2.
OUTPUT:	$\nu_2 = \lambda_1 \delta_{F_1} + (1-\lambda_1)\lambda_{21}\delta_{F_{21}} + (1-\lambda_1)(1-\lambda_{21})\delta_{F_{22}}$
	for $\lambda_{21} = \dfrac{\lvert\upsilon_2\rvert}{\lvert\upsilon_1\rvert + \lvert\upsilon_2\rvert}$ and $F_{2i} = F_2 + \upsilon_i \dfrac{F_2 m}{\lvert F_2 m\rvert} \otimes s$ for $i = 1, 2$

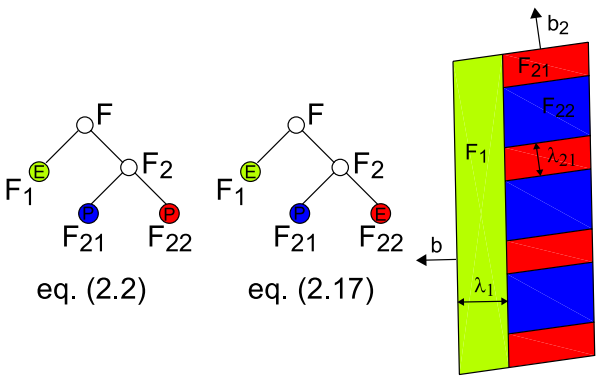


Fig. 2 Graph of a second order laminate built with (2.2) and (2.17)

with $\lambda_2 > \lambda_1$ the singular values of F, i.e. the eigenvalues of $(F^T F)^{1/2}$. The optimal microstructure is given in this case by a simple laminate with either F_+ or F_- belonging to $SO(2)$, i.e., plastic deformation is concentrated only on one of the two. As a result, it is possible to define with similar arguments another type of second order laminate whose energy bounds from above the effective energy in the case the dissipation is the dominant mechanism. The laminate would therefore present the phase F splitted into two phases: F_1 and F_2 with F_1

elastic and F_2 unstable. The latter would be then splitted into other two: an elastic F_{21} and plastic F_{22}. The corresponding graph and microstructure is depicted in Fig. 2. In this case, however, for the determination of f^{**} one would have to find the convex envelope between a parabola $W_{\mathrm{e}}(F + xa \otimes b)$ and the convex function $W_{\mathrm{CT}}^{\mathrm{qc}}(F + xa \otimes b)$ rather than between the two parabolas as in (2.12).

2.3 An approximate first order laminate

The laminate constructed above is based on assuming that the elastic and the plastic deformation are, to a good approximation, spatially separated. We consider here instead a different situation, in which a plastic microstructure is superimposed to a uniform elastic deformation. This will lead us to the determination of a different laminate, which also produces an upper bound on the sought relaxation. Choice of the best one will in the end be done by a variational criterion.

We consider the energy

$$W_3(F) = \min_{F_{\mathrm{e}}} \left\{ W_{\mathrm{e}}(F_{\mathrm{e}}) + W_1^{\mathrm{qc}}(F_{\mathrm{p}}) : F_{\mathrm{p}} = F_{\mathrm{e}}^{-1} F \right\}. \tag{2.18}$$

This corresponds to the best average energy that can be obtained by superimposing a uniform elastic deformation F_{e} to all plastic microstructures determined, for the energy W_1, in Sect. 2.1. Consider an average deformation gradient F with $\det F = 1$. Since $\det F_{\mathrm{p}} = 1$, then necessarily $\det F_{\mathrm{e}} = 1$ and $|F_{\mathrm{e}}| = |F_{\mathrm{e}}^{-1}|$. By accounting for (1.3) and (2.2), the argument in the minimization of (2.18) reads

$$\bar{W}(F, F_{\mathrm{e}}^{-1}) = \begin{cases} \dfrac{\mu}{2}(|F_{\mathrm{e}}^{-1}|^2 - 2) + \dfrac{h}{2}(|F_{\mathrm{e}}^{-1} F m|^2 - 1) & \text{if } |F_{\mathrm{e}}^{-1} F s| \le 1 \text{ and} \\ & \det F_{\mathrm{e}}^{-1} = 1, \\ \infty & \text{else.} \end{cases} \tag{2.19}$$

By introducing

$$w = \frac{Fm}{|Fm|},$$

we can express F_{e}^{-1} in general as follows

$$F_{\mathrm{e}}^{-1} = Q\left(\eta w \otimes w + \theta w \otimes w^{\perp} + \frac{1}{\eta} w^{\perp} \otimes w^{\perp}\right) \tag{2.20}$$

for some $Q \in SO(2)$, $\eta, \theta \in \mathbb{R}$, $\eta \neq 0$. Using the identities $|F_{\mathrm{e}}^{-1} w|^2 = \eta^2$ and $|F_{\mathrm{e}}^{-1} w^{\perp}|^2 = \theta^2 + 1/\eta^2$, (2.19) can be re-written as

$$\bar{W}(F; \eta, \theta) = \begin{cases} \phi(F; \eta, \theta) & \text{if } (\eta, \theta) \in \mathbb{X}, \\ \infty & \text{else.} \end{cases} \tag{2.21}$$

Here

$$\phi(F; \eta, \theta) = \eta^2 \left(\frac{\mu}{2} + \frac{h}{2}|Fm|^2\right) + \frac{\mu}{2}\left(\frac{1}{\eta^2} + \theta^2\right) - \left(\mu + \frac{h}{2}\right) \tag{2.22}$$

and

$$\mathbb{X} = \left\{ (\eta, \theta) \in \mathbb{R}^2 : \left| \left(\eta w \otimes w + \theta w \otimes w^{\perp} + \frac{1}{\eta} w^{\perp} \otimes w^{\perp}\right) Fs \right| \le 1 \right\}. \tag{2.23}$$

If $F \neq \mathrm{Id}$, the set $\mathbb{X}$ is compact and ϕ is continuous, hence, if $\mathbb{X}$ is not empty, there will exist at least a F_{e} such that the minimum in (2.18) is attained. With these definitions, we can then give the following result.

Proposition 2.7 *If $\mathbb{X}$ is not empty, then $W_3(F)$ is finite and there holds*

$$W_2^{\mathrm{qc}}(F) \le W_3(F). \tag{2.24}$$

Proof Let $F_e \in \mathbb{R}^{2\times 2}$. From the definition of W_2 we have that

$$W_2(F) \le W_e(F_e) + W_1(F_e^{-1}F).$$

Taking the quasiconvex envelope on both sides (seen as a function of F, with fixed F_e) we obtain

$$W_2^{qc}(F) \le W_e(F_e) + W_1^{qc}(F_e^{-1}F)$$

for all F, and all F_e. Taking the minimum of both sides with respect to F_e proves the assertion. □

The energy $W_3(F)$ equals the average energy of a simple laminate whose definition, however, requires that one finds a global minimum of (2.21). In order to obtain a first order laminate which is simpler to compute and at the same time still retains the upper bound on W_2^{qc}, we restrict the minimization of (2.21), and hence of (2.18), to the matrices F_e^{-1} of the type

$$F_e^{-1} = Q\left(\eta w \otimes w + \frac{1}{\eta} w^\perp \otimes w^\perp\right) \tag{2.25}$$

for some $Q \in SO(2)$ and $\eta \neq 0$. As a result, by defining

$$W_3'(F) = \min_{\eta\in\mathbb{X}_0} \bar{W}'(F;\eta) \tag{2.26}$$

with $\bar{W}'(F;\eta) = \bar{W}(F;\eta,0)$ and

$$\mathbb{X}_0 = \left\{\eta \in \mathbb{R} : \left|\left(\eta w \otimes w + \frac{1}{\eta} w^\perp \otimes w^\perp\right) Fs\right| \le 1\right\}, \tag{2.27}$$

one easily checks the bound

$$W_3(F) \le W_3'(F).$$

Let $\eta_{opt} \in \mathbb{X}_0$ be a point where the minimum of (2.26) is attained. This means that if we set

$$F_e = \left(\frac{1}{\eta_{opt}} w \otimes w + \eta_{opt} w^\perp \otimes w^\perp\right) Q^T \tag{2.28}$$

for some $Q \in SO(2)$ and $F_p = F_e^{-1}F$, then it is

$$W_3'(F) = W_e(F_e) + W_1^{qc}(F_e^{-1}F). \tag{2.29}$$

Furthermore, by definition of $\mathbb{X}_0$ necessarily the two real solutions υ_1 and υ_2 of the equation

$$\upsilon^2 + 2\upsilon \frac{F_p m \cdot F_p s}{|F_p m|} + |F_p s|^2 - 1 = 0, \tag{2.30}$$

have opposite sign. Notice that the coefficients of (2.30) remain unchanged if we replace F_p with QF_p for any $Q \in SO(2)$.

Proposition 2.8 *If $\mathbb{X}_0$ is not empty then $W_3'(F)$ is finite and there holds*

$$W_3'(F) = \lambda W_2(F_1) + (1-\lambda) W_2(F_2), \tag{2.31}$$

where

$$F_i = F + \frac{\upsilon_i}{|F_p m|} Fm \otimes s \quad i = 1, 2, \tag{2.32}$$

and

$$\lambda = \frac{|\upsilon_2|}{|\upsilon_1| + |\upsilon_2|}. \tag{2.33}$$

Box 2 Construction of a first order laminate with energy bounding from above W_2^{qc}

DATA:	$m,\ s\ \in \mathbb{R}^2$ for $F_{\mathrm{p}} = \mathrm{Id} + \gamma s \otimes m$
INPUT:	$F \in \mathbb{R}^{2\times 2}$ with $\det F = 1$
COMPUTE:	$\mathbb{X}_0$ from (2.27)
	IF $\mathbb{X}_0 = \varnothing$ STOP 'F homogeneous phase and $\nu = \delta_F$'.
	$\eta_{\mathrm{opt}} \in \underset{\eta\in\mathbb{X}_0}{\arg\min} \left(\eta^2(\frac{\mu}{2} + \frac{h}{2}\lvert Fm\rvert^2) + \frac{\mu}{2\eta^2} - (\mu + \frac{h}{2})\right)$
SET:	$w = \dfrac{Fm}{\lvert Fm\rvert}$ and $G_p = (\eta_{\mathrm{opt}} w \otimes w + \dfrac{1}{\eta_{\mathrm{opt}}} w^{\perp} \otimes w^{\perp})F$
SOLVE:	quadratic equation $\upsilon^2 + 2\upsilon \dfrac{G_p m \cdot G_p s}{\lvert G_p m\rvert} + \lvert G_p s\rvert^2 - 1 = 0$ with two real solutions υ_1 and υ_2.
OUTPUT:	$\nu = \lambda\delta_{F_1} + (1-\lambda)\delta_{F_2}$
	for $\lambda = \dfrac{\lvert\upsilon_2\rvert}{\lvert\upsilon_1\rvert + \lvert\upsilon_2\rvert}$ and $F_i = F + \upsilon_i \dfrac{Fm}{\lvert G_p m\rvert} \otimes s$ for $i = 1, 2$

Proof Let $F_{\mathrm{p}} = F_{\mathrm{e}}^{-1} F$ with F_{e} as in (2.29). From Proposition 2.1, by definition of W_1^{qc} we have then that F_{p} is supported on the matrices

$$F_{pi} = F_{\mathrm{p}} + \upsilon_i \frac{F_{\mathrm{p}} m}{\lvert F_{\mathrm{p}} m\rvert} \otimes s \quad i = 1, 2 \tag{2.34}$$

with υ_1 and υ_2 solutions of (2.30). As a result, $W_1^{\mathrm{qc}}(F_{\mathrm{e}}^{-1} F)$ in (2.29) can be expressed as follows

$$\begin{aligned} W_1^{\mathrm{qc}}(F_{\mathrm{e}}^{-1} F) &= \lambda W_1(F_{p1}) + (1-\lambda) W_1(F_{p2}) \\ &= \lambda W_{\mathrm{p}}(\gamma(F_{p1})) + (1-\lambda) W_{\mathrm{p}}(\gamma(F_{p2})), \end{aligned} \tag{2.35}$$

with λ given by (2.33) and $\gamma(F) = Fm \cdot Fs$. Notice that by construction F_{pi} are such that $\det F_{pi} = 1$ and $\lvert F_{pi} s\rvert = 1$ for $i = 1, 2$. By replacing (2.35) into (2.29) we have

$$W_3'(F) = \lambda(W_{\mathrm{e}}(F_{\mathrm{e}}) + W_{\mathrm{p}}(\gamma(F_{p1}))) + (1-\lambda)(W_{\mathrm{e}}(F_{\mathrm{e}}) + W_{\mathrm{p}}(\gamma(F_{p2}))) \tag{2.36}$$

which yields (2.31) after observing that

$$W_2(F_i) = W_{\mathrm{e}}(F_{\mathrm{e}}) + W_{\mathrm{p}}(\gamma(F_{pi})) \quad i = 1, 2, \tag{2.37}$$

with $F_i = F_{\mathrm{e}} F_{pi}$ given by (2.32). □

Box 2 finally summarizes the algorithm for the construction of the laminate.

3 Numerical relaxation

The analytical results from the previous sections give several laminates with good energy, but there is no reason to expect them to be the optimal ones (and indeed they are not). We shall use them to determine numerically a locally optimal laminate. This means that we construct a numerical algorithm which optimizes locally each of the analytically proposed laminates. We check the final result for stability against increase in the lamination order; we shall see that in all cases laminates of order up to two, corresponding to the graph depicted in Fig. 3, are sufficient to achieve local stability. Therefore we shall formulate the algorithm only for second-order laminates, higher lamination order would bring heavier notation (as well as heavier computation, of course). The fact that second laminates are sufficient is also in agreement with previous numerical results from [9] using a clustering type global optimization algorithm.

We first fix the notation with the help of Fig. 3. Figure 3a illustrates the graph of the laminate, and Fig. 3b a sketch of the microstructure. The laminate has average F, and is supported on the four matrices F_{11}, F_{12},

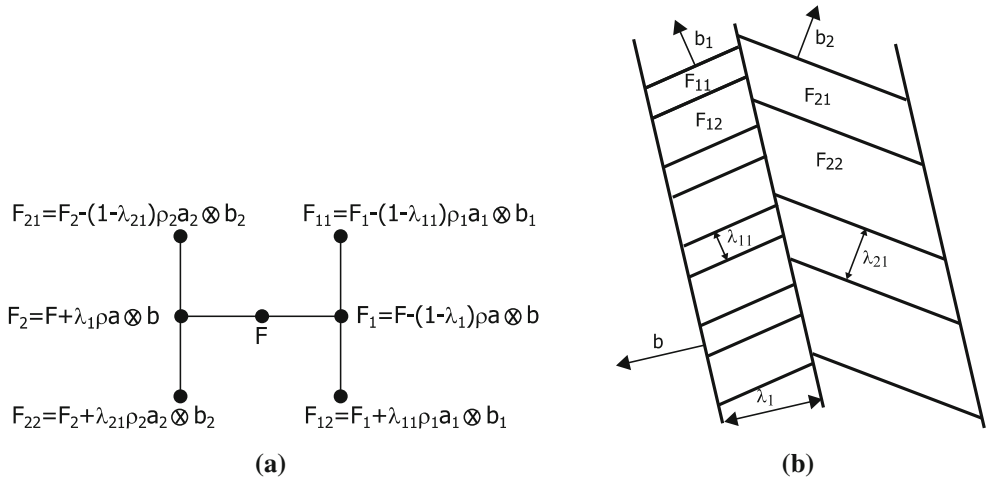


Fig. 3 **a** Graph of the second order laminate considered for the relaxation of (1.6) with **b** corresponding microstructure

F_{21} and F_{22} with volume fractions $\lambda_1\lambda_{11}$, $\lambda_1(1-\lambda_{11})$, $(1-\lambda_1)\lambda_{21}$ and $(1-\lambda_1)(1-\lambda_{21})$, respectively, for $\lambda_1,\ \lambda_{11},\ \lambda_{21} \in [0,\ 1]$. We express a generic rank-one matrix in $\mathbb{R}^{2\times 2}$ as

$$\rho a \otimes b, \tag{3.1}$$

with $a = (\cos\alpha,\ \sin\alpha)$ and $b = (\cos\beta,\ \sin\beta)$, for $\alpha,\ \beta,\ \rho \in \mathbb{R}$. The support of the laminate in Fig. 3 is then given by the matrices

$$\begin{aligned} F_{11} &= F_1 - (1-\lambda_{11})\rho_1 a_1 \otimes b_1, \quad F_{12} = F_1 + \lambda_{11}\rho_1 a_1 \otimes b_1, \\ F_{21} &= F_2 - (1-\lambda_{21})\rho_2 a_2 \otimes b_2, \quad F_{22} = F_2 + \lambda_{21}\rho_2 a_2 \otimes b_2, \end{aligned} \tag{3.2}$$

where

$$F_1 = F - (1-\lambda_1)\rho a \otimes b, \quad \text{and} \quad F_2 = F + \lambda_1 \rho a \otimes b \tag{3.3}$$

with $a_i = (\cos\alpha_i,\ \sin\alpha_i)$, $b_i = (\cos\beta_i,\ \sin\beta_i)$ for $\alpha_i,\ \beta_i,\ \rho_i \in \mathbb{R}$, $i = 1, 2$. The laminate is the measure

$$\nu = \lambda_1\lambda_{11}\delta_{F_{11}} + \lambda_1(1-\lambda_{11})\delta_{F_{12}} + (1-\lambda_1)\lambda_{21}\delta_{F_{21}} + (1-\lambda_1)(1-\lambda_{21})\delta_{F_{22}}. \tag{3.4}$$

If we denote by $q = (\alpha,\ \beta, \alpha_1, \beta_1, \alpha_2, \beta_2, \lambda_1, \lambda_{11}, \lambda_{21}, \rho, \rho_1, \rho_2)$ the degrees of freedom of ν, the corresponding energy is then equal to

$$\begin{aligned} E^{\mathrm{lc},2}(F; q) &= \langle \nu;\ W \rangle \\ &= \lambda_1\lambda_{11} W(F - (1-\lambda_1)\rho a \otimes b - (1-\lambda_{11})\rho_1 a_1 \otimes b_1) \\ &\quad + \lambda_1(1-\lambda_{11}) W(F - (1-\lambda_1)\rho a \otimes b + \lambda_{11}\rho_1 a_1 \otimes b_1) \\ &\quad + (1-\lambda_1)\lambda_{21} W(F + \lambda_1 \rho a \otimes b - (1-\lambda_{21})\rho_2 a_2 \otimes b_2) \\ &\quad + (1-\lambda_1)(1-\lambda_{21}) W(F + \lambda_1 \rho a \otimes b + \lambda_{21}\rho_2 a_2 \otimes b_2), \end{aligned} \tag{3.5}$$

with the microscopic energy $W(F)$ defined in (1.6). The best upper bound on the relaxation that can be obtained with second-order laminates is the second lamination-convex envelope of W, i.e.,

$$W^{\mathrm{lc},2}(F) = \min_{q \in \mathbb{S}} E^{\mathrm{lc},2}(F; q), \tag{3.6}$$

with the admissible domain $\mathbb{S}$ defined as

$$\mathbb{S} = \left\{ q \in \mathbb{R}^{12} : \begin{array}{l} \lambda_1, \lambda_{11}, \lambda_{21} \in [0,\ 1], \\ \det(F_{11}) > 0,\ \det(F_{12}) > 0,\ \det(F_{21}) > 0,\ \det(F_{22}) > 0 \end{array} \right\}. \tag{3.7}$$

Remark 3.1 (i) Since $E^{\mathrm{lc},2}(F;q)$ is continuous, $E^{\mathrm{lc},2}(F;q)\to\infty$ as $\det F_i\to 0$, and W grows quadratically at infinity, then (3.6) admits at least one solution.
(ii) The first Piola–Kirchhoff stress tensor of the relaxed energy can correspondingly be determined by averaging of the stress in each phase F_i. If $\bar{q}$ denotes an optimal solution that gives $W^{\mathrm{lc},2}(F)$, that is,

$$W^{\mathrm{lc},2}(F)=E^{\mathrm{lc},2}(F,\bar{q}(F)), \tag{3.8}$$

by taking the derivative with respect to F and using the chain rule we obtain

$$DW^{\mathrm{lc},2}=\frac{\partial E^{\mathrm{lc},2}}{\partial F}+\frac{\partial E^{\mathrm{lc},2}}{\partial q}:\frac{\partial q}{\partial F}. \tag{3.9}$$

Since $\bar{q}(F)$ is an optimal solution to (3.6), if $\lambda_1,\ \lambda_{11},\ \lambda_{21}\in\,]0,\ 1[$ then there holds

$$\frac{\partial E^{\mathrm{lc},2}}{\partial q}(F,\bar{q}(F))=0, \tag{3.10}$$

and (3.9) together with (3.5) yields

$$\begin{aligned}DW^{\mathrm{lc},2}(F)=\lambda_1\lambda_{11}DW(F_{11})+\lambda_1(1-\lambda_{11})DW(F_{12})\\ +(1-\lambda_1)\lambda_{21}DW(F_{21})+(1-\lambda_1)(1-\lambda_{21})DW(F_{22}).\end{aligned} \tag{3.11}$$

By direct inspection, (3.11) is then extended also to $\lambda_1,\ \lambda_{11},\ \lambda_{21}\in[0,\ 1]$.

The solution of (3.6) is computationally very expensive, for most of the algorithms require meaningful and representative sampling of the space $\mathbb{R}^{12}$ in order to locate the best choice where then one can start the local minimization [9,27,39]. We propose, instead, to perform two local minimizations assuming as initial guess the two laminates obtained in Sects. 2.2 and 2.3. We then determine local stability of either of the two local minima, with respect to increase of the order of lamination. Precisely, for every F_i in the support of the considered laminates, we verify the stability condition

$$\min_{a,b\in\mathbb{R}^2}\{W(F_i+a\otimes b)+W(F_i-a\otimes b)-2W(F_i)\}\geq 0. \tag{3.12}$$

In practice, only small values of a and b are considered, corresponding to a local check on the rank-one convexity of W at F_i. If condition (3.12) fails, then one needs to refine the laminate. In this case, if $a\otimes b$ denotes a rank-one matrix that violates (3.12), we consider the laminate obtained by splitting F_i along $a\otimes b$ with volume fraction equal to 0.5 and use this as initial guess for the local minimization of the energy corresponding to the new resulting laminate.

4 Optimality of the relaxation via polyaffine lower bounds

We now turn to checking optimality of the relaxation we obtained in the previous sections. We do this by using polyaffine functions, which are a simple but yet rather general class of quasiconvex functions [33, Theorem 5.1]. Following Ball [5] we call a function $\ell:\mathbb{R}^{2\times 2}\to\mathbb{R}$ polyaffine if it is an affine function of A and $\det A$, i.e., if

$$\ell(A)=\xi+H:A+\zeta\det A, \tag{4.1}$$

with $\xi,\ \zeta\in\mathbb{R}$, $H\in\mathbb{R}^{2\times 2}$ and $H:A=\mathrm{Tr}(A^TH)$. Consider a polyaffine function ℓ which bounds from below W, in the sense that

$$\ell(A)\leq W(A)\quad\text{for all}\quad A\in\mathbb{R}^{2\times 2}. \tag{4.2}$$

Then, since A and $\det A$ are null Lagrangians [5,20], for any $\varphi\in W_0^{1,\infty}((0,1)^2;\mathbb{R}^2)$ one has

$$\ell(A)=\int_{(0,1)^2}\ell(A)\mathrm{d}x=\int_{(0,1)^2}\ell(A+\nabla\varphi)\mathrm{d}x\leq\int_{(0,1)^2}W(A+\nabla\varphi)\mathrm{d}x,$$

and taking the infimum over all test functions φ one easily sees that (4.2) implies

$$\ell(A)\leq W^{\mathrm{qc}}(A)\quad\text{for all}\quad A\in\mathbb{R}^{2\times 2}. \tag{4.3}$$

Except for some degenerate situations, there is no single ℓ which gives a good bound for all possible A. However, in many cases of interest one can determine, for each given $F \in \mathbb{R}^{2\times 2}$, a polyaffine function ℓ which obeys (4.2) and such that it gives the optimal bound $\ell(F) \le W^{\mathrm{qc}}(F)$. We shall show that in the situation of interest here this is indeed the case for most matrices, up to a small numerical error.

Consider some matrix $F \in \mathbb{R}^{2\times 2}$. In the previous sections we have constructed a laminate giving a good bound from above on $W^{\mathrm{lc},k}(F)$. For any polyaffine function ℓ which obeys (4.2), by (4.3) we have

$$\ell(F) \le W^{\mathrm{qc}}(F) \le W^{\mathrm{lc},k}(F), \quad \text{for all} \quad k \in \mathbb{N}. \tag{4.4}$$

(In practice we deal with $k = 1$ or 2). If we can construct such a function, with additionally the property $\ell(F) = W^{\mathrm{lc},k}(F)$ for some k, then equality holds throughout and we have determined the relaxation at F. If instead we only achieve $\ell(F) < W^{\mathrm{lc},k}(F)$, then (4.4) gives nevertheless an upper and a lower bound on the relaxation, and in particular we know that the remaining error is controlled by $W^{\mathrm{lc},k}(F) - \ell(F)$. In the current situation this error will turn out to be either zero, or very small.

Polyaffine functions, as well as the more general concept of polyconvex functions, are a canonical method to obtain lower bounds on a relaxation. Numerically, an efficient algorithm for the determination of polyconvex envelopes was proposed in [8]. It is based on building a continuous piecewise multilinear approximation to the polyconvex envelope and considering the characterization of the polyconvex envelope using the Carathéodory theorem [20,41]. This permitted one to work at the same time on all matrices, without the need to treat each F individually; however, the results in [8] are based on a discretization in matrix space, and hence are affected by mesh-size discretization errors. This has lead, for example in [9], to lower bounds which are somewhat higher than the upper bounds. Our approach eliminates this difficulty, since it is mesh-free.

Given a matrix F, the search for the best polyaffine lower bound is, in principle, a finite-dimensional optimization problem. The space of all polyaffine functions is six dimensional, and can be parameterized by (ξ, H, ζ). For each H and ζ, the highest polyaffine function which obeys (4.2) is obtained by taking

$$\xi = \inf_{A\in\mathbb{R}^{2\times 2}} W(A) - (H : A + \zeta \det A).$$

Having defined ξ this way, one seeks H and ζ which maximize $\ell(F)$. In other words, we obtain a nine-dimensional minimax problem, which is in practice not easy to solve efficiently.

There are however, additional conditions that permit, in some cases, to greatly reduce the space in which one searches. These can be understood by analogy to the case of convexity: taking a convex envelope in one dimension amounts to a double-tangent construction, and one uses a straight line which has to agree *up to the gradient* with the original function at two points. Reformulating this condition in the polyaffine setting, we obtain the following result.

Lemma 4.1 *Let $F \in \mathbb{R}^{2\times 2}$, and assume that*

$$\nu = \sum_{i=1}^{k} \lambda_i \delta_{F_i}, \qquad \textit{with} \;\; \lambda_i > 0, \;\; \sum_{i=1}^{k} \lambda_i = 1, \;\; \sum_{i=1}^{k} \lambda_i F_i = F_0$$

is a laminate such that

$$W^{\mathrm{lc},k}(F) = \sum_{i=1}^{k} \lambda_i W(F_i). \tag{4.5}$$

If there is a polyaffine function ℓ such that $\ell \le W$ [in the sense of (4.3)] and

$$\ell(F) = W^{\mathrm{lc},k}(F), \tag{4.6}$$

then necessarily

$$\ell(F_i) = W(F_i) \qquad i = 1, \ldots, k. \tag{4.7}$$

If additionally W is differentiable at $F_1, \ldots, F_k$, then

$$D\ell(F_i) = DW(F_i) \qquad i = 1, \ldots, k. \tag{4.8}$$

Proof The key fact is that polyaffine functions are affine along laminates, hence

$$\ell(F) = \sum_{i=1}^{k} \lambda_i \ell(F_i) \leq \sum_{i=1}^{k} \lambda_i W(F_i).$$

If one or more of the inequalities were strict, then—since $\lambda_i > 0$—comparing with (4.5) we would get $\ell(F) < W^{\mathrm{lc},k}(F)$, against the assumption. Therefore $\ell(F_i) = W(F_i)$ for all i, and the function $A \mapsto W(A) - \ell(A)$ has absolute minima at the points F_i. If it is differentiable there, then necessarily its gradient must vanish. This concludes the proof. □

Of course, in general there is no guarantee that such a function ℓ exists, and there is no guarantee that the best laminate we have found actually gives the relaxation.

Conditions (4.7) and (4.8) will be used to verify the existence of the polyaffine function ℓ of Lemma 4.1; if such a function does not exist, we shall nevertheless use those conditions to determine a good candidate for ℓ. The way we construct ℓ will be different according to the type of laminate, so that the following cases need to be distinguished:

(i) ν is a homogeneous phase;
(ii) ν is a first order laminate;
(iii) ν is a second order laminate.

For the case (iii) we describe below the procedure only when the laminate is of the type shown in Fig. 2.

We shall therefore first construct ℓ meeting as close as possible the conditions (4.7) and (4.8), and afterwards determine

$$m = \inf_{A \in \mathbb{R}^{2\times 2}} W(A) - \ell(A). \tag{4.9}$$

If $m \geq 0$, then equality holds throughout and we are done (the case $m > 0$ is impossible, and its occurrence would indicate numerical or algorithmical errors). If, on the contrary, $m < 0$, then the function $\bar{\ell} = \ell + m$ gives a lower bound to W^{qc}, i.e., $\ell(F) + m \leq W^{\mathrm{qc}}(F)$.

Homogeneous phase: Conditions (4.7) and (4.8) become

$$\ell(F) = W(F), \quad D\ell(F) = DW(F) \tag{4.10}$$

and yield a system of five equations in the six unknowns: ξ, H, and ζ. By reparameterizing ℓ according to

$$\ell(A) = \xi' + H' : (A - F) + \zeta' \det(A - F)$$

one finds

$$\xi' = W(F) \quad \text{and} \quad H' = DW(F),$$

consequently, the polyaffine function

$$\ell(A) = W(F) + DW(F) : (A - F) + \zeta' \det(A - F)$$

obeys (4.7) and (4.8) for any $\zeta' \in \mathbb{R}$. In this case, therefore, the problem reduces to verify the existence of some $\zeta' \in \mathbb{R}$ such that the global condition $m \geq 0$ is met.

First-order laminate: To fix notation, assume that the optimal first-order laminate has the form $\nu = \lambda \delta_{F_1} + (1 - \lambda)\delta_{F_2}$, with

$$F_1 = F - (1 - \lambda)\rho a \otimes b \quad \text{and} \quad F_2 = F + \lambda \rho a \otimes b, \tag{4.11}$$

with $\lambda \in (0, 1)$, $a = (\cos\alpha,\ \sin\alpha)$, and $b = (\cos\beta,\ \sin\beta)$. Optimality implies that this is a stationary point for $E^{\mathrm{lc},1}(F; q) = \langle \nu;\ W \rangle$, with $q = (\alpha,\ \beta,\ \lambda,\ \rho)$. In this case, the conditions (4.7) and (4.8) read

$$\begin{aligned} &\ell(F_1) = W(F_1), \qquad \ell(F_2) = W(F_2) \\ &D\ell(F_1) = DW(F_1), \quad D\ell(F_2) = DW(F_2) \end{aligned} \tag{4.12}$$

which yield the following system of 10 equations in the 6 unknowns ξ, H, and ζ:

$$\begin{aligned}
\xi + H\colon F_1 + \zeta \det F_1 &= W(F_1)\\
\xi + H\colon F_2 + \zeta \det F_2 &= W(F_2)\\
H + \zeta \operatorname{cof} F_1 &= DW(F_1)\\
H + \zeta \operatorname{cof} F_2 &= DW(F_2).
\end{aligned} \tag{4.13}$$

This linear system is, from the dimensional viewpoint, overdetermined. However, the coefficients are not all independent, since the laminate we are considering is optimal. The fact that $E^{\mathrm{lc},1}$ is stationary gives the following conditions:

$$\begin{aligned}
\partial_\alpha E^{\mathrm{lc},1} &= \lambda(1-\lambda)\rho(a^\perp \otimes b)\colon (-DW(F_1) + DW(F_2)) = 0\\
\partial_\beta E^{\mathrm{lc},1} &= \lambda(1-\lambda)\rho(a \otimes b^\perp)\colon (-DW(F_1) + DW(F_2)) = 0\\
\partial_\rho E^{\mathrm{lc},1} &= \lambda(1-\lambda)(a \otimes b)\colon (-DW(F_1) + DW(F_2)) = 0\\
\partial_\lambda E^{\mathrm{lc},1} &= W(F_1) - W(F_2) + \rho(a \otimes b)\colon (\lambda DW(F_1) + (1-\lambda)DW(F_2)) = 0.
\end{aligned} \tag{4.14}$$

Here $a^\perp = (-\sin\alpha,\ \cos\alpha)$ and $b^\perp = (-\sin\beta,\ \cos\beta)$. We can then state the following result.

Proposition 4.2 *Given F, F_1 and F_2 as in (4.11) with some $\lambda \in (0,1)$, $\rho \in \mathbb{R}$, $a, b \in \mathbb{R}^2$, if the conditions (4.14) are met then the system (4.13) has one and only one solution.*

Proof Replacing the first pair of equations with their difference and their λ-weighted average, and the same for the second pair, one sees that the system (4.13) is equivalent to

$$\begin{aligned}
H\colon (F_1 - F_2) + \zeta(\det F_1 - \det F_2) &= W(F_1) - W(F_2)\\
\xi + H\colon F + \zeta \det F &= \lambda W(F_1) + (1-\lambda)W(F_2)\\
H + \zeta \operatorname{cof} F &= \lambda DW(F_1) + (1-\lambda)DW(F_2)\\
\zeta(\operatorname{cof} F_1 - \operatorname{cof} F_2) &= DW(F_1) - DW(F_2).
\end{aligned} \tag{4.15}$$

The first three equations of (4.14) imply that $DW(F_1) - DW(F_2)$ is parallel to $a^\perp \otimes b^\perp$. The same is true for the left-hand side of the last equation $(4.15)_4$. Indeed, the linearity of cof as a linear map on $\mathbb{R}^{2\times 2}$ together with (4.11) imply

$$\operatorname{cof} F_1 - \operatorname{cof} F_2 = \operatorname{cof}(F_1 - F_2) = -\rho a^\perp \otimes b^\perp.$$

Therefore $(4.15)_4$ can be solved uniquely with respect to ζ. Then $(4.15)_3$ yields a unique solution for H, and $(4.15)_2$ for ξ.

It remains to be shown that these three equations, and the last remaining of (4.14), imply $(4.15)_1$. We first observe that

$$\det F_1 - \det F_2 = \operatorname{cof} F : (F_1 - F_2)$$

hence the left-hand side of $(4.15)_1$ equals the left-hand side of $(4.15)_3$ multiplied by $F_1 - F_2 = -\rho a \otimes b$. The same is true for the corresponding right-hand sides, by $(4.14)_4$. This concludes the proof. □

Second-order laminate: Given an optimal double laminate of the type shown in Fig. 2, the conditions (4.7) and (4.8) yield a system of 15 equations in the 6 unknowns: ξ, H, and ζ, as follows

$$\begin{aligned}
\xi + H\colon F_1 + \zeta \det F_1 &= W(F_1)\\
\xi + H\colon F_{21} + \zeta \det F_{21} &= W(F_{21})\\
\xi + H\colon F_{22} + \zeta \det F_{22} &= W(F_{22})\\
H + \zeta \operatorname{cof} F_1 &= DW(F_1)\\
H + \zeta \operatorname{cof} F_{21} &= DW(F_{21})\\
H + \zeta \operatorname{cof} F_{22} &= DW(F_{22}),
\end{aligned} \tag{4.16}$$

which can be transformed into the equivalent system

$$\begin{aligned} H:\,(F_1-F_2)+\zeta(\det F_1-\det F_2) &= W(F_1)-(\lambda_{21}W(F_{21})+(1-\lambda_{21})W(F_{22}))\\ \xi+H:\,F_2+\zeta\det F_2 &= \lambda_{21}W(F_{21})+(1-\lambda_{21})W(F_{22})\\ H+\zeta\,\mathrm{cof}F_2 &= \lambda_{21}DW(F_{21})+(1-\lambda_{21})DW(F_{22})\\ \zeta\,\mathrm{cof}(F_1-F_2) &= DW(F_1)-(\lambda_{21}DW(F_{21})+(1-\lambda_{21})DW(F_{22}))\\ \xi+H:\,F_{22}+\zeta\det F_{22} &= W(F_{22})\\ H+\zeta\,\mathrm{cof}F_{22} &= DW(F_{22}), \end{aligned} \tag{4.17}$$

with $F_2=\lambda_{21}F_{21}+(1-\lambda_{21})F_{22}$. Using the optimality conditions $\partial_q E^{\mathrm{lc},2}=0$ and similar arguments as in the previous case, one can show that the Eqs. $(4.17)_2$–$(4.17)_4$ define uniquely ℓ. In the following numerical examples, we will use the polyaffine function ℓ so defined to check condition (4.9).

5 Numerical examples

We shall now discuss concrete application of the algorithm developed in the previous sections to determine the relaxation of the energy W defined in (1.6) on selected macroscopic deformation gradients F. In particular, we shall focus on the case that F is a simple shear deformation and a biaxial deformation. The algorithm is summarized in Box 3 and considers the relaxation up to a complete laminate of order two.

We take material constants as in [9]: $\mu=1.0\times10^4$MPa, $\kappa=1.5\times10^4$ MPa, $h=1.0\times10^3$ MPa and $\tau_{\mathrm{cr}}=10$ MPa. We fix a reference system in $\mathbb{R}^2$, and characterize the orientation of the slip system (s,m) through an angle ψ, by taking $s=(\cos\psi,\,\sin\psi)$ and $m=(-\sin\psi,\,\cos\psi)$. For the local minimization of (3.5), we have adopted the SQP algorithm implemented in the release 7.0 ($R14$) of MatLab and described in [42]. For more details on SQP see also [36]. All energy values below are expressed in MPa.

5.1 Simple shear

We consider macroscopic deformation gradients F of the type

$$F=\mathrm{Id}+\xi r\otimes r^{\perp}.$$

Here $\xi\in\mathbb{R}$ is the shear strain, $r=(\cos\theta,\,\sin\theta)$, $r^{\perp}=(-\sin\theta,\,\cos\theta)$ for $\theta\in[0,\,2\pi)$; following [9] we use here the slip system $(s,\,m)$ defined by $\psi=3\pi/4$. We start from the case $\theta=0$, that is $r=(1,0)$. This

Box 3 Relaxation algorithm for (1.6)

DATA:	$m,\,s\in\mathbb{R}^2$ for $F_{\mathrm{p}}=\mathrm{Id}+\gamma s\otimes m,\ tol=1e-6.$
INPUT:	$F\in\mathbb{R}^{2\times2}$ with $\det F=1$.
COMPUTE:	ν_i from algorithm in Box i for i=1,2.
FIND:	optimal ν from (3.6) using initial guess $\nu_0=\nu_i$ for $i=1,2$. WHILE (3.12) fails FIND $a\otimes b$ that violates (3.12) at the phase F_i SELECT new laminate ν_0 by splitting phase F_i along $a\otimes b$ SOLVE (3.6) with initial guess ν_0
SET:	$W^{\mathrm{lc},2}(F)=\langle\nu;W\rangle$
COMPUTE:	polyaffine ℓ from (4.7) and (4.8), and $m=\min_{A\in\mathbb{R}^{2\times2}}W(A)-\ell(A)$
OUTPUT:	IF $m>-tol$ THEN: $\ell(F)=W^{\mathrm{pc}}(F)=W^{\mathrm{qc}}(F)=W^{\mathrm{lc},2}(F)$ ELSE: $\ell(F)+m\le W^{\mathrm{pc}}(F)\le W^{\mathrm{qc}}(F)\le W^{\mathrm{lc},2}(F)$

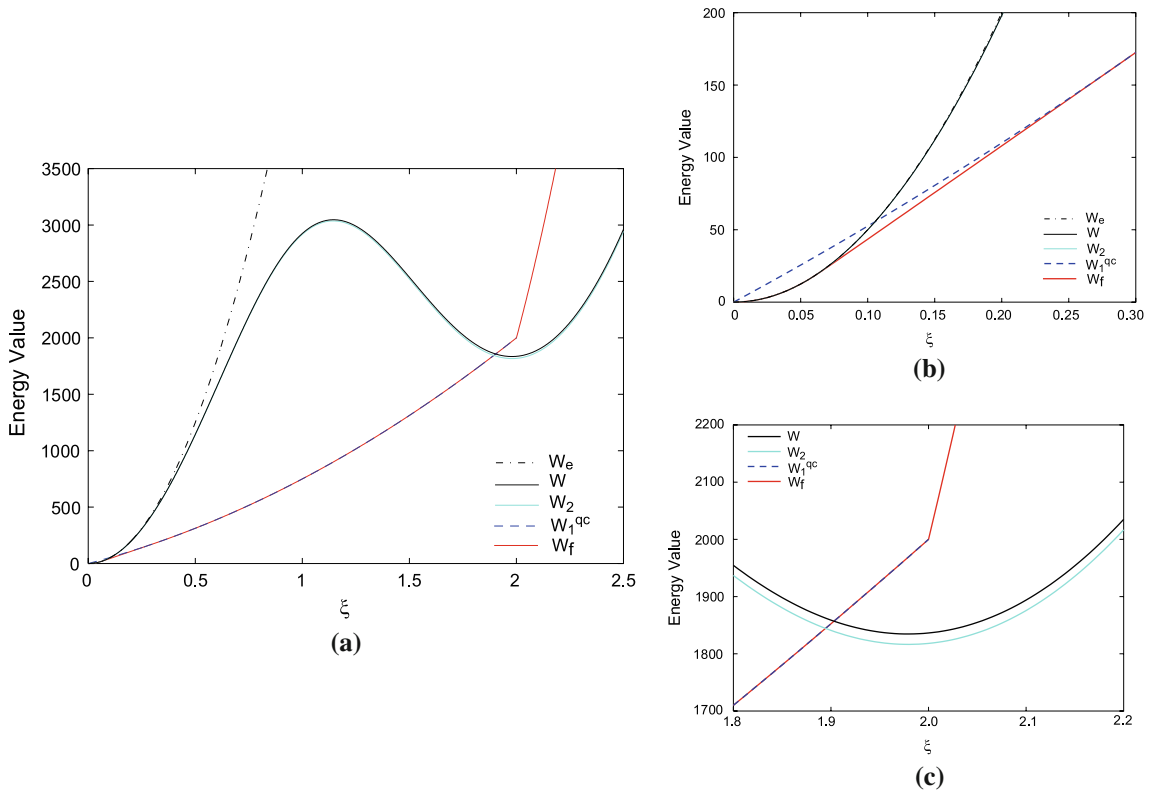


Fig. 4 Energy densities before numerical relaxation on the line $F = \mathrm{Id} + \xi r \otimes r^{\perp}$ and with $r = (1, 0)$ (see Sect. 5.1). In **a** we plot, from the higher to the lower curve at the central region $\xi \sim 1$: the elastic energy W_{e} defined in (1.3); the condensed energy W (from 1.6) and its approximation W_2 with $\tau_{\mathrm{cr}} = 0$ (from 2.5); the relaxation of the rigid-plastic energy W_1^{qc} (from 2.2) and the optimal lamination energy W_{f} (from 2.15). The two pairs (W, W_2) and $(W_1^{\mathrm{qc}}, W_{\mathrm{f}})$ are undistinguishable in this scale, except for the fact that W_1^{qc} is only defined up to $\xi = 2$. We also report enlargements of the region around $\xi = 0$ (**b**) and $\xi = 2$ (**c**)

is exactly the problem simulated in [29] where a semianalytical formula for the relaxation over first order laminates is developed.

Figure 4a reports the value of several of the energies determined analytically in Sect. 2 as functions of ξ, i.e., along a one-dimensional, rank-one section of their definition domain $\mathbb{R}^{2\times 2}$. The condensed energy W (see Eq. 1.6) is apparently not convex along this rank-one direction. The elastic energy W_{e} (see Eq. 1.3) is convex but significantly higher than W, except for small values of ξ. The analytic relaxation had been obtained in the case $\tau_{\mathrm{cr}} = 0$. Therefore we report W_2 (defined as W for $\tau_{\mathrm{cr}} = 0$; obviously $W_2 \le W$), which is seen to be very close to W, and barely distinguishable from it on this scale. Further, we report the relaxation with constrained elasticity W_1^{qc} (see Eq. 2.2) and the value $W_{\mathrm{f}}(F)$ of the energy of the second order laminate constructed in Sect. 2.2, see (2.15). From (2.6) and definition of W_{f}, it follows also $W_1^{\mathrm{qc}}(F) \ge W_{\mathrm{f}}(F)$ and $W_{\mathrm{e}}(F) \ge W_{\mathrm{f}}(F)$; both inequalities are also apparent in Fig. 4b. For low values of ξ, we observe in Fig. 4b that W_{f} is indistinguishable from W_{e}. This corresponds to the fact that a purely elastic deformation is stable, no microstructure and no plastic deformation are expected. As ξ increases, the evaluation of the convex envelope in $f(\cdot; b)$ becomes nontrivial (i.e., the two parabolas $W_1^{\mathrm{qc}}(F + xa \otimes b)$ and $W_{\mathrm{e}}(F + xa \otimes b)$, which one must consider to evaluate $W_{\mathrm{f}}(F)$, intersect each other as in Fig. 1). As a result, $W_{\mathrm{f}}(F) < W_1^{\mathrm{qc}}(F)$ and the laminate is of second order. With increasing ξ the laminate becomes then of first order, and $W_{\mathrm{f}}(F) = W_1^{\mathrm{qc}}(F)$ (see Fig. 4b) with both the phases plastic for $\xi \le 2$. In this case $W_{\mathrm{f}}(F) = W_1^{\mathrm{qc}}(F)$, since the parabola $W_1^{\mathrm{qc}}(F + xa \otimes b)$ is below $W_{\mathrm{e}}(F + xa \otimes b)$. For $\xi \ge 2$ the condition $|Fs| \le 1$, needed for $W_1^{\mathrm{qc}}(F)$ to be finite (see Eq. 2.2), is violated, and one obtains again a second-order laminate between the elastic phase and the plastic one. In this case, the elastic phase provides the major contribution to $W_{\mathrm{f}}(F)$ and determines the change of slope (see Fig. 4c). Numerical optimization has been performed, starting from the above laminates, as discussed in Sect. 3. For any given ξ we denote by ν^{ana} the best laminate constructed semianalytically as above, and by $W^{\mathrm{ana}} = \langle \nu^{\mathrm{ana}}, W \rangle$ the estimate

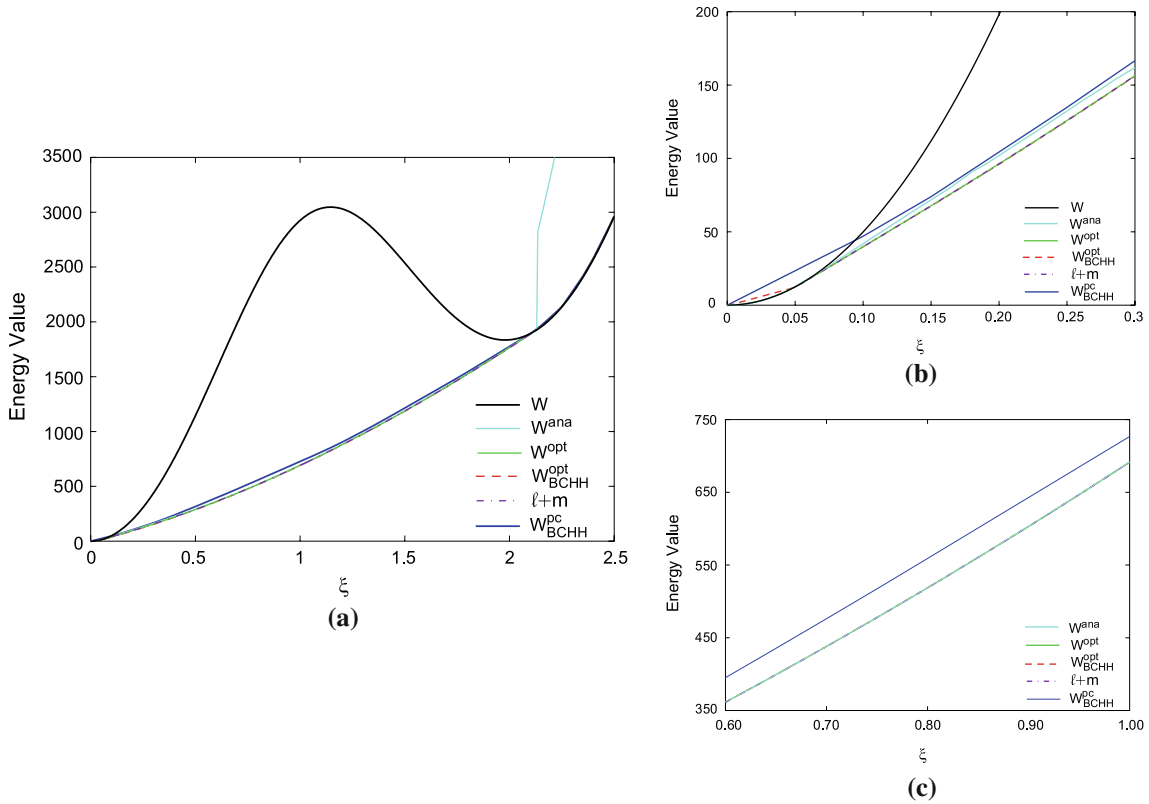


Fig. 5 Condensed energy W and estimates for its relaxation, for the same strains as Fig. 4. We report the best upper bound obtained with the analytical lamination $W^{\text{ana}} = \langle \nu^{\text{ana}}, W \rangle$, the upper bound after numerical optimization $W^{\text{opt}} = \langle \nu, W \rangle$, and the lower bound $\ell + m$. For comparison we also report the upper bound $W^{\text{opt}}_{\text{BCHH}}$ and the lower bound $W^{\text{pc}}_{\text{BCHH}}$ from [9]. In **a** we show the same domain as Fig. 4, whereas **b** and **c** show blow-ups of the region at small ξ and of the region around $\xi = 1$

on the energy it produces. The optimal laminate after numerical local minimization of (3.5) is denoted by ν, and the corresponding energy by $W^{\text{opt}} = \langle \nu,\ W \rangle \geq W^{\text{lc},2}$. Both curves are illustrated in Fig. 5a with details of the diagram around $\xi = 0$ and $\xi = 1$ in Fig. 5b, c, respectively. Both the figures show that the two curves are very close for the values of ξ where laminates are the stable phases, with a discontinuity at $\xi \simeq 2.13$ where the homogeneous phase becomes the stable phase. For $\xi < 2.13$ the semianalytical solution provides therefore a good approximation of the effective energy. Also, this Figure shows a very good quantitative agreement for the values of W^{opt} with those in [9] obtained using a global optimization algorithm, requiring consequently a significantly higher numerical effort (see also [10]).

We now turn to the optimality, which has been verified using the procedure discussed in Sect. 4. Results are also included in Fig. 5; the resulting lower bound $\ell + m$ turns out to be indistinguishable from the upper bound W^{opt} on this scale (see below for a finer analysis of the remaining difference). We also report the approximation of the polyconvex envelope realized in [9] with the procedure described in [8] (denoted by $W^{\text{pc}}_{\text{BCHH}}$). Figure 5c shows that in some regions this becomes somewhat larger than the upper bound, a fact already noticed in [9], and attributed to the discretization in the matrix space. Our method is free from such discretizations, and free from this difficulty. For instance, for $\xi = 0.10$ we have $F = \left(\begin{smallmatrix} 1 & 0.10 \\ 0 & 1 \end{smallmatrix}\right)$, $W(F) = 49.920398$, and we find the following optimal double laminate

$$F_{11} = \begin{pmatrix} 1.000268 & 0.076068 \\ -0.021716 & 0.997612 \end{pmatrix} \quad F_{12} = \begin{pmatrix} 1.180307 & -0.049463 \\ 0.205408 & 0.839252 \end{pmatrix}$$

$$F_2 = \begin{pmatrix} 0.829708 & 0.314685 \\ -0.125711 & 1.158482 \end{pmatrix}$$

$$\lambda_1 = 0.198369 \qquad \lambda_{11} = 0.767415$$

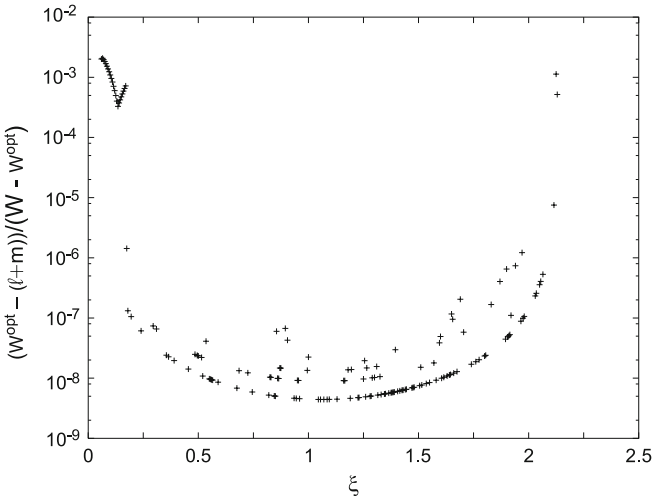


Fig. 6 Relative uncertainty on the relaxation $(W^{\mathrm{opt}} - (\ell(F) + m))/(W - W^{\mathrm{opt}})$ in logarithmic scale, on the same domain as Figs. 4 and 5

which gives $\ell(F) + m = 39.792579 \leq W^{\mathrm{qc}}(F) \leq \langle \nu, W \rangle = 39.803629$ with $\ell + m \leq W$ everywhere. This in turn means that we obtain the following two-sided bound $\ell(F) + m \leq W^{\mathrm{qc}}(F) \leq W^{\mathrm{lc},2}(F) \leq \langle \nu, W \rangle$, or that we have determined $W^{\mathrm{qc}}(F)$ up to an error of about 10^{-2}, which is three orders of magnitude smaller than the difference between the relaxed and the unrelaxed energy, $W^{\mathrm{opt}} - W \sim 10$. The same estimate applies of course to the rank-one convex and polyconvex envelopes of W [20,22]. The result of this analysis is reported in Fig. 6 for all values of ξ. We report there, in a logarithmic scale, the relative error on the relaxation, defined as the difference between the upper and lower bounds on $W^{\mathrm{qc}}(F)$ scaled by the difference between the unrelaxed and the relaxed energy.

Figure 8 shows the components of the Kirchhoff stress tensor $\tau = FP$ with P the first Piola stress tensor, and in particular that the two estimates for the Kirchhoff stress tensor obtained from our two bounds to the energy, namely, $P' = D\langle \nu, W \rangle$ and $P'' = D\ell$ are indistinguishable. For the component τ_{12} our results have also been compared with those of [9]. The little difference seen between the energies in Fig. 5 shows up more prominently on the stress field component.

Figure 7 displays the optimal laminates also for other values of ξ together with the corresponding values of $\langle \nu, W \rangle$ and $\ell + m$ and Fig. 9 depicts the value of the volume fractions λ_1 and λ_{11}. Figure 9 completely describes the volume fractions since $\lambda_2 = 1 - \lambda_1$ (and this branch is not decomposed further), and $\lambda_{12} = 1 - \lambda_{11}$. Initially, the material is in a homogeneous elastic state. Then an elastic state and a mixture of two opposite-slip plastic states appears. The volume fraction of the elastic phase starts at 100% and then decreases continuously until it vanishes at a shear $\xi = 0.170$. Both plastic phases then progress with slowly varying volume fractions until the homogeneous phase F is stable starting from $\xi = 2.135$. For the values of ξ such that the computed optimal laminate is a simple laminate, we also verify that the two phases are to a very good approximation plastic with opposite slip γ (see Eq. 1.7). This fact was assumed a priori for the approximate relaxation carried out in [29]; our results justify this assumption.

Finally, Fig. 10 presents a diagram of the different type of optimal laminates for $\theta \in [0,\ \pi]$ and $\xi \in [0,\ 2.5]$. In this case the computed optimal laminate yielding the effective energy is different according to the orientation of the shear. For instance, assuming $\theta = 5\pi/36$, for $\xi \in [0.09,\ 0.20]$ the relaxed energy is realized by a simple laminate with mixture of an elastic and plastic phase. By increasing ξ, first both phases are plastic with opposite value of the slip γ (see Eq. 1.7) and then a stable homogeneous plastic phase occurs. Table 1 reports the values of $\langle \nu,\ W \rangle$ and $\ell + m$ for $\theta = 3\pi/4$ and $\theta = \pi$ and some representative values of ξ. When $\theta = \pi$ we note that there are values of ξ such that the computed optimal laminate is a full double laminate with one elastic phase. This laminate presents a good match between upper and lower bound. As a general remark, however, it must be recalled that there might also exist other laminates yielding the same value of the energy, since in general one cannot ensure the uniqueness. The consideration of a laminate will finally depend on how well the corresponding two bounds $\langle \nu,\ W \rangle$ and $\ell(F) + m$ agree each other, by accounting also for the observations expressed in Sect. 4.

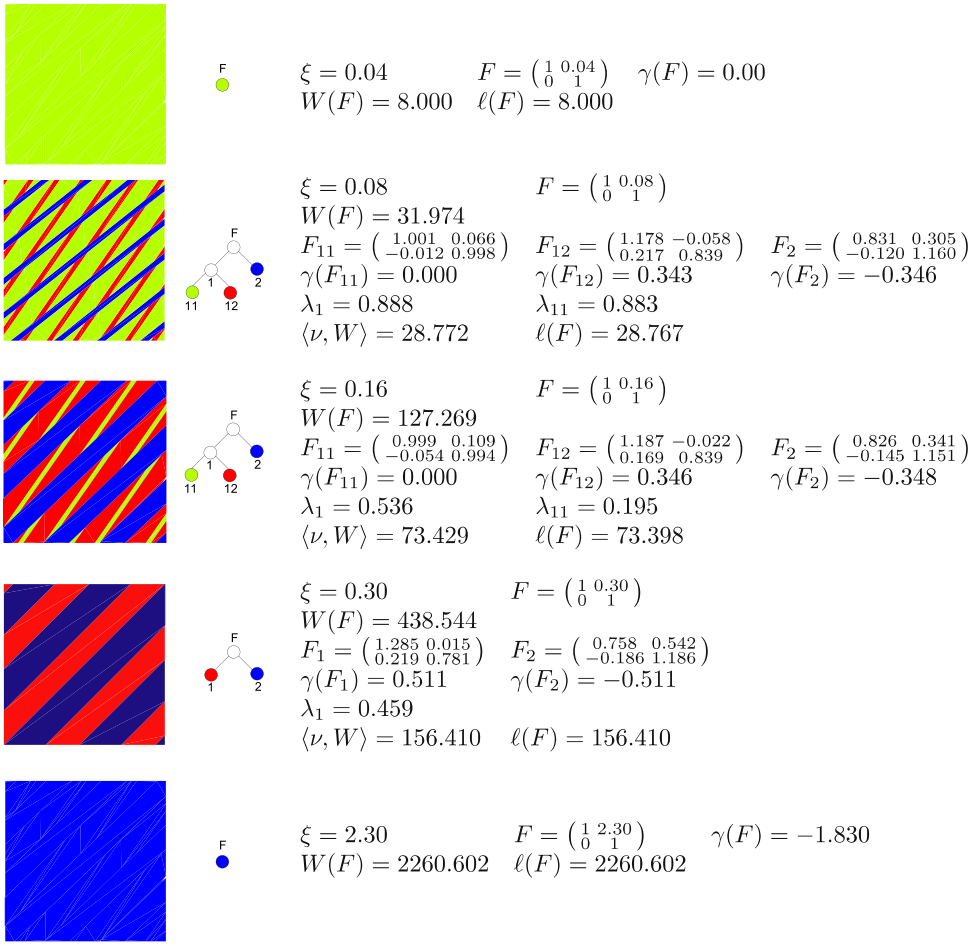


Fig. 7 Optimal laminates for different values of ξ and for $\theta = 0$, for the relaxation shown in Fig. 5

5.2 Biaxial deformation

In this example we consider the relaxation of W when the macroscopic deformation gradient F is a biaxial deformation of the type

$$F = \begin{pmatrix} \exp(\xi) & 0 \\ 0 & \exp(-\xi) \end{pmatrix}$$

with $\xi \in \mathbb{R}$. Following [29], we investigate the effect of the orientations of the slip system defined by $\psi = 65\pi/180$ (same geometry as in [29]) and $\psi = \pi/2$ on the relaxation of W. Figures 11 and 12 display the unrelaxed energy W together with the upper bound obtained with the optimal laminate $\langle \nu, W \rangle$ and the polyaffine lower bound $\ell + m$ for $\psi = 65\pi/180$ and $\psi = \pi/2$, respectively. Analogously, Tables 2 and 3 compare the type of optimal laminates for some representative values of ξ for $\psi = 65\pi/180$ and $\psi = \pi/2$, respectively.

For $\psi = 65\pi/180$ we find that where the homogeneous phase is stable up to $\xi \sim 0.040$, and that for $\xi \in [0.040, 0.080)$ it spontaneously decomposes into an elastic and plastic component. This structure was not considered in [29]. For larger ξ, i.e., for $\xi \in [0.080, 0.830]$, the optimal laminate contains two plastic deformations with opposite plastic slip γ confirming the conjecture of [29]. This difference in turn reflects into a small difference in the values of the relaxed energy as illustrated in Fig. 11b and Table 2.

In the case $\psi = \pi/2$, from (1.7) we have that $\gamma(F) = 0$ for each ξ, which implies that the homogeneous phase has no elastic deformation (this geometry has not been analysed in [29]). However, this appears not to

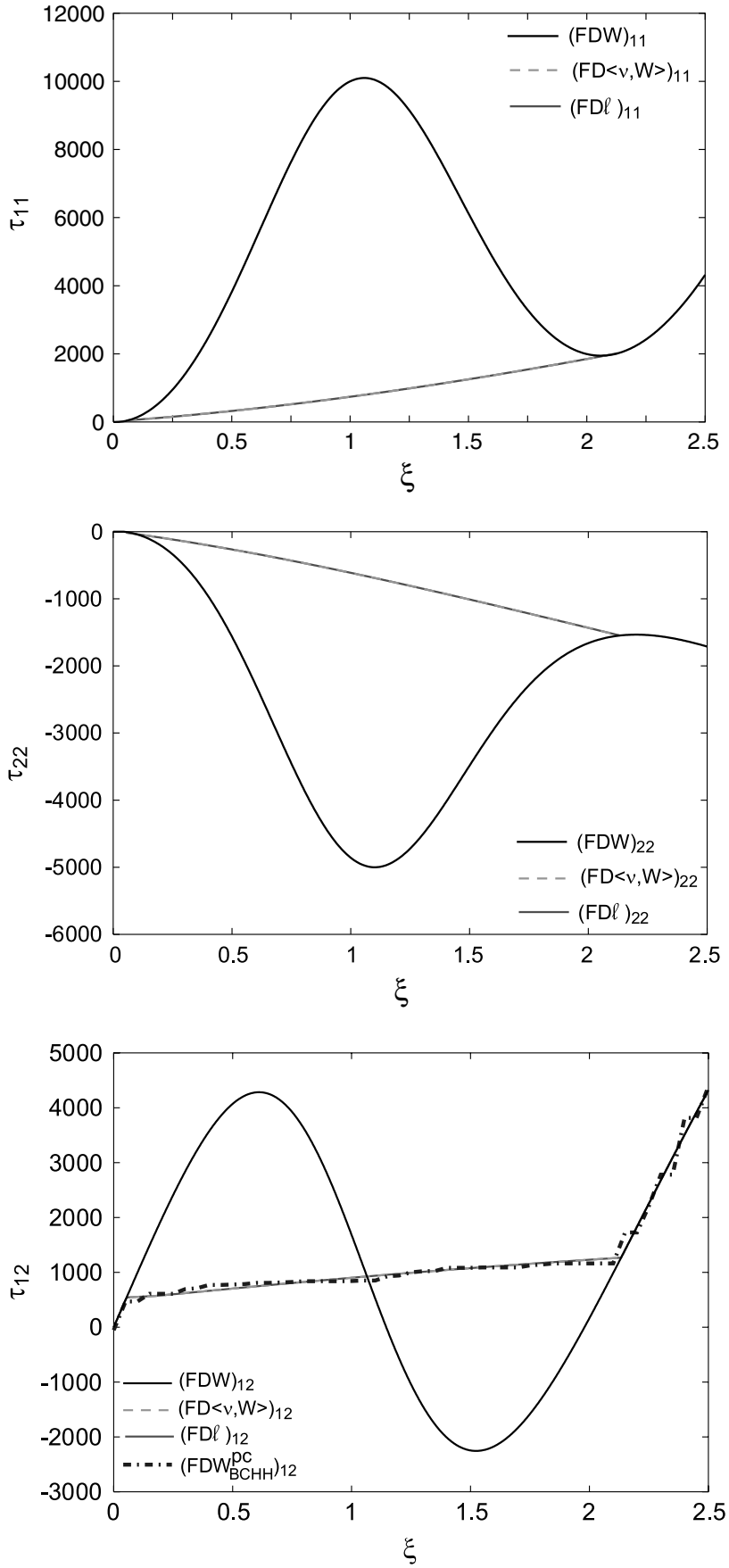


Fig. 8 Kirchhoff stress components for different values of ξ, $\theta = 0$ and $\psi = 3\pi/4$. Geometry as in Fig. 5

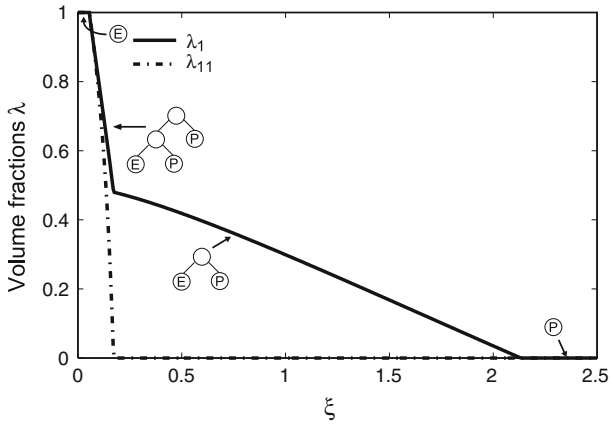


Fig. 9 Volume fractions λ_1 and λ_{11} for different values of ξ and for $\theta = 0$, $\psi = 3\pi/4$. Geometry as in Fig. 5

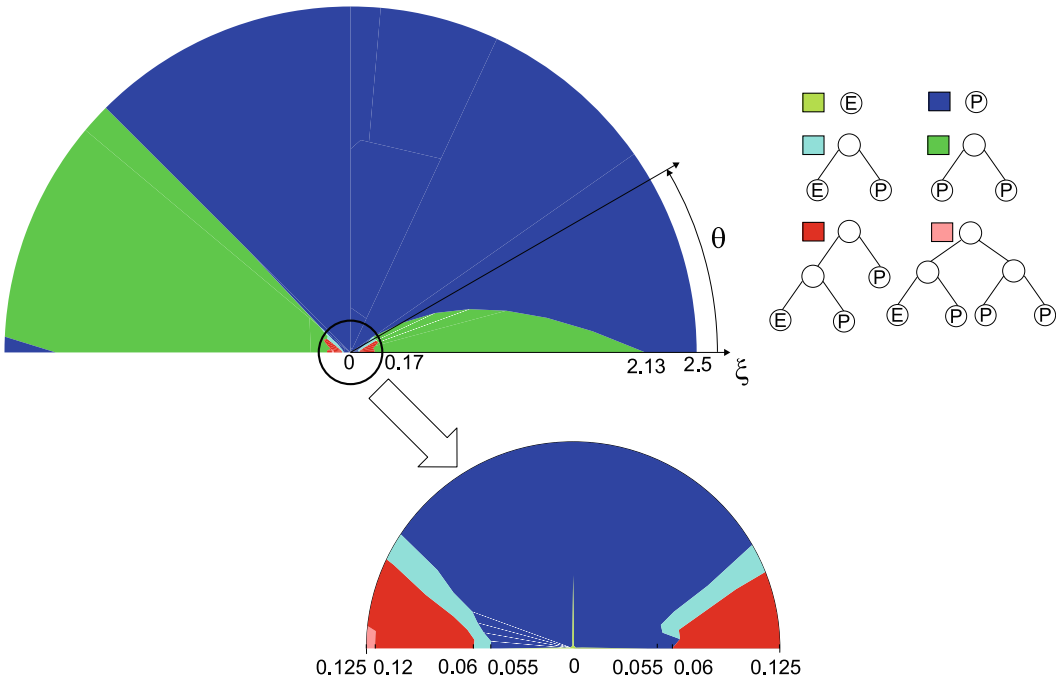


Fig. 10 Phase diagram in the plane (ξ, θ) of the type of optimal laminates for the relaxation of W when $F = \mathrm{Id} + \xi r \otimes r^{\perp}$ with $r = (\cos\theta,\ \sin\theta)$, and detail for $\xi \in [0,\ 0.125]$ (see Sect. 5.1)

be stable. For $\xi \in [0.035,\ 0.065]$ a second-order laminate is formed, which mixes elastic and plastic phases; for $\xi > 0.065$ a simple laminate is obtained with both plastic phases of opposite slip.

The quality of our relaxation can also be appreciated indirectly looking at Fig. 13 where the components of the Kirchhoff stress tensor for the two energies $\langle \nu,\ W \rangle$ and $\ell(F)$ are coincident whereas they slightly differ from those associated with the approximate relaxation of [29]. We remark that, up to a certain overestimation of the component τ_{12} of the stresss (see Fig. 13a), the approximate relaxation from [29] gives very good results. Finally, in the case $\psi = 0$ one obtain a stable homogeneous purely elastic phase (i.e., the laminate is trivial, and $\gamma(F) = 0$ for each ξ).

6 Conclusions

We have proposed an efficient algorithm for the numerical relaxation of the energy density modeling the elastoplastic behaviour of single crystals with one active single slip system in two dimensions. Our strategy

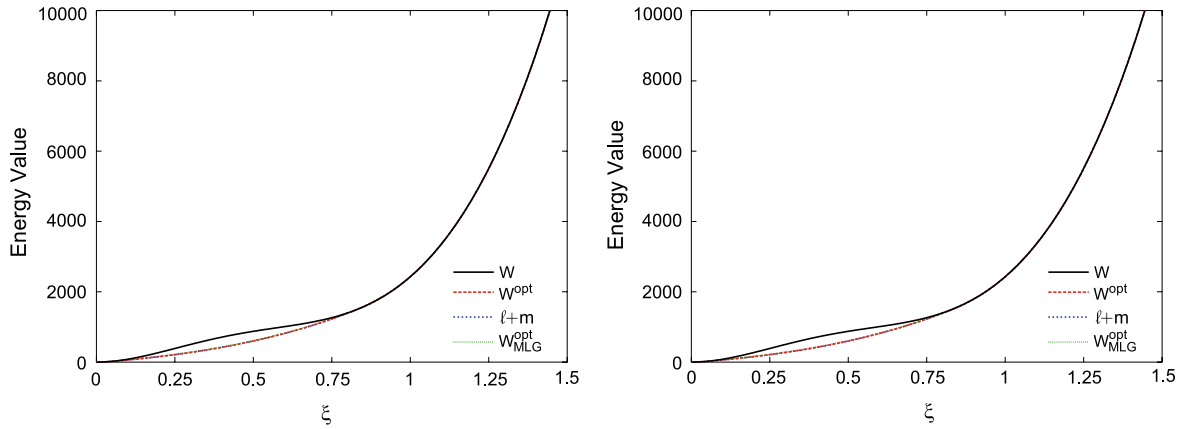


Fig. 11 Relaxed energy for the biaxial loading discussed in Sect. 5.2 with $\psi = 65\pi/180$ (same geometry as in [29]) (**a**) and diagram zoom for $\xi \in [0,\ 0.60]$ (**b**)

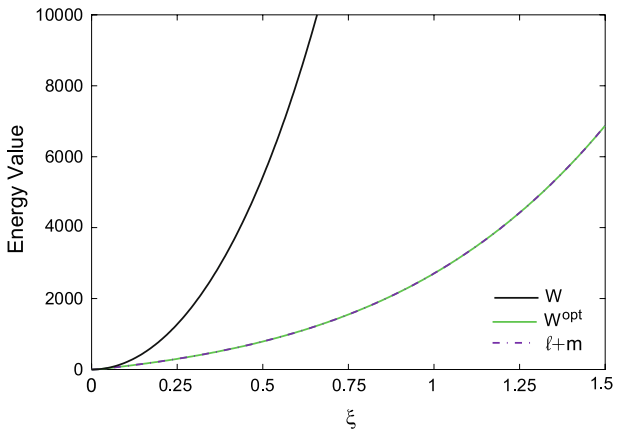


Fig. 12 Relaxed energy for the biaxial loading discussed in Sect. 5.2 with $\psi = \pi/2$

Table 1 Relaxed energy and type of the optimal laminate for the simple shear geometry discussed in Sect. 5.1 for $\theta = 3\pi/4$ and $\theta = \pi$

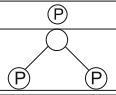
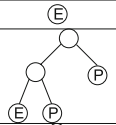
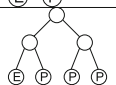
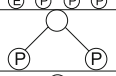
θ	ξ	optimal laminate	W	$\langle \nu, W \rangle$	$\ell + m$
$3\pi/4$	0.001	Ⓔ	0.005	0.005	0.005
	1.000	Ⓟ	463.632	463.632	463.632
	2.300		2425.450	2283.042	2283.042
π	0.040	Ⓔ	8.000	8.000	8.000
	0.060		17.997	17.833	17.833
	0.125		77.889	53.720	53.709
	0.250		307.308	125.857	125.857
	2.300	Ⓟ	2260.602	2260.602	2260.602

Table 2 Relaxed energy for the biaxial loading discussed in Sect. 5.2 with type of optimal laminate for $\psi = 65\pi/180$ (same geometry as in [29]) and some representative values of ξ, compared with the result $W^{\text{opt}}_{\text{MLG}}$ from [29]

ψ	ξ	optimal laminate	W	$\langle \nu, W \rangle$	$\ell(F)+m$	$\langle \nu, W \rangle$ [29]
$65\pi/180$	0.040	Ⓟ	14.703	14.703	14.703	14.703
	0.050	Ⓔ Ⓟ	22.484	21.910	21.910	22.484
	0.150	Ⓟ Ⓟ	169.306	106.517	106.517	114.450
	1.000	Ⓟ	2428.858	2428.858	2428.858	2428.858

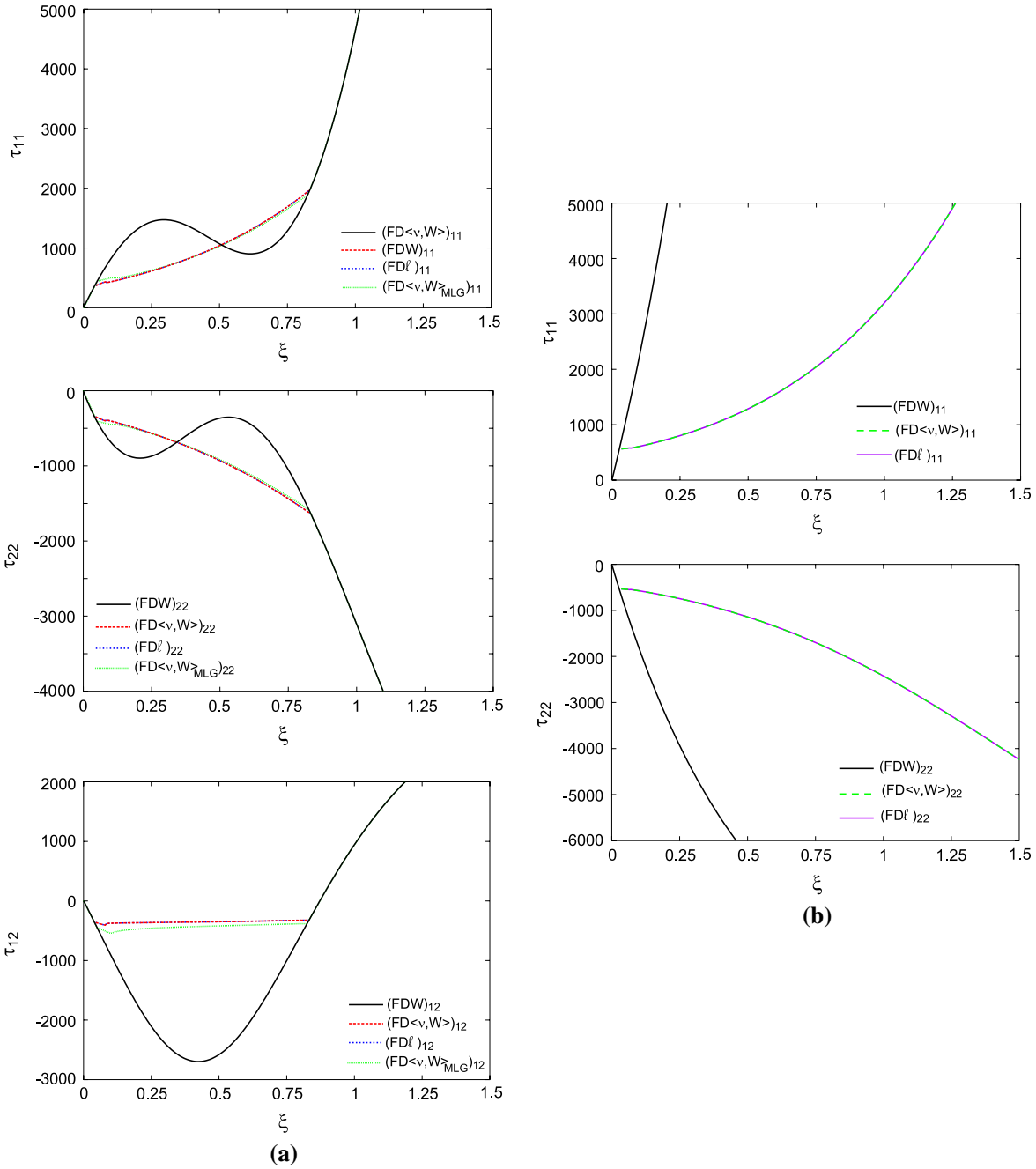
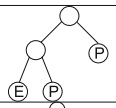
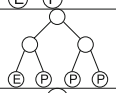
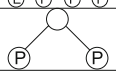


Fig. 13 Kirchhoff stress components for the biaxial loading discussed in Sect. 5.2 with $\psi = 65\pi/180$ (**a**) and $\psi = \pi/2$ (**b**). In this last case, note that $\tau_{12} = 0$. The geometry for $\psi = 65\pi/180$ corresponds to Fig. 8 of [29], and in that case the results from [29] are also reported

Table 3 Relaxed energy for the biaxial loading discussed in Sect. 5.2 with type of optimal laminate for $\psi = \pi/2$ and some representative values of ξ

ψ	ξ	optimal laminate	W	$\langle \nu, W \rangle$	$\ell(F) + m$
$\pi/2$	0.040		32.017	28.817	28.811
	0.060		72.086	51.073	51.062
	1.000		27621.957	2708.206	2708.206

exploits in an essential manner the structure of the problem in suggesting good initial guesses for the evaluation of an optimal laminate, and thereby avoids the use of a brute-force global optimization algorithm. The precision of our relaxation over laminates has been assessed by computing at each macroscopic strain a polyaffine function which coincides with the unrelaxed energy on the support of the laminate and checking that it is below the condensed energy, up to a very small error. This has lead us to a guaranteed lower bound to $W^{\mathrm{qc}}(F)$ which is free from mesh-size errors, at variance with algorithms based on discretization in matrix space. We illustrated a practical application of our algorithm to determine the relaxation of W when F describes a simple shear and a biaxial deformation. In both cases, we have obtained a good approximation of the quasiconvex envelope and of the Kirchhoff stress components, with the two bounds very close to each other.

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References

1. Adams, J., Conti, S., DeSimone, A., Dolzmann, G.: Relaxation of some transversally isotropic energies and applications to smectic A elastomers. Math. Mod. Meth. Appl. Sci. **18**, 1–20 (2008)
2. Allaire, G.: Shape optimization by the homogenization method, vol. 146 of Applied Mathematical Sciences, Springer, New York (2002)
3. Asaro, R.J.: Micromechanics of crystals and polycrystals. Adv. Appl. Mech. **23**, 1–115 (1983)
4. Aubry, S., Fago, M., Ortiz, M.: A constrained sequential-lamination algorithm for the simulation of sub-grid microstructure in martensitic materials. Comput. Meth. Appl. Mech. Eng. **192**, 2823–2843 (2003)
5. Ball, J.M.: Convexity conditions and existence theorems in nonlinear elasticity. Arch. Rat. Mech. Anal. **63**, 337–403 (1977)
6. Ball, J.M., James, R.D.: Fine phase mixtures as minimizer of energy. Arch. Rat. Mech. Anal. **100**, 13–52 (1987)
7. Ball, J.M., James, R.D.: Proposed experimental tests for the theory of fine microstructures and the two-well problem. Philos. Trans R. Soc. Lond. A **338**, 389–450 (1992)
8. Bartels, S.: Reliable and efficient approximation of polyconvex envelopes. SIAM J. Numer. Anal. **43**, 363–385 (2005)
9. Bartels, S., Carstensen, C, Hackl, K., Hoppe, U.: Effective relaxation for microstructure simulations: algorithms and applications. Comput. Meth. Appl. Mech. Eng. **193**, 5143–5175 (2004)
10. Bartels, S., Carstensen, C., Conti, S., Hackl, K., Hoppe, U., Orlando, A.: Relaxation and the computation of effective energies and microstructures in solid mechanics. In: Mielke A. (ed.) Analisys, Modeling and Simulation of Multiphase Problems. Springer, Berlin 197–224 (2006)
11. Bhattacharya, K., Dolzmann, G.: Relaxation of some multiwell problems. Proc. R. Soc. Edin. A **131**, 279–320 (2001)
12. Carstensen, C.: Numerical analysis of microstructure. In: Blowey, J.F., Coleman, J.P., Craig, A.W. (eds.) Theory and Numerics of Differential Equations, Durham 2000. Springer, New York (2001)
13. Carstensen, C., Hackl, K., Mielke, A.: Non-convex potentials and microstructures in finite-strain plasticity. Proc. R. Soc. Lond. A **458**, 299–317 (2002)
14. Conti, S., DeSimone, A., Dolzmann, G.: Soft elastic response of stretched sheets of nematic elastomers: a numerical study. J. Mech. Phys. Solids **50**, 1431–1451 (2002)
15. Conti, S.: Microstructure and relaxation in single-crystal plasticity. Oberwolfach Rep. **2**, 3000–3003 (2005)
16. Conti, S.: Relaxation of single-slip single-crystal plasticity with linear hardening. In: Gumbsch, P. (ed.) Proceedings of Multiscale Material Modeling Conference. Freiburg, 18–22 September (2006) 30–35
17. Conti, S., Ortiz, M.: Dislocation microstructures and the effective behavior of single crystals. Arch. Ration. Mech. Anal. **176**, 103–147 (2005)
18. Conti, S., Theil, F.: Single-slip elastoplastic microstructures. Arch. Ration. Mech. Anal. **178**, 125–148 (2005)
19. Conti, S., Hauret, P., Ortiz, M.: Concurrent multiscale computing of deformation microstructure by relaxation and local enrichment with application to single-crystal plasticity. Multiscale Model. Simul. **6**, 135–157 (2007)

20. Dacorogna, B.: Direct Methods in the Calculus of Variations, vol. 78 of Applied Mathematical Sciences. Springer, USA (1989)
21. DeSimone, A., Dolzmann, G.: Macroscopic response of nematic elastomers via relaxation of a class of $SO(3)$-invariant energies. Arch. Rat. Mech. Anal. **161**, 181–204 (2002)
22. Dolzmann, G.: Variational Methods for Crystalline Microstructure—Analysis and Computation, Lecture Notes in Mathematics 1803. Springer, Berlin (2003)
23. Dolzmann, G.: Numerical computation of rank-one convex envelopes. SIAM J. Numer. Anal. **36**, 1621–1635 (1999)
24. Hackl, K., Hoppe, U.: On the calculation of microstructures for inelastic materials using relaxed energies. In: Miehe Ch. (ed.) IUTAM Symposium on Computational Mechanics of Solid Materials at Large Strains. Kluwer, Dordrecht (2002)
25. Kohn, R.V.: The relaxation of a double-well energy. Contin. Mech. Thermodyn. **3**, 193–236 (1991)
26. Kohn, R.V., Strang, G.: Optimal design and relaxation of variational problems I, II, III, Comm. Pure Appl. Math. **39**, 113–137, 139–182, 353–377 (1986)
27. Kruzik, M., Luskin, M.: The computation of martensitic microstructures with piecewise laminates. J. Sci. Comput. **19**, 293–308 (2003)
28. Miehe, C., Lambrecht, M.: Analysis of microstructure development in shearbands by energy relaxation of incremental stress potentials: large strain theory for standard dissipative solids. Int. J. Numer. Meth. Eng. **58**, 1–41 (2003)
29. Miehe, C., Lambrecht, M., Gürses, E.: Analysis of material instabilities in inelastic solids by incremental energy minimization and relaxation methods: evolving deformation microstructures in finite plasticity. J. Mech. Phys. Solids **52**, 2725–2769 (2004)
30. Mielke, A.: Relaxation via Young measures of material models for rate-independent inelasticity. In: Miehe Ch. (ed.) IUTAM Symposium on Computational Mechanics of Solid Materials at Large Strains. Kluwer, Dordrecht (2002)
31. Mielke, A.: Finite elastoplasticity, Lie groups and geodesics on SL(d). In: Newton, P., Weinstein, A., Holmes, P.J. (eds.) Geometry, Dynamics, and Mechanics. Lecture Notes in Mathematics 1278. Springer, New-York (2002)
32. Mielke, A.: Evolution in rate-independent systems (Chap. 6). In: Dafermos, C., Feireisl, E. (eds.) Handbook of Differential Equations: Evolutionary Equations. vol. 2. Elsevier, Amsterdam (2005)
33. Morrey, C.B.: Quasi-convexity and the lower semicontinuity of multiple integrals. Pacific J. Math. **2**, 25–53 (1952)
34. Müller, S.: Variational models for microstructure and phase transitions. In: Hildebrandt S., Struwe M. (eds.) Calculus of Variations and Geometric Evolution Problems. Lecture Notes in Mathematics 1713. Springer, Berlin (1999)
35. Müller, S., Šverák, V.: Convex integration with constraints and applications to phase transitions and partial differential equations. J. Eur. Math. Soc. **1**, 393–442 (1999)
36. Nocedal, J., Wright, S.: Numerical Optimization. Springer, New York (2006)
37. Ortiz, M., Repetto, E.A.: Nonconvex energy minimization and dislocation structures in ductile single crystals. J. Mech. Phys. Solids **47**, 397–462 (1999)
38. Ortiz, M., Repetto, E.A., Stainer, L.: A theory of subgrain dislocation structures. J. Mech. Phys. Solids **48**, 2077–2114 (2000)
39. Pardalos, P.M., Romeijn, H.E.: Handbook of Global Optimization, Vol. 2. Springer, Berlin (2002)
40. Pedregal, P.: Parametrized Measures and Variational Principles. Birkhäuser, Basel (1997)
41. Roubíček, T.: Relaxation in Optimization Theory and Variational Calculus. Walter de Gruyter, Berlin (1996)
42. Schittkowski, K.: NLQPL: A FORTRAN-subroutine solving constrained nonlinear programming problems. Ann. Oper. Res. **5**, 485–500 (1985)
43. Smyshlyaev, V.P., Willis, J.R.: On the relaxation of a three-well energy. Proc. R. Soc. A **455**, 779–814 (1999)