FINITE ORDER RANK-ONE CONVEX ENVELOPES AND COMPUTATION OF MICROSTRUCTURES WITH LAMINATES IN LAMINATES

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ABSTRACT. Finite order rank-one convex envelopes are introduced and it is shown that the i-th order laminated microstructures, or laminates in laminates, can be solved by any of the k-th order rank-one convex envelopes with $k \geq i$. It is also shown that in finite element approximations of microstructures, replacing the nonquasiconvex potential energy density by its k-th order rank-one convex envelope, one can generally obtain sharper numerical results. Especially, for crystalline microstructures with laminates in laminates of order no greater than $k+1$, numerical results with up to the computer precision can be obtained. Numerical examples on the first and second order rank-one convex envelopes for Ericksen and James two dimensional model for elastic crystals are given. A numerical example on finite element approximations of a crystalline microstructure by using the first order rank-one convex envelope and the periodic relaxation method is also presented. The methods turn out to be very successful for microstructures with laminates in laminates.

1. INTRODUCTION

In a well known geometrically nonlinear theory of martensitic microstructures [1, 3], microstructures are characterized by energy minimizing sequences which consist of increasingly fine oscillations and lead to Young measures of gradients which are known to be the limit distribution of the gradients in a neighbourhood of each point [2]. The theory leads to the consideration of the problem of minimizing an integral functional

$$F(u;\ \Omega) = \int_\Omega f(\nabla u(x))\, dx \tag{1}$$

with a nonquasiconvex integrand $f : R^{mn} \to R^1$ [19, 8] in a set of admissible functions

$$\mathbb{U}(u_0;\ \Omega) = \{u \in W^{1,p}(\Omega; R^m) : u = u_0,\ \text{on } \partial\Omega\}, \tag{2}$$

where $\Omega \subset R^n$ is a bounded open set with a Lipschitz continuous boundary $\partial\Omega$ and $1 < p < \infty$.

Such a variational problem provides a natural setting for a finite element approximation of crystalline microstructures. Unfortunately, numerical analysis and experiments

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reveal that a direct implementation of a finite element discretization to the problem generally produces large truncation errors which are known to be mainly caused by the energy accumulation on the transition layers and the boundary layer and which can cause serious problems in the finite element approximations [5, 6, 7, 12, 13, 14, 18, 21]. Some numerical methods have been developed recently to tackle such difficulties [15, 16, 17], and they turned out to be successful, especially for the first order laminated microstructures where a combination of the mesh transformation method and the periodic relaxation method can completely avoid the formation of transition layers and a boundary layer [17]. However, it is noticed that, for crystalline microstructures more complicated than the first order laminates, transition layers are generally inevitable if a conforming finite element method is applied to the nonquasiconvex variational problem

$$\inf_{u \in \mathbb{U}(u_0;\, \Omega)} \int_\Omega f(\nabla u(x))\, dx \tag{3}$$

even if the mesh is aligned with the interfaces between laminates, since the displacements across such interfaces are no longer continuous.

In the present paper, a new approach for computing crystalline microstructures with finite order laminates in laminates is developed by introducing the finite order rank-one convex envelopes $R_k f$ of f (see section 2). We shall see that the transition layers between laminated microstructures with orders no greater than k can be avoided, if the integrand f in (3) is replaced by its k-th order rank-one convex envelope $R_k f$ and thus all the laminates of order less than or equal to k will appear as affine functions in the finite element solutions with the information of the laminates being given as a result of the computation of $R_k f$. Potentially, we can combine the method with the finite element method to solve problems with nonlinear boundary conditions, that is, in each step of an iterative method searching for a minimizer, we replace the integrand f by its k-th order rank-one convex envelope $R_k f$ and compute on each piecewise linear element the value of $R_k f$ by the method given in this paper. The advantage is that the finite element solutions for the new problem have much less oscillations and thus can be approximated with much higher precision. In fact, theoretically speaking, such replacements generally produce sharper numerical results. Furthermore, the information on the laminates in laminates obtained by the method can be used to construct good initial deformation for finite element approximations to compute at mesoscopic scale more details such as the needle-like microstructures near the interface areas. The investigations in these directions will not be discussed in this paper. Numerical computations of rank-one convex envelopes, which is a key issue of the present paper, attracts a lot of attention recently [9, 10, 11, 20]. In section 3, to simplify the computation, a new formula of the rank-one convex envelopes is introduced in which $R_k f$ is expressed as a unconstrained optimization problem with $(m+n)(2^k-1)$ variables. The main idea is that we restrict the search for optimization in the rank-one directions $\phi \otimes \theta$ which can be viewed as searching for ϕ and θ in two unit spheres S^{m-1} and S^{n-1} centered at 0 in R^m and R^n respectively, thus the condition of rank-one connections is automatically satisfied. In section 4, numerical examples on the first and second order rank-one convex envelopes of Ericksen and James two dimensional model for elastic crystals [5, 6, 12] are given, a simple and highly efficient algorithm and high precision numerical results on the first and second order laminated microstructures are presented. A numerical example of finite element approximation using $R_1 f$ and the periodic relaxation method is also given. The numerical results show that the methods given in this paper are very efficient for microstructures with laminates in laminates.

2. Finite order rank-one convex envelopes

Let $f : R^{mn} \to R^1 \cup \{\infty\}$ be continuous.

Definition 2.1. Let $R_1 f : R^{mn} \to R^1 \cup \{\infty\}$ be defined by

$$R_1 f(A) = \inf\{\lambda f(A_0) + (1-\lambda) f(A_1) : \lambda \geq 0,\ A = \lambda A_0 + (1-\lambda)A_1, \quad \operatorname{rank}(A_0 - A_1) \leq 1\}, \tag{4}$$

and let $R_k f : R^{mn} \to R^1 \cup \{\infty\}$ be defined by

$$R_k f(A) = R_1(R_{k-1} f)(A). \tag{5}$$

We call $R_k f$ the k-th order rank-one convex envelope of f.

To see the relationship between the finite order rank-one convex envelope $R_k f$ and the rank-one convex envelope Rf, which is the greatest rank-one convex function less than or equal to f, recall that [8]

$$Rf(A) = \inf\{\sum_{i=1}^{N} \lambda_i f(A_i) : \sum_{i=1}^{N} \lambda_i A_i = A, \text{and } (\lambda_i,\ A_i) \text{ satisfy } (\mathrm{H}_N),\ \forall N\}, \tag{6}$$

where $(\lambda_i,\ A_i)$ are said to satisfy (H_N) if $\lambda_i > 0$, $\sum_{i=1}^{N} \lambda_i = 1$ and

(1): $N = 2$, then $\operatorname{rank}(A_1 - A_2) \leq 1$,

(2): $N > 2$, then up to a permutation, $\operatorname{rank}(A_1 - A_2) \leq 1$ and if

$$\begin{cases} \mu_1 = \lambda_1 + \lambda_2, & B_1 = \frac{\lambda_1 A_1 + \lambda_2 A_2}{\lambda_1 + \lambda_2}, \\ \mu_i = \lambda_{i+1}, & B_i = A_{i+1},\ 2 \leq i \leq N-1, \end{cases}$$

then (μ_i, B_i) satisfy (H_{N-1}).

Definition 2.2. $(\lambda_{i_1}, \lambda_{i_1 i_2}, \ldots, \lambda_{i_1 i_2 \cdots i_k}, A_{i_1 i_2 \cdots i_k})$, $i_\nu \in \{0,1\}$, $0 \leq \nu \leq k$ are said to satisfy (R_k) if $\lambda_{i_1 \cdots i_\nu} \geq 0$ for $\nu = 1, \cdots, k$, $\lambda_0 + \lambda_1 = 1$, $\lambda_{i_1 \cdots i_{\nu-1} 0} + \lambda_{i_1 \cdots i_{\nu-1} 1} = 1$, for $\nu = 2, \cdots, k$ and

(i): $\operatorname{rank}(A_{i_1 \cdots i_{k-1} 0} - A_{i_1 \cdots i_{k-1} 1}) \leq 1$,

(ii): let $A_{i_1 \cdots i_\nu} = \lambda_{i_1 \cdots i_\nu 0} A_{i_1 \cdots i_\nu 0} + \lambda_{i_1 \cdots i_\nu 1} A_{i_1 \cdots i_\nu 1}$, then

$$\operatorname{rank}(A_{i_1 \cdots i_{\nu-1} 0} - A_{i_1 \cdots i_{\nu-1} 1}) \leq 1,\ \forall \nu = k-1, \cdots, 2.$$

An equivalent definition of the finite order rank-one convex envelopes can be given as follows:

Definition 2.3. $R_k f : R^{mn} \to R^1 \cup \{\infty\}$ is said to be the k-th order rank-one convex envelope of f, if

$$R_k f(A) = \inf\{ \sum_{i_1, \ldots, i_k = 0}^{1} \lambda_{i_1} \lambda_{i_1 i_2} \cdots \lambda_{i_1 i_2 \cdots i_k} f(A_{i_1 i_2 \cdots i_k}) : \tag{7}$$

$$\sum_{i_1,\ldots,i_k=0}^{1} \lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1 i_2\cdots i_k} A_{i_1 i_2\cdots i_k} = A,$$
$$(\lambda_{i_1}, \lambda_{i_1 i_2}, \ldots, \lambda_{i_1 i_2\cdots i_k}, A_{i_1 i_2\cdots i_k}) \text{ satisfy } (\mathrm{R}_k)\}.$$

Lemma 2.1. *We have*

$$f \geq R_1 f \geq R_2 f \geq \cdots \geq R_k f \geq \cdots \geq Rf \tag{8}$$

and

$$\lim_{k\to\infty} R_k f(A) = Rf(A),\ \forall A \in R^{mn}. \tag{9}$$

Proof. Since the inequalities (8) are direct consequences of the definitions of $R_k f$ and Rf, we only need to show (9). Let $(\mu_i,\ B_i)$ satisfy (H_k) and $A = \sum_{i=1}^{k} \mu_i B_i$. Let $b_j(\alpha)$ be the j bits binary representation of $0 \leq \alpha \leq 2^j - 1$, that is

$$b_j(\alpha) = \beta_1\beta_2\cdots\beta_j,\quad \beta_i \in \{0,1\},\quad \text{and } \sum_{i=1}^{j} \beta_i 2^{j-i} = \alpha.$$

Define

$$A_{b_k(0)} = B_1,\quad A_{b_k(1)} = B_2,$$
$$A_{b_k(\alpha)} = B_i,\quad 2^{i-2} \leq \alpha \leq 2^{i-1} - 1,\quad 3 \leq i \leq k$$

and

$$\lambda_{b_j(0)} = \Big(\sum_{i=1}^{k-j+1} \mu_i\Big)^{-1} \sum_{i=1}^{k-j} \mu_i,\quad 1 \leq j \leq k,$$
$$\lambda_{b_j(1)} = \Big(\sum_{i=1}^{k-j+1} \mu_i\Big)^{-1} \mu_{k-j+1},\quad 1 \leq j \leq k,$$
$$\lambda_{b_j(\alpha)} = \frac{1}{2},\quad 2 \leq \alpha \leq 2^j - 1,\quad 2 \leq j \leq k.$$

Then, it is not difficult to verify that $(\lambda_{i_1}, \lambda_{i_1 i_2}, \ldots, \lambda_{i_1 i_2\cdots i_k}, A_{i_1 i_2\cdots i_k})$ satisfy (R_k), and $\sum_{i_1,\ldots,i_k=0}^{1} \lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1 i_2\cdots i_k} A_{i_1 i_2\cdots i_k} = A$. This implies

$$R_k f(A) \leq \inf\{\sum_{i=1}^{k} \mu_i f(B_i) : \sum_{i=1}^{k} \mu_i B_i = A, \text{and } (\mu_i,\ B_i) \text{ satisfy } (\mathrm{H}_k)\}. \tag{10}$$

Thus, (9) follows as a consequence of (6), (8) and (10). $\square$

Lemma 2.2. *Let*

$$W_k(f) = \{A \in R^{mn} : A = \sum_{i_1,\ldots,i_k=0}^{1} \lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1 i_2\cdots i_k} A_{i_1 i_2\cdots i_k}, \tag{11}$$
$$(\lambda_{i_1}, \lambda_{i_1 i_2}, \ldots, \lambda_{i_1 i_2\cdots i_k}, A_{i_1 i_2\cdots i_k}) \textit{ satisfy } (R_k), \textit{ and } f(A_{i_1 i_2\cdots i_k}) = \min_{B\in R^{mn}} f(B)\},$$

which is the $k-$th order rank-one convex hull of the set $\{C \in R^{mn} : f(C) = \min_{B\in R^{mn}} f(B)\}$. *Then, for all* $A \in W_k(f)$, *we have*

$$R_k f(A) = \min_{B\in R^{mn}} f(B). \tag{12}$$

On the other hand, if $\lim\limits_{\|B\|\to\infty} f(B) > \min\limits_{B\in R^{mn}} f(B)$ *and* (12) *is satisfied, then* $A \in W_k(f)$.

Proof. By (11) and definition 2.3, for all $A \in W_k(f)$, we have

$$\min_{B\in R^{mn}} f(B) \le R_k f(A) \le \sum_{i_1,\dots,i_k=0}^{1} \lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1 i_2\cdots i_k} f(A_{i_1 i_2\cdots i_k}).$$

Since $f(A_{i_1 i_2\cdots i_k}) = \min_{B\in R^{mn}} f(B)$ and $\sum_{i_1,\dots,i_k=0}^{1} \lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1 i_2\cdots i_k} = 1$, (9) follows.

Next, assume that A satisfies (12). It follows from (7) and (12) that there exists a sequence $\{(\lambda^j_{i_1}, \lambda^j_{i_1 i_2}, \dots, \lambda^j_{i_1 i_2\cdots i_k}, A^j_{i_1 i_2\cdots i_k})\}_{j=1}^{\infty}$ which satisfy (R_k) and

$$\sum_{i_1,\dots,i_k=0}^{1} \lambda^j_{i_1}\lambda^j_{i_1 i_2}\cdots\lambda^j_{i_1 i_2\cdots i_k} A^j_{i_1 i_2\cdots i_k} = A,$$

$$\lim_{j\to\infty} \sum_{i_1,\dots,i_k=0}^{1} \lambda^j_{i_1}\lambda^j_{i_1 i_2}\cdots\lambda^j_{i_1 i_2\cdots i_k} f(A^j_{i_1 i_2\cdots i_k}) = \min_{B\in R^{mn}} f(B).$$

Since $0 \le \lambda^j_{i_1 i_2\cdots i_\nu} \le 1$ and $A^j_{i_1 i_2\cdots i_k}$ are bounded by assumption, it follows that there is a subsequence, denoted again by $\{(\lambda^j_{i_1}, \lambda^j_{i_1 i_2}, \dots, \lambda^j_{i_1 i_2\cdots i_k}, A^j_{i_1 i_2\cdots i_k})\}_{j=1}^{\infty}$, such that

$$\lim_{j\to\infty} (\lambda^j_{i_1}, \lambda^j_{i_1 i_2}, \dots, \lambda^j_{i_1 i_2\cdots i_k}, A^j_{i_1 i_2\cdots i_k}) = (\lambda_{i_1}, \lambda_{i_1 i_2}, \dots, \lambda_{i_1 i_2\cdots i_k}, A_{i_1 i_2\cdots i_k}).$$

This implies that

$$\sum_{i_1,\dots,i_k=0}^{1} \lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1 i_2\cdots i_k} A_{i_1 i_2\cdots i_k} = A,$$

$$\sum_{i_1,\dots,i_k=0}^{1} \lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1 i_2\cdots i_k} f(A_{i_1 i_2\cdots i_k}) = \min_{B\in R^{mn}} f(B).$$

Now, by these relations, it is easily verified that $A \in W_k(f)$. □

Definition 2.4. The set $(\lambda_{i_1}, \lambda_{i_1 i_2}, \dots, \lambda_{i_1 i_2\cdots i_k}, A_{i_1 i_2\cdots i_k})$ is said to be a representation of A in $W_k(f)$, if $(\lambda_{i_1}, \lambda_{i_1 i_2}, \dots, \lambda_{i_1 i_2\cdots i_k}, A_{i_1 i_2\cdots i_k})$ satisfy (R_k) and

- **(a):** $A = \sum_{i_1,\dots,i_k=0}^{1} \lambda_{i_1}\lambda_{i_1 i_2}\cdots\lambda_{i_1 i_2\cdots i_k} A_{i_1 i_2\cdots i_k}$,
- **(b):** $f(A_{i_1 i_2\cdots i_k}) = \min_{B\in R^{mn}} f(B)$.

Theorem 2.1. *Assume* $A \in W_k(f)$. *Then,* $u(x) = Ax$ *is a solution to the problem*

$$\inf_{u\in \mathbb{U}(Ax,\,\Omega)} \int_\Omega R_k f(\nabla u(x))\,dx. \tag{13}$$

Assume $A \in W_{k+1}(f) \setminus W_k(f)$ *and* $(\lambda_{i_1}, \lambda_{i_1 i_2}, \dots, \lambda_{i_1 i_2\cdots i_{k+1}}, A_{i_1 i_2\cdots i_{k+1}})$ *is a representation of* A *in* $W_{k+1}(f)$. *Then,the problem* (13) *has a minimizing sequence leading* *to a first order laminated microstructure which has a homogeneous Young measure of gradients*

$$\nu_x \equiv \nu = \lambda_0 \delta_{A_0} + \lambda_1 \delta_{A_1}, \tag{14}$$

where A_0 and A_1 are defined by (ii) in Definition 2.2.

Proof. The first part of the theorem is obvious. It follows from $A \in W_{k+1}(f) \setminus W_k(f)$ that $\operatorname{rank}(A_0 - A_1) \le 1$, $\lambda_0 > 0$, $\lambda_1 > 0$, $\lambda_0 + \lambda_1 = 1$ and

$$R_k f(A_0) = R_k f(A_1) = \min_{B \in R^{mn}} R_k f(B) = \min_{B \in R^{mn}} f(B).$$

Thus, a minimizing sequence of the problem (13), which leads to the Young measure (14), can be constructed in a standard way [1, 8, 18] as a simple laminate with gradients oscillating between A_0 and A_1. □

Theorem 2.2. *Assume $A \in W_k(f)$. Let $(\lambda_{i_1}, \lambda_{i_1 i_2}, \ldots, \lambda_{i_1 i_2 \ldots i_k}, A_{i_1 i_2 \cdots i_k})$ be a representation of A in $W_k(f)$. Then, the problem*

$$\inf_{u \in \mathbb{U}(Ax,\, \Omega)} \int_\Omega f(\nabla u(x))\, dx \tag{15}$$

has a minimizing sequence which produces a microstructure with laminates in laminates of order no greater than k and which has a Young measure of gradients

$$\nu_x \equiv \nu = \sum_{i_1, i_2, \cdots, i_k = 0}^{1} \lambda_{i_1} \lambda_{i_1 i_2} \cdots \lambda_{i_1 i_2 \cdots i_k} \delta_{A_{i_1 i_2 \cdots i_k}}. \tag{16}$$

Proof. By lemma 2.2, we have

$$\sum_{i_1, i_2, \cdots, i_k = 0}^{1} \lambda_{i_1} \lambda_{i_1 i_2} \cdots \lambda_{i_1 i_2 \cdots i_k} f(A_{i_1 i_2 \cdots i_k}) = R_k f(A) = \min_{B \in R^{mn}} f(B). \tag{17}$$

Let A_{i_1}, $A_{i_1 i_2}$, $\ldots$, $A_{i_1 i_2 \cdots i_{k-1}}$ be defined by the Definition 2.2. Without loss of generality, we may assume that $A \in W_k(f) \setminus W_{k-1}(f)$ and $A_{i_1 \cdots i_\nu} \in W_{k-\nu}(f) \setminus W_{k-\nu-1}(f)$. Then, as in the proof of Theorem 2.1, A_0 and A_1 can be used to construct a simple banded structure with the ratio of band width being λ_0 to λ_1. Similarly, on the bands where the gradient is $A_{i_1 \cdots i_\nu}$, $A_{i_1 \cdots i_\nu 0}$ and $A_{i_1 \cdots i_\nu 1}$ can be used to construct a simple banded structure with the ratio of band width being $\lambda_{i_1 \cdots i_\nu 0}$ to $\lambda_{i_1 \cdots i_\nu 1}$. The successive constructions will finally lead to the expected structure of laminates in laminates of order k. (Details of constructions of first and second order laminated microstructures can be found in [18, 3]). □

Theorem 2.3. *For any $k \ge 1$ and any $u_0 \in W^{1,p}(\Omega;\, R^m)$, we have*

$$\inf_{u \in \mathbb{U}(u_0,\, \Omega)} \int_\Omega R_k f(\nabla u(x))\, dx = \inf_{u \in \mathbb{U}(u_0,\, \Omega)} \int_\Omega f(\nabla u(x))\, dx. \tag{18}$$

Proof. Let $u_i \in \mathbb{U}(u_0;\, \Omega)$ be a minimizing sequence of the problem

$$\inf_{u \in \mathbb{U}(u_0,\, \Omega)} \int_\Omega R_k f(\nabla u(x))\, dx.$$

Since f is continuous so is $R_k f$, without loss of generality, we may assume that u_0 and u_i are piece wise affine and ∇u_i take only finite different values $\{B^i_j\}_{j=1}^{N_i}$ on a finite partition $\{\Omega^i_j\}_{j=1}^{N_i}$ of Ω. Thus, we may write

$$\int_\Omega R_k f(\nabla u_i(x))\,dx = \sum_{j=1}^{N_i} R_k f(B^i_j)\,\mathrm{meas}(\Omega^i_j). \tag{19}$$

On each Ω^i_j, by the definition of $R_k f(B^i_j)$, it is easily seen that

$$R_k f(B^i_j)\,\mathrm{meas}(\Omega^i_j) \geq \inf_{u\in\mathbb{U}(u_i|_{\Omega^i_j};\,\Omega^i_j)} \int_{\Omega^i_j} f(\nabla u(x))\,dx.$$

By (19), this gives

$$\int_\Omega R_k f(\nabla u_i(x))\,dx \geq \inf_{u\in\mathbb{U}(u_0;\,\Omega)} \int_\Omega f(\nabla u(x))\,dx. \tag{20}$$

This completes the proof, since $R_k f \leq f$. □

Remark 2.1. Under certain growth and coercivity conditions, (18) is a direct consequence of

$$Qf \leq Rf \leq R_k f \leq f$$

and (see [8])

$$\inf_{u\in\mathbb{U}(u_0,\,\Omega)} \int_\Omega Qf(\nabla u(x))\,dx = \inf_{u\in\mathbb{U}(u_0,\,\Omega)} \int_\Omega f(\nabla u(x))\,dx.$$

where Qf is the quasiconvex envelope of f. It is interesting to notice here that in Theorem 2.3 the equation (18) is obtained without using any growth and coercivity condition.

Remark 2.2. Since rank one convexity does not imply quasiconvexity [8], microstructures other than finite and infinite order laminates in laminates can exist even when the boundary condition is affine. Hence, it is necessary to consider finite element approximations of the problem (13). Lemma 2.1 and Theorem 2.3 imply that sharper numerical results can generally be obtained by solving (13) instead of (15), since all the laminates in laminates of order no greater than k appear to be affine functions in this case, and the information of the laminates are recovered by the representations of the gradients of the corresponding affine functions in $W_k(f)$.

Remark 2.3. Compared with the problem (15), a minimizing sequence of the problem (13) generally contains much less oscillations, since oscillations corresponding to laminates in laminates of order no greater than k do not necessarily show up explicitly in the gradients, and thus the complexity of a finite element approximation is much reduced.

3. Reformulate $R_k f$ as a unconstrained optimization problem

To simplify the calculation of $R_k f(A)$, we reformulate it in the following way. Let $A \in R^{mn}$. Let $(\lambda_{i_1}, \lambda_{i_1 i_2}, \ldots, \lambda_{i_1 i_2 \cdots i_k}, A_{i_1 i_2 \cdots i_k})$ satisfy (R_k) and

$$A = \sum_{i_1,\ldots,i_k=0}^{1} \lambda_{i_1} \lambda_{i_1 i_2} \cdots \lambda_{i_1 i_2 \cdots i_k} A_{i_1 i_2 \cdots i_k}. \tag{21}$$

By definition 2.2, we have

$$A = \lambda_0 A_0 + \lambda_1 A_1, \ \ \operatorname{rank}(A_0 - A_1) \le 1, \ \ \lambda_0 \ge 0, \lambda_0 + \lambda_1 = 1. \tag{22}$$

Thus, there exist $\theta_- \in S^{m-1}$, $\phi_- \in S^{n-1}$, $\gamma_- \in R^1$ and $\tau_- \in [0,\ \pi/2]$ such that

$$A_0 = A^0(A, \theta_-, \phi_-, \tau_-, \gamma_-) \equiv A + \gamma_- \sin^2(\tau_-)\, \phi_- \otimes \theta_-, \tag{23}$$

$$A_1 = A^1(A, \theta_-, \phi_-, \tau_-, \gamma_-) \equiv A - \gamma_- \cos^2(\tau_-)\, \phi_- \otimes \theta_-, \tag{24}$$

where $\tau_- = \arcsin(\sqrt{(\lambda_1)})$ and S^{i-1} is the unit sphere in R^i centered at 0. Similarly, since

$$\begin{gathered} A_{i_1 \ldots i_\nu} = \lambda_{i_1 \ldots i_\nu 0} A_{i_1 \ldots i_\nu 0} + \lambda_{i_1 \ldots i_\nu 1} A_{i_1 \ldots i_\nu 1}, \\ \operatorname{rank}(A_{i_1 \ldots i_{\nu-1} 0} - A_{i_1 \ldots i_{\nu-1} 1}) \le 1, \\ \lambda_{i_1 \ldots i_\nu} \ge 0, \ \ \lambda_{i_1 \ldots i_{\nu-1} 0} + \lambda_{i_1 \ldots i_{\nu-1} 1} = 1, \end{gathered}$$

there exist $\phi_{i_1 \ldots i_\nu} \in S^{m-1}$, $\theta_{i_1 \ldots i_\nu} \in S^{n-1}$, $\gamma_{i_1 \ldots i_\nu} \in R^1$ and $\tau_{i_1 \ldots i_\nu} \in [0,\ \pi/2]$ such that

$$\begin{aligned} A_{i_1 \ldots i_\nu 0} &= A^0(A_{i_1 \ldots i_\nu}, \theta_{i_1 \ldots i_\nu}, \phi_{i_1 \ldots i_\nu}, \tau_{i_1 \ldots i_\nu}, \gamma_{i_1 \ldots i_\nu}), \\ A_{i_1 \ldots i_\nu 1} &= A^1(A_{i_1 \ldots i_\nu}, \theta_{i_1 \ldots i_\nu}, \phi_{i_1 \ldots i_\nu}, \tau_{i_1 \ldots i_\nu}, \gamma_{i_1 \ldots i_\nu}). \end{aligned}$$

Consequently, we have

$$A_{i_1 \cdots i_k} = A + \sum_{j \in I_{i_1 \cdots i_k}} \gamma_{j^-} ((1 - i(j)) \sin^2(\tau_{j^-}) - i(j) \cos^2(\tau_{j^-})) \phi_{j^-} \otimes \theta_{j^-}, \tag{25}$$

where the index set $I_{i_1 \cdots i_k} = \{i_1, i_1 i_2, \ldots, i_1 i_2 \cdots i_k\}$ and

$$i(j) = i_\nu, \quad \text{if } j = i_1 \cdots i_\nu, \tag{26}$$

$$j^- = \begin{cases} -, & \text{if } j = i_1, \\ i_1 \cdots i_{\nu-1}, & \text{if } j = i_1 \cdots i_\nu. \end{cases} \tag{27}$$

On the other hand, let $A_{i_1 \cdots i_k}$ be defined by (25), and let

$$\lambda_j = (1 - i(j)) \cos^2(\tau_{j^-}) - i(j) \sin^2(\tau_{j^-}), \ \ j \in I_{i_1 \cdots i_k}. \tag{28}$$

Then, it is easily verified that $(i_1, i_1 i_2, \ldots, i_1 i_2 \cdots i_k, A_{i_1 \cdots i_k})$ satisfy (R_k) and (21) holds. Consequently, we have

Theorem 3.1. *Let $A \in R^{mn}$. Let $A_{i_1 \cdots i_k}$ and λ_j, $j \in I_{i_1 \cdots i_k}$ be defined by* (25) *and* (28) *respectively. Then, we have*

$$R_k f(A) = \inf \sum_{i_1,\ldots,i_k=0}^{1} \lambda_{i_1} \lambda_{i_1 i_2} \cdots \lambda_{i_1 \cdots i_k} f(A_{i_1 \cdots i_k}), \tag{29}$$

where the infimum is taken among all $\{(\theta_{j^-}, \phi_{j^-}, \tau_{j^-}, \gamma_{j^-}),\ j \in I_{i_1 \cdots i_k}\}$ with $\theta_{j^-} \in S^{n-1}$, $\phi_{j^-} \in S^{m-1}$, $\tau_{j^-} \in [0,\ \pi/2]$ and $\gamma_{j^-} \in R^1$.

By Theorem 3.1, to calculate $R_k f(A)$ is to solve a nonlinear unconstrained optimization problem with $(m+n)(2^k-1)$ variables. For example, the first and second order rank-one convex envelope can be written as

$$R_1 f(A) = \inf\{\cos^2(\tau) f(A+\gamma \sin^2(\tau)\phi\otimes\theta) + \sin^2(\tau) f(A-\gamma \cos^2(\tau)\phi\otimes\theta)\}, \tag{30}$$

$$\begin{aligned} R_2 f(A) = \inf\{ &\cos^2(\tau_0)\cos^2(\tau) f(A+\gamma \sin^2(\tau)\phi\otimes\theta + \gamma_0 \sin^2(\tau_0)\phi_0\otimes\theta_0) \\ &+ \sin^2(\tau_0)\cos^2(\tau) f(A+\gamma \sin^2(\tau)\phi\otimes\theta - \gamma_0 \cos^2(\tau_0)\phi_0\otimes\theta_0) \\ &+ \cos^2(\tau_1)\sin^2(\tau) f(A-\gamma \cos^2(\tau)\phi\otimes\theta + \gamma_1 \sin^2(\tau_1)\phi_1\otimes\theta_1) \\ &+ \sin^2(\tau_1)\sin^2(\tau) f(A-\gamma \cos^2(\tau)\phi\otimes\theta - \gamma_1 \cos^2(\tau_1)\phi_1\otimes\theta_1)\}. \end{aligned} \tag{31}$$

Remark 3.1. In fact, (25)-(29) give an equivalent definition of the finite order rank-one convex envelope $R_k f$ of f. From the computational point of view, this definition yields a simplified code, while from the application point of view, the quantities involved in the optimization have obvious physical meanings. For example, θs are the unit normals to the interfaces between the laminates, and $\cos^2(\tau)$s and $\sin^2(\tau)$s are related to the ratios of band width of the corresponding laminates, *etc.*

4. Numerical Examples

In this section, we consider the Ericksen-James two dimensional energy model for elastic crystals [5, 6, 12] with $f(A) = \phi(A^T A)$ and

$$\phi(C) = \kappa_1(\operatorname{tr} C - 2)^2 + \kappa_2 C_{12}^2 + \kappa_3((\frac{C_{11}-C_{22}}{2})^2 - \varepsilon^2)^2, \tag{32}$$

where $C = \nabla u^T \nabla u$ is the right Cauchy-Green strain tensor, $\kappa_i > 0$, $i = 1,2,3$ are constant elastic moduli, and $\varepsilon > 0$ is the transformation strain.

It is well known [5, 6, 12] that the Ericksen-James energy has two symmetry related rotationally invariant elastic energy wells $SO(2)U_0$ and $SO(2)U_1$, where

$$U_0 = \begin{pmatrix} \sqrt{1-\varepsilon} & 0 \\ 0 & \sqrt{1+\varepsilon} \end{pmatrix}, \quad U_1 = \begin{pmatrix} \sqrt{1+\varepsilon} & 0 \\ 0 & \sqrt{1-\varepsilon} \end{pmatrix}, \tag{33}$$

and for a rotational matrix, where we denote $\eta_1 = \sqrt{1-\varepsilon}$ and $\eta_2 = \sqrt{1+\varepsilon}$,

$$R^\pm = \begin{pmatrix} \eta_1\eta_2 & \pm\varepsilon \\ \mp\varepsilon & \eta_1\eta_2 \end{pmatrix}, \tag{34}$$

U_0 and $R^\pm U_1$ are in rank-one connection, more precisely

$$R^\pm U_1 = U_0 + \mathbf{a}^\pm \otimes \mathbf{n}^\pm, \tag{35}$$

where $\mathbf{a}^\pm = \sqrt{2}\varepsilon(\eta_1,\ \mp\eta_2)^T$ and $\mathbf{n}^\pm = \frac{1}{\sqrt{2}}(1,\ \pm 1)^T$. In our numerical experiments, we take $\kappa_1 = 10$, $\kappa_2 = 3$, $\kappa_3 = 1$, $\varepsilon = 0.1$.

First, we consider affine boundary conditions $u(x) = R(\alpha)A_\lambda^- x$ on $\partial\Omega$ with $R(\alpha)$ being a rotational matrix and

$$A_\lambda^- = (1-\lambda)U_0 + \lambda R^- U_1, \quad 0 < \lambda < 1. \tag{36}$$

By [3], the Young measure of gradients derived from any minimizing sequence satisfying such a boundary condition is homogeneous and unique and is given by

$$\mu_x^\lambda \equiv \mu^\lambda = (1-\lambda)\delta_{R(\alpha)A_0} + \lambda\delta_{R(\alpha)A_1}, \tag{37}$$

where δ_E is the Dirac measure centered at E. Thus, the numerical results of $R_1 f(R(\alpha)A_\lambda^-)$ are expected to have

$$\theta = (\cos(\frac{\pi}{4}),\ -\sin(\frac{\pi}{4}))^T, \tag{38}$$

$$\phi = \pm\ (\cos(\alpha + \arctan(\frac{\eta_2}{\eta_1})),\ \sin(\alpha + \arctan(\frac{\eta_2}{\eta_1})))^T, \tag{39}$$

$$\tau = \arccos(\sqrt{\lambda}) \text{ or } \arcsin(\sqrt{\lambda}), \tag{40}$$

$$\gamma = 2\,\varepsilon \tag{41}$$

and

$$R_1 f(R(\alpha)A_\lambda^-) = 0. \tag{42}$$

In our algorithm, inexact linear search is applied to θ, ϕ, γ and τ successively. To be more precise, starting from an initial value $(\theta_0, \phi_0, \gamma_0, \tau_0)$, searching first along the descent direction with respect to θ, and then along the descent directions with respect to ϕ_0 and γ_0 successively, followed by the search for τ. The numerical experiments showed that the search for τ is usually more delicate, a simple local search along the descent direction with respect to τ often leads to a local minimizer. We found that a gradient method combined with a sectioning search turned out to be successful. The idea is that when the gradient respect to τ at τ_i is small, we search for τ_{i+1} in the set $[\tau_i - K\Delta\tau,\ \tau_i + K\Delta\tau]$ by the golden section search, where $\Delta\tau$ is the step length of the last search for τ and K is a parameter which is taken to be 5 in our numerical experiments. The above precedure is repeated until convergence is achieved, that is for example the increments of $(\theta, \phi, \gamma, \tau)$ are sufficiently small in a complete iteration cycle. Even though it is a local optimization algorithm, the numerical experiments showed that a global minimizer for $\lambda \in [0.05,\ 0.995]$ can always be located in at most five tries with the initial data $\theta_0 = (1,\ 0)^T$, $\tau_0 = \pi/4$, $\gamma_0 \in (0.05,\ 0.5)$ and $\phi_0 = (\cos(\alpha\pi/4),\ \sin(\alpha\pi/4))^T$, $\alpha = 0, \pm1, \pm2$ respectively. The numerical results of $R_1 f(R(\alpha)A_\lambda^-)$ for various λ and α are shown in table 1, where $E_r(\cdot)$ is the relative error of the corresponding quantity. We see that the algorithm produces very sharp numerical results (up to the machine precision!), especially for λ close to 0 or 1 when finite element methods usually can not find the microstructure. Furthermore, our numerical experiments showed that the algorithm is hundreds of times faster than finite element methods in obtaining a numerical approximation of a simple laminate.

Next, we consider numerical computations of $R_2 f$. Let

$$A_{\lambda,\mu,\sigma} = (1-\sigma)A_\mu^+ + \sigma Q_{\lambda,\mu}A_\lambda^-, \tag{43}$$

where A_λ^- is defined by (36),

$$A_\mu^+ = (1-\mu)U_0 + \mu R^+ U_1, \tag{44}$$

and $Q_{\lambda,\mu} = R(\alpha_{\lambda,\mu})$ is a rotational matrix with

$$\alpha_{\lambda,\mu} = \arctan\Big(\frac{a\sqrt{a^2+b^2-\eta_1^2\eta_2^2} - b\eta_1\eta_2}{b\sqrt{a^2+b^2-\eta_1^2\eta_2^2} + a\eta_1\eta_2}\Big), \tag{45}$$

TABLE 1. Numerical results for $R_1 f(R(\alpha)A_\lambda^-)$.

λ	α	$R_1 f(R(\alpha)A_\lambda^-)$	$E_r(\theta)$	$E_r(\phi)$	$E_r(\lambda)$	$E_r(\gamma)$
0.01	0	2.9×10^{-23}	6.5×10^{-12}	1.4×10^{-10}	3.6×10^{-9}	1.2×10^{-9}
0.50	0	7.2×10^{-27}	6.7×10^{-15}	4.3×10^{-13}	4.2×10^{-12}	2.4×10^{-15}
0.99	0	3.0×10^{-23}	7.2×10^{-12}	1.4×10^{-10}	3.7×10^{-11}	1.3×10^{-9}
0.15	$\pi/12$	2.3×10^{-25}	6.0×10^{-14}	3.4×10^{-12}	6.0×10^{-11}	2.2×10^{-11}
0.35	$\pi/8$	9.6×10^{-27}	7.2×10^{-15}	5.2×10^{-13}	6.7×10^{-12}	1.4×10^{-12}
0.48	$\pi/4$	3.7×10^{-27}	4.9×10^{-17}	3.1×10^{-13}	3.1×10^{-12}	1.1×10^{-13}
0.74	$\pi/3$	5.2×10^{-26}	2.2×10^{-14}	1.3×10^{-12}	6.9×10^{-12}	5.8×10^{-12}
0.87	$-\pi/6$	2.1×10^{-25}	7.0×10^{-14}	3.4×10^{-12}	9.2×10^{-12}	2.3×10^{-11}
0.995	$2\pi/3$	4.7×10^{-23}	1.5×10^{-11}	2.5×10^{-10}	3.5×10^{-11}	2.3×10^{-9}

and where $a=\eta_1\eta_2(1-2\lambda\mu\varepsilon^2)$, $b=(\lambda+\mu)\varepsilon-2\lambda\mu\varepsilon^3$. It is easily verified that $\operatorname{rank}(Q_{\lambda,\mu}A_\lambda^- - A_\mu^+)=1$. For given $\lambda,\ \mu,\ \sigma\in(0,\ 1)$, denote $C^{\lambda,\mu}=Q_{\lambda,\mu}A_\lambda^- - A_\mu^+$, we expect to have, for the numerical results of $R_2 f(A_{\lambda,\mu,\sigma})$,

$$\theta=\frac{\operatorname{sign}(C_{11}^{\lambda,\mu})}{\sqrt{(C_{11}^{\lambda,\mu})^2+(C_{12}^{\lambda,\mu})^2}}(C_{11}^{\lambda,\mu},\ C_{12}^{\lambda,\mu})^T,\quad \theta^\pm=\frac{1}{\sqrt{2}}(1,\ \pm1)^T, \tag{46}$$

$$\phi_1:\phi_2=C_{21}^{\lambda,\mu}:C_{11}^{\lambda,\mu},\quad \phi^+=\frac{1}{\sqrt{2}}\begin{pmatrix}\eta_1\\-\eta_2\end{pmatrix},\quad \phi^-=\frac{1}{\sqrt{2}}Q_{\lambda,\mu}\begin{pmatrix}\eta_1\\\eta_2\end{pmatrix}, \tag{47}$$

$$\tau=\arcsin\sqrt{\sigma},\quad \tau^+=\arcsin\sqrt{\mu},\quad \tau^-=\arcsin\sqrt{\lambda}, \tag{48}$$

$$\gamma=\left(\operatorname{tr}\left(C^{\lambda,\mu}\right)^T C^{\lambda,\mu}\right)^{1/2},\quad \gamma^\pm=2\,\varepsilon, \tag{49}$$

and

$$R_2 f(A_{\lambda,\mu,\sigma})=0. \tag{50}$$

In our numerical experiments, inexact linear search along descent directions is applied successively to $\theta^\pm$, $\phi^\pm$, $\gamma^\pm$ and $\tau^\pm$, followed by a golden section search for $\tau^\pm$ as in the case of $R_1 f$, then a similar search is applied to θ, ϕ, γ and τ. The procedure is repeated until a convergence, say the increments in a complete iteration are sufficiently small, is achieved. An approximation for a global minimizer of $R_2 f(A_{\lambda,\mu,\sigma})$ can usually be found in a few tries as in the case of $R_1 f$. Numerical results of $R_2 f(A_{\lambda,\mu,\sigma})$ for various $(\lambda,\ \mu,\ \sigma)$ are shown in table 2, where $\lambda=\sigma$, $\lambda^-=\lambda$, $\lambda^+=\mu$, and where the quantities in the $+$ and $-$ rows correspond to the variables with superscripts $+$ and $-$ respectively. Numerical experiments on $R_2 f(A_{\lambda,\mu,\sigma})$ also suggest that the solution of $R_2 f(A)$ is not unique (see Table 3). It is worth pointing out that while the algorithm given here can obtain very sharp numerical results for second order laminates, the finite element methods generally fail so far to produce reasonably accurate numerical results for such laminates.

TABLE 2. Numerical results for $R_2 f(A_{\lambda^-,\lambda^+,\lambda})$.

	λ	$R_2 f(A_{\lambda^-,\lambda^+,\lambda})$	$E_r(\theta)$	$E_r(\phi)$	$E_r(\tau)$	$E_r(\gamma)$
	0.5	1.4×10^{-26}	1.4×10^{-14}	1.7×10^{-14}	9.2×10^{-17}	1.6×10^{-15}
$+$	0.5	1.5×10^{-26}	1.7×10^{-16}	5.8×10^{-13}	5.8×10^{-12}	2.4×10^{-14}
$-$	0.5	1.3×10^{-26}	9.9×10^{-15}	6.1×10^{-13}	6.1×10^{-12}	6.4×10^{-15}
	0.31	8.3×10^{-26}	2.5×10^{-13}	4.5×10^{-14}	1.1×10^{-14}	9.1×10^{-13}
$+$	0.73	6.0×10^{-26}	7.7×10^{-15}	1.4×10^{-12}	7.5×10^{-12}	1.0×10^{-11}
$-$	0.22	1.4×10^{-25}	5.0×10^{-14}	2.3×10^{-12}	3.9×10^{-11}	2.0×10^{-11}
	0.85	2.7×10^{-26}	3.3×10^{-15}	5.2×10^{-15}	2.5×10^{-12}	9.4×10^{-16}
$+$	0.64	3.3×10^{-26}	7.0×10^{-15}	9.9×10^{-13}	7.1×10^{-12}	4.7×10^{-12}
$-$	0.72	2.5×10^{-26}	1.1×10^{-14}	8.8×10^{-13}	5.2×10^{-12}	7.3×10^{-12}

TABLE 3. Global and local minimizers of $R_2 f(A_{\lambda,\mu,\sigma})$.

		solution 1	solution 2
	$R_2 f(A_{\lambda,\mu,\sigma})$	1.41538×10^{-26}	5.36675×10^{-26}
$\lambda = 0.5$	$\arctan(\theta_1/\theta_2)$	-1.45482×10^{-14}	4.710914311897866
$\mu = 0.5$	$\arctan(\phi_1/\phi_2)$	1.523225189602783	3.092546824279279
$\sigma = 0.5$	$\arcsin(\sqrt{\sigma})$	0.7853981633974487	0.78539844951448412
	γ	-0.01002509414234170	0.01002526347478143

Finally, we consider to solve the problem

$$\text{(P)} \quad \inf_{u \in \mathbb{U}(Ax,\, \Omega)} \int_\Omega f(\nabla u(x))\, dx$$

by using the first order rank-one convex envelope $R_1 f$ and by using the mesh transformation method and the periodic relaxation method [16, 17], that is, we apply the mesh transformation method and the periodic relaxation method to the problem

$$(\mathrm{R_1P}) \quad \inf_{u \in \mathbb{U}(Ax,\, \Omega)} \int_\Omega R_1 f(\nabla u(x))\, dx.$$

As in [17] (see also [15, 16]), let $D = (-1,\ 1)^2$, and let a family of regular triangulations $\mathfrak{T}_h(D)$ [4] for $h_N = 2\sqrt{2}/N$ with $N \geq 2$ be introduced by the lines

$$\begin{cases} x = -1 + \frac{2}{N} i, & 0 \leq i \leq N; \\ y = -1 + \frac{2}{N} j, & 0 \leq j \leq N; \\ y = \ \ x - \frac{2}{N} k, & -N+1 \leq k \leq N-1. \end{cases}$$

Denote $\mathbb{U}_h(D)$ the set of piece wise affine conforming finite element functions. Denote

$$S_1^{\pm} = \{(\pm 1,\ y) : |y| \leq 1\}, \quad S_2^{\pm} = \{(x,\ \pm 1) : |x| \leq 1\}, \quad V(D) = \{(\pm 1,\ \pm 1)\},$$

which are the four sides and the four vertices of D respectively.

For a given $R \in SO(2)$, define

$$\begin{aligned} P(D;\ R) = \{ & L \in W^{1,\infty}(D; R^2) : L^{-1} \in W^{1,\infty}(L(D); R^2) \text{ and } \det \nabla L > 0, \\ & a.e. \text{ in } D,\ L(x) = R(x), \forall x \in V(D), (L-R)|_{S_i^+} = (L-R)|_{S_i^-},\ i = 1,2\}, \end{aligned}$$

$$\tilde{\mathbb{U}}(A;D) = \{u \in W^{1,\infty}(D;\ R^2) : u(x) = A\,x, \forall x \in V(D),$$
$$(u(x) - A\,x)|_{S_i^+(D)} = (u(x) - A\,x)|_{S_i^-(D)},\ i = 1,2\},$$

where by $g|_{S_i^+} = g|_{S_i^-}$ we mean that

$$g(x,1) = g(x,-1),\ \ \forall x \in [-1,1], \quad \text{and}\ \ g(1,y) = g(-1,y),\ \ \forall y \in [-1,1].$$

Define

$$P(D) = \{L \in P(D;\ R) : \text{for some } R \in SO(2)\},$$
$$P_h(D) = \{L \in P(D) : L|_K \text{ is affine } \forall K \in \mathfrak{T}_h\},$$
$$\tilde{\mathbb{U}}_h(A;D) = \mathbb{U}_h(D) \cap \tilde{\mathbb{U}}(A;D).$$

The deduced discrete problem is

$$(51) \qquad (\mathrm{DR_1P}) \quad \begin{cases} \text{find } (u,\ L) \in \tilde{\mathbb{U}}_h(0;\ D) \times P_h(D) \text{ such that} \\ R_1F(u,L;\ D) = \inf_{(u',L') \in \tilde{\mathbb{U}}_h(0;\ D) \times P_h(D)} R_1F(u',L';\ D), \end{cases}$$

where

$$(52) \qquad R_1F(u,L;\ D) = \int_D R_1f(A + \nabla u(x)(\nabla L(x))^{-1}) \det \nabla L(x)\,dx.$$

In our numerical experiments, the problem $(\mathrm{DR_1P})$ is solved by the conjugate gradient method, in which the gradient of $R_1f(B)$ is given by

$$(53) \qquad \nabla R_1f(B) = \cos^2\tau\,\nabla f(B + \gamma\,\sin^2\tau\,\phi \otimes \theta) + \sin^2\tau\,\nabla f(B - \gamma\,\cos^2\tau\,\phi \otimes \theta),$$

where $(\theta,\phi,\tau,\gamma)$ is a minimizer of (30).

In the numerical example presented below, we set $A = A_{\lambda,\mu,\sigma}$ with $\lambda = 0$, $\mu = \sigma = 0.5$ (see (43)) and $N = 4$. Thus, the Young measure is given by [1, 3] (see also (16) and (43))

$$(54) \qquad \nu_x \equiv \nu = \frac{1}{2}\delta_{Q_{0,1/2}U_0} + \frac{1}{4}\delta_{U_0} + \frac{1}{4}\delta_{R^+U_1}.$$

Let $(u_h,\ L_h)$ be a numerical solution to (51), and let

$$A_h(x) = A + \nabla u_h(x)\,(\nabla L_h(x))^{-1}.$$

Denote

$$D(Q_{0,1/2}U_0) = \{x \in D : \|A_h(x) - Q_{0,1/2}U_0\| < \|A_h(x) - A_\mu^+\|\},$$
$$\sigma_h = \operatorname{meas} D(Q_{0,1/2}U_0) / \operatorname{meas} D,$$
$$e(\sigma) = |\sigma - \sigma_h|$$
$$e_\infty(Q_{0,1/2}U_0) = \max\{\|A_h(x) - Q_{0,1/2}U_0\| : x \in D(Q_{0,1/2}U_0)\}.$$

For an element $K \in \mathfrak{T}_h(D)$ such that $\overset{\circ}{K} \subset D \setminus D(Q_{0,1/2}U_0)$, let $(\theta_K^+, \phi_K^+, \lambda_K^+, \gamma_K^+)$ be the numerical solution of $R_1f(A_h(K))$. Denote

$$A_h^+(K) = A_h(K) + \lambda_K^+\,\gamma_K^+\,\phi_K^+ \otimes \theta_K^+,$$
$$A_h^-(K) = A_h(K) - (1 - \lambda_K^+)\,\gamma_K^+\,\phi_K^+ \otimes \theta_K^+,$$
$$e(\lambda^+) = \max\{|\lambda^+ - \frac{1}{2}| : \overset{\circ}{K} \subset D \setminus D(Q_{0,1/2}U_0)\},$$
$$e_\infty(U_0) = \max\{\min\{\|A_h^\pm(K) - U_0\|\} : \overset{\circ}{K} \subset D \setminus D(Q_{0,1/2}U_0)\},$$

$$e_\infty(R^+U_1) = \max\{\min\{\|A_h^\pm(K) - R^+U_1\|\} : \overset{\circ}{K} \subset D \setminus D(Q_{0,1/2}U_0)\}.$$

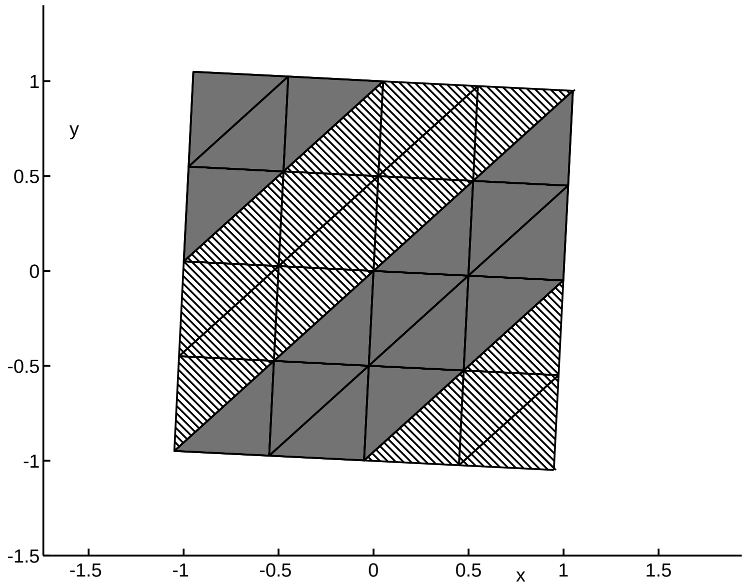

Figure 1. A periodic brick of laminates in laminates.

Analytically, for the Young measure to be in the form of (53), we expect

$$e(\sigma) = e(\lambda^+) = e_\infty(Q_{0,1/2}U_0) = e_\infty(U_0) = e_\infty(R^+U_1) = 0.$$

The results of a numerical experiment are shown in table 4. Figure 1 shows a periodic brick given by a numerical solution of ($\mathrm{DR_1P}$), where the black and white stripes represent the laminates oscillating between U_0 and R^+U_1, and where on the grey elements the deformation gradient is about $Q_{0,1/2}U_0$.

Table 4. Numerical results of ($\mathrm{DR_1P}$).

$R_1F(u, L; D)$	$e(\sigma)$	$e(\lambda^+)$	$e_\infty(Q_{0,1/2}U_0)$	$e_\infty(U_0)$	$e_\infty(R^+U_1)$
3.3×10^{-24}	3.0×10^{-13}	1.5×10^{-10}	1.9×10^{-12}	5.5×10^{-11}	4.3×10^{-11}

The above numerical experiments show that microstructures with laminates in laminates can be solved with high precision by applying the finite order rank-one convex envelope. We also see that a combination of the finite order rank-one convex envelope and the periodic relaxation method is very successful (for a comparison see for example [21]) and thus is worth of further investigations on its applications to nonquasiconvex variational problems with boundary conditions which do not lead to homogeneous microstructures with laminates in laminates.

References

[1] J. M. Ball and R. D. James, *Fine phase mixtures as minimizers of energy.* Arch. Rat. Mech. Anal., 100(1987), pp. 13-52.

[2] J.M. Ball, *A version of the fundamental theorem for Young measures.* In Partial Differential Equations and Continuum models of Phase Transitions, Lecture Notes in Physics, No. 344, M. Rascle, D. Serre and M. Slemrod, eds., Springer-Verlag, New York (1989), pp. 207-215.

[3] J. M. Ball and R. D. James, *Proposed experimental test of a theory of fine microstructure and the two-well problem.* Phil. Trans. R. Soc. Lond. 338A(1992), pp. 389-450.

[4] P.G. Ciarlet, The Finite Element Method for Elliptic Problems. North-Holland, Amsterdam, 1978.

[5] C. Collins, *Computation of Twinning.* In Microstructure and Phase Transitions, IMA Volumes in Mathematics and Its Applications, Vol.54, J. Ericksen, R. James, D. Kinderlehrer and M. Luskin, eds, Springer-Verlag, New York, (1993), pp. 39-50.

[6] C. Collins, M. Luskin and J. Riordan, *Computational results for a two-dimensional model of crystalline microstructure*, in Microstructure and Phase Transitions, IMA Volumes in Mathematics and Its Applications, Vol.54, J. Ericksen, R. James, D. Kinderlehrer and M. Luskin, eds, Springer-Verlag, New York, (1993), pp. 51-56.

[7] C. R. Collins, *Convergence of a reduced integration method for computing microstructures.* SIAM J. Numer. Anal., 35(1998), pp. 1271-1298.

[8] B. Dacorogna, Direct Methods in the Calculus of Variations, Applied Mathematical Sciences, 78, Springer-Verlag, Berlin, 1989.

[9] G. Dolzmann and N. J. Walkington, *Bounds on the effective energy by rank-one convexification*, in Enumath 97, H. -G. Bock, F. Brezzi, R. Glowinski, G. Kanschat, Y. A. Kuznetsov, J. Périaux, R. Rannacher, eds., (1998), pp. 270-277.

[10] G. Dolzmann, *Numerical computation of rank-one convex envelopes.* SIAM J. Numer. Anal., 36(1999), pp. 1621-1635.

[11] G. Dolzmann and N. J. Walkington, *Estimates for numerical approximations of rank-one convex envelopes.* To appear in Numer. Math..

[12] P.-A. Gremaud, *Numerical analysis of a nonconvex variational problem related to solid-solid phase transitions.* SIAM J. Numer. Anal., 31(1994), pp. 111-127.

[13] Z.-P. Li, *Simultaneous numerical approximation of microstructures and relaxed minimizers.* Numer. Math., 78 (1997), pp. 21-38.

[14] Z.-P. Li, *Laminated microstructure in a variational problem with a non-rank-one connected double well potential.* J. Math. Anal. Appl., 217(1998), pp. 490-500.

[15] Z.-P. Li, *Rotational transformation method and some numerical techniques for computing microstructures.* Math. Models Meth. Appl. Sci., 8(1998), pp. 985-1002.

[16] Z.-P. Li, *A mesh transformation method for computing microstructures.* Research Report No.24, Institute of Mathematics and School of Mathematical Sciences, Peking University, 1998

[17] Z.-P. Li, *A periodic relaxation method for computing microstructures.* Appl. Numer. Math., 32(2000), pp. 291-303.

[18] M. Luskin, *On the computation of crystalline microstructure.* Acta Numerica 5(1996), pp. 191-257.

[19] C. B. Morrey, **Multiple Integrals in the Calculus of Variations**. Springer-Verlag, New York, 1966.

[20] J. Matoušek and P. Plechàč, *On functional separately convex hulls*, Discrete and Comp. Geometry, 19(1998), pp. 105-130.

[21] R. A. Nicolaides, N. Walkinton and H. Wang, *Numerical methods for a nonconvex optimization problem modeling martensitic microstructure.* SIAM J. Sci. Comput., 18(1997), pp. 1122-1141.