ROTATION TRANSFORMATION METHOD AND SOME NUMERICAL TECHNIQUES FOR THE COMPUTATION OF MICROSTRUCTURES

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Abstract. A rotation transformation method and an incremental crystallization method are developed to overcome some of the difficulties involved in the computation of microstructures. The numerical method based on these techniques is proved to converge. To increase further the accuracy of the computation, a technique is applied to remove the boundary effect of the numerical solutions. Numerical results for a double well problem are given to show the efficiency of the techniques.

1. Introduction

In many physical problems, for example in material sciences and nonlinear elasticity [1, 2], one is often lead to consider problems of minimizing an integral functional

$$F(u;\ \Omega) = \int_\Omega f(\nabla u(x))\, dx \tag{1.1}$$

in a set of admissible functions

$$\mathbb{U}(u_0;\ \Omega) = \{u \in W^{1,p}(\Omega; R^m) : u = u_0, \text{ on } \partial\Omega\}, \tag{1.2}$$

where $\Omega \in R^n$ is a bounded open set with a Lipschitz continuous boundary, and where the integrand $f : R^{mn} \to R^1$ is continuous, nonquasiconvex [3, 4] and satisfies

(h1): $\max\{0, a_1 + b_1|\xi|^p\} \le f(\xi) \le a_2 + b_2|\xi|^p$,
(h2): $|f(\xi) - f(\eta)| \le C(1 + |\xi|^{p-1} + |\eta|^{p-1})(|\xi - \eta|)$,

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where $a_1 \in R^1$, $a_2 > 0$, $b_2 \geq b_1 > 0$ and $C > 0$ are constants. It is well known that, in general, such a problem fails to have a solution [3, 4, 5], and the minimizing sequences of $F(\cdot;\ \Omega)$ in $\mathbb{U}(u_0;\ \Omega)$, which develop finer and finer oscillations, can converge in the sense of Young measures and lead to microstructures [1, 2, 6, 7]. To compute the microstructures , or more precisely, to find numerically a minimizing sequence of $F(\cdot;\ \Omega)$ in $\mathbb{U}(u_0;\ \Omega)$ consisting of finer and finer oscillations, with finite element method for instance, involves many difficulties (see [8] for a review). Many numerical methods have been developed to compute the microstructures, for example gradient iterative methods [9, 10], methods using simulated annealing and Monte Carlo techniques [11, 12] and multilevel techniques [13].

It has long been realized that the local minimizers of the corresponding discrete problems not only depend on the original problem but also depend strongly on the mesh and the shape functions. A mesh which is not compatible with the microstructure, i.e. the planes across which the finite element deformation gradients can be discontinuous are not parallel to the interfaces of the microstructure, may produce oscillations which do not converge to the microstructures of the original problem and lead to a pseudo-microstructure (see Sec. 3 for an example), in other words, the sequence with such oscillations is not a minimizing sequence of the original problem. Thus, to choose the right orientation of the mesh, or alternatively the right orientation of the reference configuration is of crucial importance to the computation of microstructures (see [8, 10]).

The purpose of the present paper is to develop an efficient high accuracy numerical method for double well problems with linear boundary data. Double well problems have important applications in material sciences [1], and an efficient high accuracy numerical method for such problems with linear boundary data will provide us a basic tool to study further the numerical computations of microstructures for the double well problems in the general cases.

It is known that with a right orientation the corresponding numerical solutions converge to the right microstructures for multiple well problems [14, 15, 16]. Hence, it makes sense to introduce the orientation as a unknown to the discrete problem. This motivates the rotation transformation method in which a finite element deformation u and a rotation transformation matrix

$R \in SO(n)$ are to be found to minimize the functional

$$\int_{\hat{\Omega}} f(\nabla u(x) R^{-1})\, dx,$$

where $\hat{\Omega} \subset R^n$ is such that $\bigcap_{R \in SO(n)} R(\hat{\Omega}) \supset \Omega$ (see Sec.2 for details). It is shown in Sec. 2 that the finite element solutions thus obtained can be used to construct a minimizing sequence of $F(\cdot;\ \Omega)$ in $\mathbb{U}(u_0;\ \Omega)$.

One of the other main difficulties is that the patches of the numerical microstructures forms in the various parts of the domain may not be compatible to each other and thus result in energy accumulation in the interface areas of these patches (see Sec. 3 for an example). In other words, local minimizers are usually obtained even if the mesh is well orientated. To overcome this difficulty, the incremental crystallization method is introduced in Sec. 3. The idea is to compute first on a small subset of the domain to produce a crystal core, that is a numerical microstructure defined on the small subset, and then to let the crystal grow in a neighborhood of the core incrementally until the whole domain is covered. The method can be viewed as a simulated crystallization procedure.

To satisfy the boundary conditions, a boundary layer usually forms in the numerical solutions, this causes energy accumulation near the boundary. Such a boundary effect is a factor that affects the accuracy of the computation of microstructures. The effect reduces as the mesh refines. Thus, to obtain numerical results with high accuracy usually needs the mesh to be sufficiently fine. The following technique, which we call the boundary layer removal technique, can be used to reduce the boundary effect. In the discrete problems, Ω is replaced by a slightly bigger open set $\Omega' \supset \overline{\Omega}$ and the boundary condition is set to

$$u = u_0 \qquad \text{on } \partial\Omega', \tag{1.3}$$

furthermore, a term of the form

$$\mu h^{-q} \int_{\Omega'} |u - u_0|^p \, dx, \tag{1.4}$$

where h is the mesh size and $\mu > 0$, $q \in (0,\ p)$ are parameters, is added to the functional $F(u; \Omega')$ to be minimized. The extra term (1.4) guarantees that any weakly convergent minimizing sequence $\{u_h\}$ of the resulted functional

$$F_\mu(u; \Omega') = F(u; \Omega') + \mu h^{-q} \int_{\Omega'} |u - u_0|^p \, dx$$

in $W^{1,p}(\Omega'; R^m)$ must satisfy

$$u_h \rightharpoonup u_0 \qquad \text{in } W^{1,p}(\Omega'; R^m), \tag{1.5}$$

where "$\rightharpoonup$" means "converges weakly to". By Sobolev's imbedding theorems [17], (1.5) implies

$$u_h \longrightarrow u_0 \qquad \text{in } L^p(\partial\Omega; R^m). \tag{1.6}$$

That is the boundary condition is satisfied by the sequence $\{u_h|_\Omega\}$ in a weaker sense. We take $\{u_h|_\Omega\}$ as the numerical microstructure to the original problem. The technique removes the boundary layer, and thus can produce better approximations. Furthermore, the technique can be used naturally in the rotation transformation method to guarantee its convergence (see Sec. 2 and Sec. 3).

In Sec. 2, the rotation transformation method is given and the convergence of the method is proved. In Sec. 3, implementation of the rotation transformation method is discussed and the incremental crystallization technique is introduced. Numerical results are given and compared in Sec. 3 which show the efficiency of the techniques developed in this paper.

2. Rotation transformation method

Let $\Omega \subset R^n$ be a bounded open set with a Lipschitz continuous boundary. Let $f : R^{mn} \to R^1$ be a continuous function satisfying (h1) and (h2) with $p > 1$. Consider the problem of minimizing the functional

$$F(u;\ \Omega) = \int_\Omega f(\nabla u(x))\, dx \tag{2.1}$$

in a set of admissible functions

$$\mathbb{U}((A, a); \Omega) = \{u \in W^{1,p}(\Omega; R^m) : u(x) = A\,x + a, \text{ on } \partial\Omega\}. \tag{2.2}$$

Without loss of generality, assume

$$\Omega \subset B(0; r), \tag{2.3}$$

where $B(0; r) = \{x \in R^n : \|x\| < r\}$ is a ball in R^n. Define

$$\hat{\Omega} = (-r,\ r)^n. \tag{2.4}$$

We have obviously

$$\Omega \subset B(0; r) = \bigcap_{R \in SO(n)} R(\hat{\Omega}), \tag{2.5}$$

where $SO(n)$ is the set of all $n \times n$ rotational transformation matrices with the determinant $\det R = 1$. $\hat{\Omega}$ will serve as the working domain for our numerical computation.

Lemma 2.1. *For any $R \in SO(n)$, we have*

$$\inf_{u \in \mathbb{U}((A,a);R(\hat{\Omega}))} \frac{1}{\mathrm{meas}(\hat{\Omega})} F(u;\ R(\hat{\Omega})) = \inf_{u \in \mathbb{U}((A,a);\Omega)} \frac{1}{\mathrm{meas}(\Omega)} F(u;\ \Omega), \tag{2.6}$$

where $\mathrm{meas}(\cdot)$ *is the Lebesgue measure in R^n.*

Proof. It is well known [3, 7, 18] that

$$Qf(A) = \inf_{u \in \mathbb{U}((A,a);\Omega')} \frac{1}{\mathrm{meas}(\Omega')} F(u;\ \Omega')$$

for all bounded open set $\Omega' \subset R^n$, where $Qf(\cdot)$ is the quasiconvex envelope of $f(\cdot)$ [3, 4, 5]. Thus the lemma follows, since $\mathrm{meas}(\hat{\Omega}) = \mathrm{meas}(R(\hat{\Omega}))$ for all $R \in SO(n)$. □

Lemma 2.2. *For any $R \in SO(n)$ and $u \in \mathbb{U}((A,a);R(\hat{\Omega}))$, let $\hat{u}(x) : \hat{\Omega} \to R^m$ be defined by*

$$\hat{u}(x) = u(R\,x) - A\,R\,x - a. \tag{2.7}$$

Then $\hat{u} \in \mathbb{U}((0,0);\hat{\Omega})$ and

$$\int_{\hat{\Omega}} f(A + \nabla \hat{u}(x) R^{-1})\, dx = F(u;\ R(\hat{\Omega})). \tag{2.8}$$

Proof. $\hat{u} \in \mathbb{U}((0,0);\hat{\Omega})$ follows directly from (2.7) and (2.3). By a change of integral variables, we have

$$\int_{R(\hat{\Omega})} f(\nabla u(y))\, dy = \int_{\hat{\Omega}} f(A + \nabla \hat{u}(x) R^{-1}) \det R\, dx.$$

Since $\det R = 1$, (2.8) follows. □

Lemma 2.3. *Let $R \in SO(n)$. Define*

$$F(u, R;\ \hat{\Omega}) = \int_{\hat{\Omega}} f(A + \nabla u(x) R^{-1})\, dx. \tag{2.9}$$

Then

$$\inf_{u \in \mathbb{U}((0,0);\hat{\Omega})} \frac{1}{\mathrm{meas}(\hat{\Omega})} F(u, R;\ \hat{\Omega}) = \inf_{u \in \mathbb{U}((A,a);\Omega)} \frac{1}{\mathrm{meas}(\Omega)} F(u;\ \Omega). \tag{2.10}$$

Proof. The lemma is a direct corollary of lemma 2.1 and lemma 2.2. □

Let $\mathfrak{T}_h$ be regular triangulations of $\hat{\Omega}$ with mesh sizes h [19]. Let

$$\mathbb{U}_h = \{u \in (C(\overline{\hat{\Omega}}))^m : u|_K \text{ is affine } \forall K \in \mathfrak{T}_h \text{ and } u = 0 \text{ on } \partial\hat{\Omega}\}, \tag{2.11}$$

and

$$\mathbb{U}_h((A, a); \hat{\Omega}) = \{u(x) = A\,x + a + u'(x) : u' \in \mathbb{U}_h\}. \tag{2.12}$$

The key step of the rotation transformation method is to solve the following discrete problem :

$$(DP) \quad \begin{cases} \text{find } (u,\ R) \in \mathbb{U}_h((0,0);\ \hat{\Omega}) \times SO(n) \text{ such that} \\ F(u, R;\ \hat{\Omega}) = \inf_{(u',R') \in \mathbb{U}_h((0,0);\ \hat{\Omega}) \times SO(n)} F(u', R';\ \hat{\Omega}). \end{cases} \tag{2.13}$$

Theorem 2.1. *The problem (DP) has at least one solution.*

Proof. Since (h1) implies the boundedness of a minimizing sequence of (DP), the continuity of $f(\cdot)$ and the relative compactness of bounded subset in $\mathbb{U}_h((0,0);\ \hat{\Omega}) \times SO(n)$ give the theorem. □

Theorem 2.2. *Let $(u_{h_i},\ R_{h_i}) \in \mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \times SO(n)$ be a sequence of minimizers of $F(\cdot,\cdot;\ \hat{\Omega})$ in $\mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \times SO(n)$ with $\lim_{i\to\infty} h_i = 0$. Then*

$$\lim_{i\to\infty} F(u_{h_i},\ R_{h_i};\ \hat{\Omega}) = \inf_{u \in \mathbb{U}((A,a);\hat{\Omega})} F(u,\ \hat{\Omega}). \tag{2.14}$$

Proof. It follows from lemma 2.3 that

$$\inf_{u \in \mathbb{U}((A,a);\hat{\Omega})} F(u;\ \hat{\Omega}) = \inf_{u \in \mathbb{U}((0,0);\hat{\Omega})} F(u, R_{h_i};\ \hat{\Omega}) \le F(u_{h_i}, R_{h_i};\ \hat{\Omega}). \tag{2.15}$$

On the other hand, for any fixed $R \in SO(n)$, we have

$$F(u_{h_i}, R_{h_i};\ \hat{\Omega}) \le \inf_{u \in \mathbb{U}_{h_i}((0,0);\hat{\Omega})} F(u, R;\ \hat{\Omega}). \tag{2.16}$$

By the standard finite element approximation theory [19], we have

$$\lim_{h_i \to 0} \inf_{u \in \mathbb{U}_{h_i}((0,0);\hat{\Omega})} F(u, R;\ \hat{\Omega}) = \inf_{u \in \mathbb{U}((0,0);\hat{\Omega})} F(u, R;\ \hat{\Omega}). \tag{2.17}$$

Combining (2.17) with (2.15), (2.16) and (2.10), we obtain (2.14). □

Corollary 2.1. *As a consequence of lemma 2.1 and theorem 2.2, we have*

$$\begin{aligned} Qf(A) &= \frac{1}{\mathrm{meas}(\Omega)} \inf_{u \in \mathbb{U}((A,a);\Omega)} F(u;\ \Omega) \\ &= \frac{1}{\mathrm{meas}(\hat{\Omega})} \lim_{h \to 0} \inf_{(u,R) \in \mathbb{U}_h((0,0);\ \hat{\Omega}) \times SO(n)} F(u, R;\ \hat{\Omega}), \end{aligned}$$

where $Qf(\cdot)$ is the quasiconvex envelope of $f(\cdot)$ [3, 4, 5].

Theorem 2.3. *Let $(u_{h_i},\ R_{h_i}) \in \mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \times SO(n)$ be a sequence of minimizers of $F(\cdot,\cdot;\ \hat{\Omega})$ in $\mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \times SO(n)$ with $\lim_{i\to\infty} h_i = 0$. Assume that there exists a $R \in SO(n)$ such that*

$$\lim_{i \to \infty} R_{h_i} = R. \tag{2.18}$$

Then $\{u_{h_i}\}$ is a minimizing sequence of $F(\cdot, R;\ \hat{\Omega})$ in $\mathbb{U}((0,0);\ \hat{\Omega})$, that is $\{u_{h_i}\} \subset \mathbb{U}((0,0);\ \hat{\Omega})$ and

$$\lim_{i \to \infty} F(u_{h_i}, R;\ \hat{\Omega}) = \inf_{u \in \mathbb{U}((0,0);\hat{\Omega})} F(u, R;\ \hat{\Omega}). \tag{2.19}$$

Proof. Since $\mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \subset \mathbb{U}((0,0);\hat{\Omega})$ for all h_i, we only need to show (2.19). In view of (2.17), it is sufficient to prove that

$$\lim_{i \to \infty} (F(u_{h_i}, R;\ \hat{\Omega}) - F(u_{h_i}, R_{h_i};\ \hat{\Omega})) = 0. \tag{2.20}$$

Since, by (h1), u_{h_i} are uniformly bounded in $W^{1,p}(\hat{\Omega};\ R^m)$, $\nabla u_{h_i} R_{h_i}^{-1}$ and $\nabla u_{h_i} R^{-1}$ are uniformly bounded in $L^p(\hat{\Omega}; R^m)$ and by (2.18), taking a subsequence if necessary, we have

$$\nabla u_{h_i}(R^{-1} - R_{h_i}^{-1}) \longrightarrow 0, \quad \text{a.e. in } \hat{\Omega}.$$

Thus, (2.20) follows from the inequality

$$|f(A + \nabla u_{h_i} R^{-1}) - f(A + \nabla u_{h_i} R_{h_i}^{-1})| \le \hat{L} |\nabla u_{h_i}|^p |R^{-1} - R_{h_i}^{-1}|,$$

which is a consequence of (h2), the uniform boundedness of ∇u_{h_i} in $L^p(\hat{\Omega};\ R^m)$ and (2.18). □

As a consequence of theorem 2.3 and lemmas 2.1-2.3, we have

Corollary 2.2. *Let* $(u_{h_i}, R_{h_i}) \in \mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \times SO(n)$ *be minimizers of* $F(\cdot,\cdot;\hat{\Omega})$ *in* $\mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \times SO(n)$ *with* $\lim_{i\to\infty} h_i = 0$ *such that* (2.18) *is satisfied. Let* $\tilde{u}_{h_i} : R_{h_i}(\hat{\Omega}) \to R^m$ *be defined by*

$$\tilde{u}_{h_i}(x) = A\,x + a + u_{h_i}(R_{h_i}^{-1}(x)), \tag{2.21}$$

Then $\tilde{u}_{h_i} \in \mathbb{U}((A,a);\ R_{h_i}(\hat{\Omega}))$ *and*

$$\lim_{i\to\infty} F(\tilde{u}_{h_i};\ R_{h_i}(\hat{\Omega})) = \inf_{u\in\mathbb{U}((A,a);\hat{\Omega})} F(u,\ \hat{\Omega}). \tag{2.22}$$

Proof. It is obvious that $\tilde{u}_{h_i} \in \mathbb{U}((A,a);\ R_{h_i}(\hat{\Omega}))$. By lemma 2.2, we have

$$F(\tilde{u}_{h_i};\ R_{h_i}(\hat{\Omega})) = F(u_{h_i}, R_{h_i};\ \hat{\Omega}).$$

Without loss generality, we assume that $\lim_{i\to\infty} R_{h_i} = R$ for some $R \in SO(n)$. Thus (2.22) follows from (2.6), (2.10), (2.19) and (2.20). □

It is well known that under the hypotheses (h1) and (h2), for any $R \in SO(n)$ there exists a minimizing sequence $\{u_i\}$ such that [7]

$$u_i(x) - A\,x - a \rightharpoonup 0 \qquad \text{in } W^{1,p}(R(\hat{\Omega});\ R^m), \tag{2.23}$$

and it is proved by Kinderlehrer and Pedredal [20, 21] that such a minimizing sequence satisfies

(C): $\{|\nabla u_i|^p\}$ are precompact [22] in $W^{1,p}(R(\hat{\Omega});\ R^m)$.

To guarantee that the obtained numerical solutions satisfy (2.23) and thus satisfy also the condition (C), we added a penalty term

$$\mu h^{-q} \int_{\hat{\Omega}} |u(x)|^p\, dx$$

to $F(u, R;\ \hat{\Omega})$ in (DP) with $\mu > 0$ and $0 < q < p/2$.

If the sequence $u_i = \tilde{u}_{h_i}$ defined by (2.21) satisfies (2.23), then it can be used to construct a minimizing sequence of $F(\cdot;\ \Omega)$ in $\mathbb{U}((A,a);\ \Omega)$ as follows.

Denote

$$\delta_i = \min\{1,\ \max\{h_i,\ \int_{R_{h_i}(\hat{\Omega})} |\tilde{u}_{h_i}(x) - A\,x - a|^p\, dx\}\}, \tag{2.24}$$

$$\Omega(\xi) = \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) < \xi\}. \tag{2.25}$$

Let $\varphi_i : R^n \to [0,\ 1]$ be such that $\varphi_i \in C_0^\infty(R^n)$,

$$\varphi_i(x) = \begin{cases} 1, & \text{if } x \in \Omega \setminus \Omega(2\delta_i^{1/\hat{p}}); \\ 0, & \text{if } x \in R^n \setminus (\Omega \setminus \Omega(h_i)), \end{cases} \tag{2.26}$$

where $\hat{p} > p$ is a constant and

$$|\nabla \varphi_i| \le \delta_i^{-1/\hat{p}}. \tag{2.27}$$

Define $\bar{u}_i : R_{h_i}(\hat{\Omega}) \to R^m$ by

$$\bar{u}_i(x) = A\,x + a + \varphi_i(x)(\tilde{u}_{h_i}(x) - A\,x - a). \tag{2.28}$$

Theorem 2.4. *Let $(u_{h_i},\ R_{h_i}) \in \mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \times SO(n)$ be minimizers of $F(\cdot,\cdot;\ \hat{\Omega})$ in $\mathbb{U}_{h_i}((0,0);\ \hat{\Omega}) \times SO(n)$ with $\lim_{i\to\infty} h_i = 0$ such that (2.18) is satisfied. Assume that $u_i = \tilde{u}_{h_i}$ defined by (2.21) satisfies (2.23) and the condition (C). Let $\{\bar{u}_i\}$ be given by (2.28). Then $\{\bar{u}_i|_\Omega\}$ is a minimizing sequence of $F(\cdot;\ \Omega)$ in $\mathbb{U}((A,a);\ \Omega)$, that is*

$$\bar{u}_i|_\Omega \in \mathbb{U}((A,a);\ \Omega), \quad \forall i \tag{2.29}$$

and

$$\lim_{i\to\infty} F(\bar{u}_i;\ \Omega) = \inf_{u\in\mathbb{U}((A,a);\Omega)} F(u;\ \Omega). \tag{2.30}$$

Proof. (2.29) follows directly from (2.26) and (2.28). Suppose that (2.30) is not true, then we would have

$$\lim_{i\to\infty} F(\bar{u}_i;\ \Omega) - \inf_{u\in\mathbb{U}((A,a);\Omega)} F(u;\ \Omega) = \beta > 0. \tag{2.31}$$

By (2.23) and (C), and by rescaling and periodic extension, we can show [7] that there exists a minimizing sequence $\{v_i\}$ of $F(\cdot;\ \Omega)$ in $\mathbb{U}((A,a);\ \Omega)$ such that

$$v_i(x) - A\,x - a \rightharpoonup 0 \qquad \text{in } W^{1,p}(\Omega;\ R^m), \tag{2.32}$$

$$\lim_{i\to\infty} F(v_i;\ \Omega) = \inf_{u\in\mathbb{U}((A,a);\Omega)} F(u;\ \Omega), \tag{2.33}$$

and

(C′): $\{|\nabla v_i|^p\}$ are precompact in $W^{1,p}(\Omega);\ R^m)$.

It follows from (2.32) and Kondrachov compactness theorems [23] that

$$v_i(x) - A\,x - a \longrightarrow 0 \qquad \text{in } L^p(\Omega;\ R^m),$$

Without loss of generality, we may assume that $\{v_i\}$ are such that

$$\int_\Omega |v_i(x) - A\,x - a|^p\,dx \le \delta_i \quad \forall i, \tag{2.34}$$

where δ_i is defined by (2.24). Let

$$\xi_i = 3\delta_i^{1/\hat p}. \tag{2.35}$$

Define $w_i : R_{h_i}(\hat\Omega) \to R^m$ by

$$w_i(x) = (1 - \varphi_i(x))\tilde u_{h_i}(x) + \varphi_i(x)v_i(x).$$

Then, it is easily verified that $w_i \in \mathbb{U}((A,a);\ R_{h_i}(\hat\Omega))$ and

$$w_i(x) = \begin{cases} \tilde u_{h_i}(x), & \text{if } x \in R_{h_i}(\hat\Omega) \setminus \Omega, \\ v_i(x), & \text{if } x \in \Omega \setminus \Omega(\xi_i). \end{cases} \tag{2.36}$$

Thus, noticing that $\tilde u_{h_i}|_{\Omega\setminus\Omega(\xi_i)} = \bar u_i|_{\Omega\setminus\Omega(\xi_i)}$ and $f(\cdot)$ is nonnegative, we have

$$\begin{aligned} &F(w_i;\ R_{h_i}(\hat\Omega)) - F(\tilde u_{h_i};\ R_{h_i}(\hat\Omega)) \\ =&F(v_i;\ \Omega\setminus\Omega(\xi_i)) + F(w_i;\ \Omega(\xi_i)) - F(\bar u_i;\ \Omega) + F(\bar u_i;\ \Omega(\xi_i)) - F(\tilde u_{h_i};\ \Omega(\xi_i)) \\ \le&F(v_i;\ \Omega) + F(w_i;\ \Omega(\xi_i)) - F(\bar u_i;\ \Omega) + F(\bar u_i;\ \Omega(\xi_i)) \\ =&F_1 + F_2 + F_3 + F_4. \end{aligned} \tag{2.37}$$

It follows from (2.33) that

$$\lim_{i\to\infty} F_1 = \inf_{u\in\mathbb{U}((A,a);\Omega)} F(u,\ \Omega). \tag{2.38}$$

Since

$$\begin{aligned} \nabla w_i(x) =&(1-\varphi_i(x))\nabla\tilde u_{h_i}(x) + \varphi_i(x)\nabla v_i(x) \\ &- (\tilde u_{h_i}(x) - A\,x - a)\otimes\nabla\varphi_i(x) + (v_i(x) - A\,x - a)\otimes\nabla\varphi_i(x), \end{aligned}$$

it follows from (2.1) and $0 \le \varphi_i \le 1$ that

$$\begin{aligned} 0 \le F_2 \le&c_1\,\mathrm{meas}(\Omega(\xi_i)) + 4^{p-1}c_2\int_{\Omega(\xi_i)} (|\nabla\tilde u_{h_i}|^p + |\nabla v_i|^p \\ &+ |(\tilde u_{h_i}(x) - A\,x - a)\otimes\nabla\varphi_i|^p + |(v_i(x) - A\,x - a)\otimes\nabla\varphi_i|^p)\,dx \\ =&I_1 + I_2 + I_3 + I_4 + I_5. \end{aligned}$$

Since $\tilde{u}_{h_i}$ satisfies (2.23), by Kondrachov compactness theorems [23], we have $\lim_{i\to\infty}\delta_i = 0$ (see (2.24)) and hence

$$\lim_{i\to\infty} I_1 = c_1 \lim_{i\to\infty} \text{meas}(\Omega(\xi_i)) = 0.$$

Thus, by (C) and (C′), we have also

$$\lim_{i\to\infty}(I_2 + I_3) = 0.$$

By (2.24), (2.34) and (2.27), we have

$$\begin{aligned} 0 \le I_4 \le & 4^{p-1} c_2 \delta_i^{-p/\hat{p}} \int_{\Omega(\xi_i)} |\tilde{u}_{h_i}(x) - A\,x - a|^p\,dx \le 4^{p-1} c_2 \delta_i^{\frac{\hat{p}-p}{\hat{p}}} \\ 0 \le I_5 \le & 4^{p-1} c_2 \delta_i^{-p/\hat{p}} \int_{\Omega(\xi_i)} |v_i(x) - A\,x - a|^p\,dx \le 4^{p-1} c_2 \delta_i^{\frac{\hat{p}-p}{\hat{p}}}. \end{aligned}$$

Thus, recalling that $\lim_{i\to\infty}\delta_i = 0$, we obtain

$$\lim_{i\to\infty} F_2 = \lim_{i\to\infty}(I_1 + I_2 + I_3 + I_4 + I_5) = 0. \tag{2.39}$$

Since

$$\nabla \bar{u}_{h_i}(x) = (1 - \varphi_i(x))A + \varphi_i(x)\nabla\tilde{u}_{h_i}(x) + (\tilde{u}_{h_i}(x) - A\,x - a) \otimes \nabla\varphi_i(x),$$

with similar arguments as in the proof of (2.39), we obtain

$$\lim_{i\to\infty} F_4 = 0. \tag{2.40}$$

Thus, as a result of (2.22) and (2.37)-(2.40), we see that (2.31) would lead to

$$\lim_{i\to\infty} F(w_i;\ R(\hat{\Omega})) - \inf_{u\in\mathbb{U}((A,a);\ R_{h_i}(\hat{\Omega}))} F(u;\ R_{h_i}(\hat{\Omega})) \le -\beta < 0.$$

This is a contradiction, since $w_i \in \mathbb{U}((A,a);\ R_{h_i}(\hat{\Omega}))$. □

Corollary 2.3. *Let $\{\tilde{u}_{h_i}\}$ be defined by (2.21). Let the assumptions of theorem 2.4 be satisfied. Then*

$$\lim_{i\to\infty} F(\tilde{u}_{h_i}; \Omega) = \inf_{u\in\mathbb{U}((A,a);\Omega)} F(u,\ \Omega). \tag{2.41}$$

and

$$\begin{cases} \tilde{u}_{h_i} \to A\,x + a & \text{in } L^q(\partial\Omega;\ R^m),\ \forall q \in [1,\ \frac{(n-1)p}{n-p}),\ \text{if } p < n; \\ \tilde{u}_{h_i} \to A\,x + a & \text{in } L^q(\partial\Omega;\ R^m),\ \forall q \in [1,\ +\infty),\ \text{if } p = n; \\ \tilde{u}_{h_i} \to A\,x + a & \text{in } (C(\bar{\Omega}))^m,\ \text{if } p > n. \end{cases} \tag{2.42}$$

Proof. Let $\bar{u}_{h_i}$ be defined by (2.28). Then, we have

$$F(\tilde{u}_{h_i};\,\Omega) = F(\bar{u}_{h_i};\,\Omega) + F(\tilde{u}_{h_i};\,\Omega(\xi_i)) - F(\bar{u}_{h_i};\,\Omega(\xi_i)),$$

where $\Omega(\xi_i)$ is defined by (2.24), (2.25) and (2.35) as in theorem 2.4. With similar arguments as in the proof of theorem 2.4, we get

$$\lim_{i\to\infty}(F(\tilde{u}_{h_i};\,\Omega(\xi_i)) - F(\bar{u}_{h_i};\,\Omega(\xi_i))) = 0.$$

Thus, (2.41) follows from (2.30). (2.42) is a consequence of

$$\tilde{u}_{h_i} \rightharpoonup A\,x + a \quad \text{in } W^{1,p}(\Omega;\ R^m)$$

and the Sobolev's imbedding theorems [17]. □

3. Implementation of the rotation transformation method and incremental crystallization

The key to the application of the rotation transformation method is to solve the discrete problem

$$(DP) \quad \begin{cases} \text{find } (u_h,\ R_h) \in \mathbb{U}_h((0,0);\ \hat{\Omega}) \times SO(n) \text{ such that} \\ F(u_h, R_h;\ \hat{\Omega}) = \inf_{(u',R')\in\mathbb{U}_h((0,0);\,\hat{\Omega})\times SO(n)} F(u', R';\ \hat{\Omega}). \end{cases} \tag{3.1}$$

Noticing that in the convergence analysis of the method (see theorem 2.4 and its proof), rather than the boundary condition

$$u_h = 0 \qquad \text{on } \partial\hat{\Omega}, \tag{3.2}$$

the condition

$$\lim_{h\to 0}\int_{\hat{\Omega}} |u_h|^p\,dx = 0 \tag{3.3}$$

plays a key role, so instead of considering problem (3.1), we consider the following discrete problem:

$$(DP') \begin{cases} \text{find } (u_h,\ R_h) \in \mathbb{U}_h((0,0);\ \hat{\Omega}) \times SO(n) \text{ such that} \\ F_\mu(u_h, R_h;\ \hat{\Omega}) = \inf_{(u',R')\in\mathbb{U}_h((0,0);\,\hat{\Omega})\times SO(n)} F_\mu(u', R';\ \hat{\Omega}), \end{cases} \tag{3.4}$$

where

$$F_\mu(u, R;\ \hat{\Omega}) = \int_{\hat{\Omega}} f(A + \nabla u(x)R^{-1})\,dx + \mu h^{-q}\int_{\hat{\Omega}} |u(x)|^p\,dx, \tag{3.5}$$

and where in (3.5) $\mu > 0$ and $q \in (0,\ p)$ are parameters. In general, the minimizing sequences produced by the discrete problems (3.4) satisfies (3.3) (see (1.5) and (1.6)). It is also natural for us to apply at this stage the boundary layer removal technique described in Sec. 1 by taking a slightly bigger open set $\hat{\Omega}'$ such that $\hat{\Omega}' \supset \overline{\hat{\Omega}}$ which we still denote by $\hat{\Omega}$.

Remark 3.1. Convergence analysis and error estimates for the discrete problems in which the functional is added with an extra term

$$\mu h^{-q} \int_{\hat{\Omega}} |u(x)|^p \, dx \tag{3.6}$$

can be found in [24] where the problem is considered in a more general setting.

Example. Let $n = 2$, $m = 2$ and let $\Omega = B(0;\ 1)$ be the unit ball centered at the origin $(0,\ 0)$. Let $A = 0$ and $a = 0$. Let

$$f(P) = \langle P - B,\ P - B\rangle\langle P + B,\ P + B\rangle \qquad \forall P \in R^{2\times 2}, \tag{3.7}$$

where $\langle D,\ E\rangle = \mathrm{tr}(DE^T)$ and

$$B = \begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{3.8}$$

It is easily seen that $f(P)$ is an energy density with double wells B and $-B$ which are not rank-one connected.

It is known [25] that

$$\inf_{u \in \mathbb{U}((0,0);\, \Omega')} F(u;\ \Omega') = 4(\det B)^2 \operatorname{meas}(\Omega') = \frac{1}{4} \operatorname{meas}(\Omega'), \tag{3.9}$$

for all bounded open sets $\Omega' \subset R^2$, and it is also known [25] that the problem of minimizing $F(\cdot;\ \Omega)$ in $\mathbb{U}((0,0);\ \Omega)$ has a laminated microstructure which is the fine scaled oscillations between the two states C and $-C$ with $C \in R^{2\times 2}$ uniquely determined by the solution of the linear equations

$$\alpha C + \operatorname{adj} C = \beta B, \tag{3.10}$$

where $\operatorname{adj} C$ is the cofactor matrix of C and

$$\alpha = \frac{7 + \sqrt{45}}{2}, \qquad \beta = \sqrt{\frac{\sqrt{45}(7 + \sqrt{45})}{2}}. \tag{3.11}$$

It follows from (3.10) and (3.11) that

$$\begin{cases} c_{11} & = & \frac{\beta(2\alpha-1)}{2(\alpha^2-1)}, \\ c_{22} & = & \frac{\beta(\alpha-2)}{2(\alpha^2-1)}, \\ c_{12} & = & c_{21} = -\frac{\beta\sqrt{(2\alpha-1)(\alpha-2)}}{2(\alpha^2-1)}. \end{cases} \tag{3.12}$$

Let $\vec{n} = (n_x, n_y)^T$ be the unit normals of the interface between the two states C and $-C$ with $n_x > 0$. It follows from $C = \vec{c} \otimes \vec{n}$ and (3.12) that

$$\frac{n_y}{n_x} = \frac{c_{12}}{c_{11}} = -\sqrt{\frac{\alpha-2}{2\alpha-1}}.$$

Let $\phi_{\vec{n}}$ be the angle between $\vec{n}$ and the unit vector $(1,0)^T$, then

$$\phi_{\vec{n}} = -arctg\sqrt{\frac{\alpha-2}{2\alpha-1}}. \tag{3.13}$$

To solve the problem with the rotation transformation method, we take $\hat{\Omega} = [-1,\ 1]^2$ and introduce on $\hat{\Omega}$ regular triangulations $\mathfrak{T}_h$ for $h = \frac{2}{N}$ with $N \geq 2$ by using the following lines

$$\begin{cases} x & = & -1 + \frac{2}{N}i, & i = 0, 1, \ldots, N; \\ y & = & -1 + \frac{2}{N}j, & j = 0, 1, \ldots, N; \\ y & = & x - \frac{2}{N}k, & k = -N+1, -N, \ldots, N-1. \end{cases} \tag{3.14}$$

For the mesh introduced by (3.14), there are three groups of parallel planes, with normal $\vec{n}_1 = (1,\ 0)^T$, $\vec{n}_2 = (0,\ 1)^T$ and $\vec{n}_3 = (\frac{\sqrt{2}}{2},\ -\frac{\sqrt{2}}{2})^T$ respectively, across which the deformation gradients can be discontinuous. Suppose that under the rotation transformation

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix},$$

the planes corresponding to $\vec{n}_3$ are transformed to the planes with normal $\vec{n}$, then we have

$$\theta = \frac{\pi}{4} - \text{arctg}\sqrt{\frac{\alpha-2}{2\alpha-1}}. \tag{3.15}$$

Hence, this is one of the rotation angles we can expect to obtain from the numerical computations.

In the numerical experiments, the discrete problems (3.4) were solved by the conjugate gradient method with a linear search. The initial deformation was a small random perturbation of the origin and the initial rotation angle was set to 0. The parameters in (3.5) are set to $\mu = 1$ and $q = 1.5$. Figure 1 shows a numerical result obtained by the conjugate gradient method without using the rotation transformation method, where in figure 1 we have $D \approx CR(\theta)$ and $-D \approx -CR(\theta)$ with θ given by (3.15). Figure 2 shows a numerical result given by the rotation transformation method.

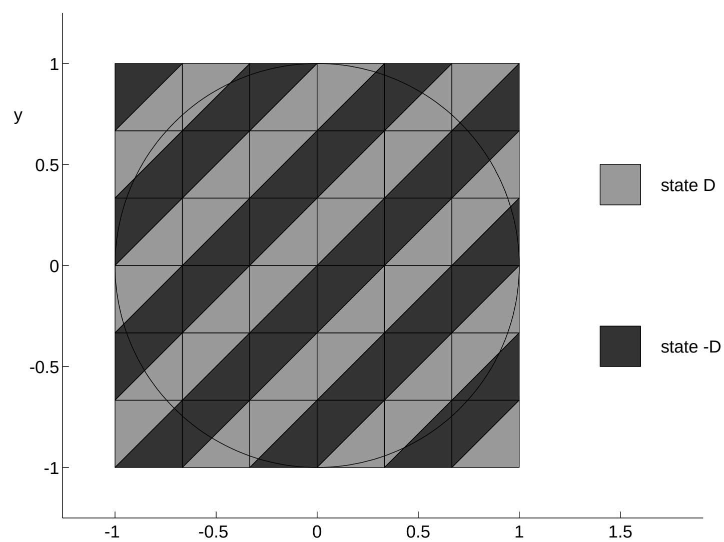

FIGURE 1. Numerical pseudo-microstructure with $N = 6$ obtained without using rotation transformation method

To increase further the accuracy, after the convergence criterion is satisfied, the parameter μ in (3.5) can be reduced gradually from the initial value to a level of h^q, as long as the inequality

$$\int_{\hat{\Omega}} |u_h^{\mu}|^p \, dx \leq L \int_{\hat{\Omega}} |u_h^{\mu_0}|^p \, dx \tag{3.16}$$

is satisfied for a given constant $L > 1$. The numerical results with $N = 6$ obtained by the conjugate gradient method (C-G) and by the rotation transformation method combined with the conjugate gradient method (R-T) are compared in table 1, where $e_r(F(u;\, \Omega))$ and $e_r(\theta)$ are relative errors for $F(u;\, \Omega)$ and θ respectively, and where the results for (R-T-μ) is obtained by further

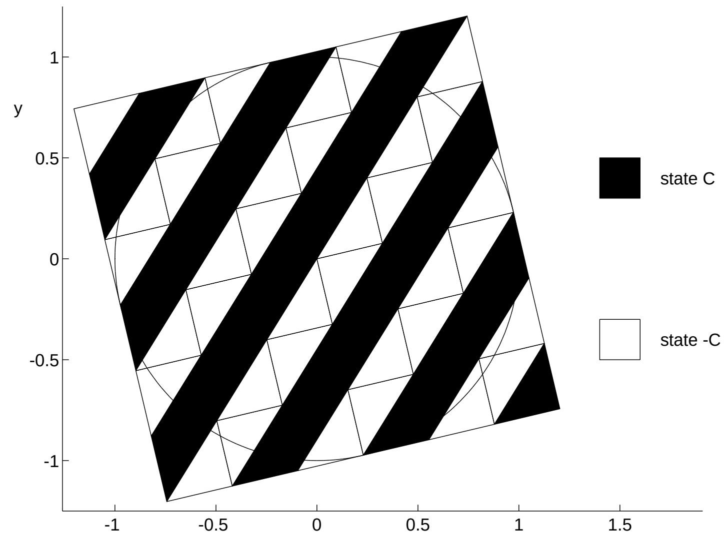

FIGURE 2. Numerical microstructure with $N = 6$ obtained by the rotation transformation method

iterations, after the convergence is achieved in (R-T) method, in which μ is reduced gradually to 0.1 from the original value of 1.

method	$e_r(F(u;\ \Omega))$	$e_r(\theta)$	$\|u\|_{L^2(\Omega;\ R^m)}$
C-G	0.4448×10^0	not applicable	0.787251×10^{-1}
R-T	0.3605×10^{-1}	0.8628×10^{-10}	0.17100
R-T-μ	0.3668×10^{-3}	$< 10^{-13}$	0.17570

TABLE 1. Comparison of numerical ($N = 6$) results.

As is shown, the rotation transformation method combined with the conjugate gradient method works very well for the coarse mesh. However, as the number of the elements increases, local minimizers are usually obtained (see figure 3).

In general, the rotation transformation method can be used together with other techniques such as simulated annealing and Monte Carlo techniques [11, 12] to overcome the difficulty. We present yet another approach: the incremental crystallization method. The solution procedure is as follows.

For simplicity, we take $N = kM$, $M = 1, 2, \cdots$, $k \geq 2$ and $h = 2/N$, where k is the increment. Instead of solving problem (3.4) directly by the conjugate

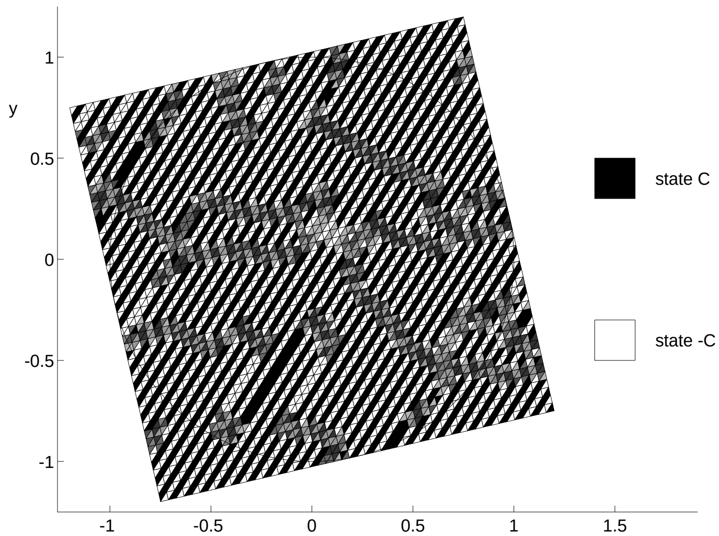

FIGURE 3. Numerical microstructure with $N = 50$ obtained by the rotation transformation method

gradient method, $2M+1$ smaller problems

$$(DP_i') \quad \begin{cases} \text{find } (u_h^i,\ R_h) \in \mathbb{U}_h((0,0);\ \hat{\Omega}) \times SO(n) \text{ such that} \\ F_\mu(u_h^i, R_h;\ \hat{\Omega}_i) = \inf_{(u',R') \in \mathbb{U}_h((0,0);\ \hat{\Omega}) \times SO(n)} F_\mu(u', R';\ \hat{\Omega}_i). \end{cases} \tag{3.17}$$

for $i = 1, 2, \cdots, 2M+1$ are solved. Where $\hat{\Omega}_i$ in (3.17) are defined by

$$\hat{\Omega}_i = \begin{cases} (-1+(i-1)kh,\ -1+ikh) \times (-1,\ -1+kh), & \text{if } i \le M, \\ (-1,\ 1) \times (-1,\ 1), & \text{if } i = 2M+1, \\ (-1,\ 1) \times (-1+(i-M-1)kh,\ -1+(i-M)kh), & \text{otherwise.} \end{cases}$$

The subproblems (DP_i') are solved by the conjugate gradient method. In the solution procedure, the i-th subproblem is solved on $\hat{\Omega}_i$ and thus $u_h^i(x_\tau)$ remains unchanged for all nodes $x_\tau \notin \bar{\hat{\Omega}}$. The rotation transformation matrix $R(\theta)$, or rather the rotation angle θ, is a global variable and is inherited from one step to the next. The step $M+1$ and the step $2M+1$, in which $\hat{\Omega}_{M+1} = \bigcup_{i=1}^{M} \hat{\Omega}_i$ and $\hat{\Omega}_{2M+1} = \bigcup_{i=1}^{2M+1} \hat{\Omega}_i$ respectively, are designed to coordinate further the u_h^is obtained in the previous steps.

To apply the incremental crystallization method to our example, the increment $k = 3$ is taken and the parameters μ and q in (3.5) are taken to be 1 and 1.5 respectively. A numerical result is shown in figure 4.

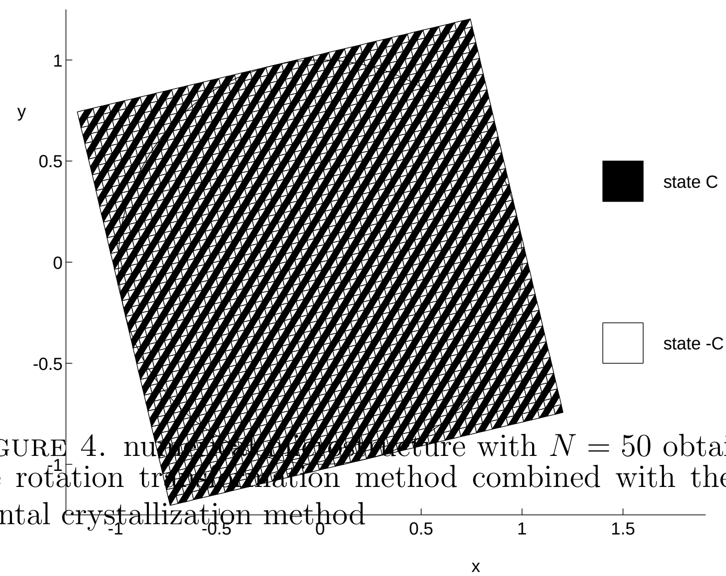

FIGURE 4. numerical microstructure with $N = 50$ obtained by the rotation transformation method combined with the incremental crystallization method

In table 2, the numerical results with $N = 50$ obtained by the rotation transformation method (R-T) and by the rotation transformation method combined with the incremental crystallization method (R-T + INCR) are compared with the analytical results, where the results for (R-T + INCR-μ) is obtained by further iterations, after the convergence in the last step (step $2M + 1$) of the (R-T + INCR) method is achieved, in which μ is reduced gradually to 0.0085 from the original value of 1.

method	$e_r(F(u;\ \Omega))$	$e_r(\theta)$	$\|u\|_{L^2(\Omega;\ R^m)}$
R-T	1.2701	0.2127×10^{-1}	0.28177×10^{-1}
R-T + INCR	0.3290×10^{-2}	0.1553×10^{-11}	0.20966×10^{-1}
R-T + INCR-μ	0.9400×10^{-7}	$< 10^{-13}$	0.21146×10^{-1}

TABLE 2. Comparison of numerical ($N = 50$) results.

As is clearly shown by table 2, the rotation transformation method combined with the incremental crystallization method, (R-T + INCR) and (R-T + INCR-μ) in particular, produces very sharp numerical results for double well problems. Numerical experiments show that the incremental crystallization method not only provides sharper numerical results but also increases further the efficiency of the rotation transformation method. In our numerical experiments for double well problems, the rotation transformation method combined with the incremental crystallization method can easily converge to the global minimizer without taking any other measure to aviod beeing traped into a local minimizer.

References

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

[2] Z.-P. Li, *Existence of minimizers and microstructures in nonlinear elasticity.* **Nonlinear Anal.: Theo., Meth. Appl., 27**(1996), 297-308.

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

[4] J. M. Ball and F. Murat $W^{1,p}$*-quasiconvexity and variational problems for multiple integrals.* **J. Funct. Anal., 58**, (1984)225-253.

[5] E. Acerbi and N. Fusco, *Semicontinuity problems in the calculus of variations.* **Arch. Rat. Mech. Anal. 86**(1984), 125-145.

[6] 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.

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

[8] M. Luskin, *On the computation of crystalline microstructure.* **Acta Numerica**, 1996.

[9] C. Collins and M Luskin, *The computation of the austenitic-martensitic phase transition.* In **Partial Differential Equations and Continuum Models of Phase Transitions** Lecture Nodes in Physics, Vol. 344, M. Rascle, D. Serre and M. Slemrod, eds, Springer-Verlag, New York, (1989), pp. 34-50.

[10] 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.

[11] M. Luskin and L. Ma, *Numerical optimization of the micromagnetics energy*, in **Mathematics in Smart Materials**, SPIE, (1993), pp. 19-29.

[12] P. Gremaud, *Numerical optimization and quasiconvexity*, **Euro. J. Appl. Math. 6**, (1995) 69-82.

[13] Z.-P. Li, *Simultaneous numerical approximation of microstructures and relaxed minimizers*. Research Report No.26, Institute of Mathematics and School of Mathematical Sciences, Peking University, 1996. To appear in **Numer. Math.**.

[14] C. Collins and M. Luskin, *Optimal-order error estimates for the finite element approximation of the solution of a nonconvex variational problem.* **Math. Comput., 57**(1991), 621-637.

[15] M. Chipot, *Numerical analysis of oscillations in nonconvex problems.* **Numer. Math., 59** (1991), 747-767.

[16] M. Chipot, C. Collins and D. Kinderlehrer, *Numerical analysis of oscillations in multiple well problems.* **Numer. Math., 70** (1995), 259-282.

[17] R.A. Adams, **Sobolev Spaces**. Academic Press, New York, 1975.

[18] G. Buttazzo, **Semicontinuity, Relaxation and Integral Representation in the Calculus of Variations**. Pitman Research Notes in Mathematics Series 207. Longman, 1989.

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

[20] D. Kinderlehrer and P. Pegregal, *Characterizations of Young measures generated by gradients.* **Arch. Rational Mech. Anal., 115**(1991), 329-365.

[21] D. Kinderlehrer and P. Pegregal, *Weak convergence of integrands and the Young measure representation.* **SIAM J. Math. Anal., 23**(1992), 1-19.

[22] I. Diestel and J. J. Uhl, Jr., **Vector Measures**, American Mathematical Society, Mathematical Surveys N0.15. Providence, 1977.

[23] M. S. Berger, **Nonlinearity and Functional Analysis**. Academic Press, New York, 1977.

[24] Z.-P. Li, *Computation of microstructures by using quasiconvex envelope.* Research Report No.61, Institute of Mathematics and Department of Mathematics, Peking University, 1995.

[25] Z.-P. Li, *Laminated microstructure in variational problems with non-rank-one connected double well potential*, Report No.53, Institute of Mathematics and School of Mathematical Sciences, Peking University, 1996. To appear in **J. Math. Anal. Appl.**.

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