APPROXIMATIONS OF THE LAMINATED MICROSTRUCTURES

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Abstract. The theory of approximation of the microstructures associated with the orthorhombic to monoclinic and cubic to tetragonal transformations is presented. The error estimates derived in this paper show that macroscopic discrete quantities cannot converge faster then $\mathcal{O}(\sqrt{h})$ in order to allow for the unlimited oscillations to develop. The Discrete Uncertainty Principle is proven. It indicates that we cannot approximate macroscopic and microscopic properties of the laminated microstructures with an unlimited precision at the same time.

1. Introduction

We present further development of the approximation theory of the martensitic transformations. This approximation theory was first setup and successfully addressed in [CL] and [CKL] in the case of one-dimensional model problem and in [CCK] and [G] in the case of the two-dimensional transformations. The truly multi-dimensional approximation theory was developed in [L, 1996a] using some unique properties of the martensitic transformations. The goal of this paper is to derive new results concerning the properties of the finite element approximations of highly oscillatory structures described by the Young measures and to improve some of the already established error estimates in this context. The particular problems which we consider in this paper are the approximation of the face-centered cubic to face-centered tetragonal and the orthorombic to monoclinic martensitic transformations. These transformations are transitions between typical equilibrium states of the shape memory alloys. The characteristic internal structures of these states are found on a nano-scale. Therefore their bulk elastic properties are desribed, within the continuum modeling, by the Young measures.

The deformation gradients of the approximate martensitic transformations converge weakly but not strongly to the gradient of the resulting deformation. As a consequence of this deficiency, the limiting deformation lacks any point-wise meaning. If the construction of the approximate deformations would be associated with the energy minimization, the total energy of the limiting deformation would be too high compare to the limit of the total energies of the approximate deformations. This seems to be a typical failure of the mathematical models which are constructed to characterize bulk behaviour utilizing the microscopic – atomic or molecular – description of the material properties.

Numerical optimizations of the non-convex free energies exhibit dependencies on the discrete data, such as the spatial discretization, the initial guess and properties of the finite element space used in the calculations, [CL], [C]. This means that local minima, rather then the global minimum, are computed.

The presented paper characterizes the order of the convergence of various quantities as the successive oscillations are created on the finest scale possible. We show that macroscopic quantities, such as the deformation itself cannot converge faster then $\mathcal{O}(h^{1/2})$ in order to allow for unlimited oscillations to develop. In fact, we show that this condition is equivalent to the convergence of

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the discrete Young measures to the appropriate limiting probability distribution of the equilibrium states.

The paper is organized as follows. In the second paragraph we summarize the notation and the basic definitions we use throughout the text, including the basic properties of the martensitic variants and the discrete approximation of the Young measures. The third paragraph contains the convergence theory of the conforming and non-conforming approximations of the Young measures associated with the martensitic transformations and the error analysis of these finite element approximations. In the paragraph four we establish the sufficient and necessary condition to obtain appropriate microscopic description using the macroscopic control of the convergence. More precisely, we establish a theorem (Theorem 4.3) which links the convergence of the discrete Young measures with the convergence of the discrete deformations itself. The connection between the convergence of the two quantities is provided by the Discrete Uncertainty Principle.

We developed our convergence and approximation theory using the simple but long overlooked fact that certain directional derivatives of the discrete deformations are continuous. This fact was first observed, proved and used in [L, 1996a].

2. Formulation of the problem

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with the Lipschitz boundary, and $u = u(x,t) = \{u_i(x,t)\}_{i=1}^3$ be the deformation. The deformation gradient $\nabla u(x) \in \mathcal{M}^{3\times 3}$, where $\mathcal{M}^{3\times 3}$ denotes the space of 3×3 real matrices, is computed with respect to the coordinate system associated with the undeformed domain Ω. The matrix multiplication in the space $\mathcal{M}^{3\times 3}$ is understood in the sense $A \cdot B \stackrel{\text{def}}{=} \operatorname{Tr}(A^T B)$ where the matrix $A^T B$ is obtained by the standard matrix multiplication. Consequently, the matrix norm is given by $|A| = \sqrt{A^T \cdot A}$ which is the natural Euclidian norm on the space $\mathbb{R}^{3\times 3}$.

The following subparagraphes are intended to summarize the technical tools we need in the course of the proofs and to describe the problem at hand. Though self-consistent, the summary is not explanatory. The details can be found in the literature which is referenced in this overview.

Martensitic deformations. We refer to *martensite or martensitic deformation* as to being a continuous deformation with discontinuous deformation gradients which oscillate among a finite number of known matrices. These matrices are called *martensitic variants.* We refer to *austenite or austenitic deformation* as to being a continuous deformation with the deformation gradient given by the identity matrix.

The complete description of the martensitic deformation consists in determination of the set of the variants $\{F_1, \ldots, F_N\}$. They must inherit the (crystal) symmetry of the unstressed, referential, configuration given by the variant F_1. Thus it is required that

$$\{R_i F_1 R_i^T \mid R_i \in \mathcal{Q}\} = \{F_1, \ldots, F_N\}. \tag{2.1}$$

Here, $\mathcal{Q}$ is the symmetry group of the referential configuration and F_1 is some positive definite matrix. In the case of the change in the crystal structure from face-centered cubic (austenite) to face-centered tetragonal (martensite), which covers e.g. transformations in $InTl$, $\mathcal{Q}$ consists of 24 rotations which map cube into itself, i.e. $N = 24$. Those are three rotations with the axis e_i, four π rad rotations with the axis perpendicular to e_i, for $i = 1, 2, 3$, and identity. The vectors $\{e_1, e_2, e_3\}$ form an orthonormal basis in $\mathbb{R}^3$. Since $\mathcal{Q}$ is a group, there are precisely three distinct matrices $(24/8 = 3)$ of the form $R_i F_1 R_i^T$. The martensitic variants are

$$\mathcal{V} \stackrel{\text{def}}{=} \{F_i = \nu_1 \mathrm{I} + (\nu_2 - \nu_1) e_i \otimes e_i, i = 1, 2, 3\}, \tag{2.2}$$

where $\nu_i > 0$, $\nu_1 \neq \nu_2$ and $e_i \otimes e_i \in \mathcal{M}^{3\times 3}$ is the tensor product given by $(a \otimes b)_{ij} = a_i b_j$. The rotations $R_i \in \mathcal{Q}$ are given by $R_i = \sum_{i=1}^{3}(-1)^{\alpha(i)} e_{\beta(i)} \otimes e_i$, where $\alpha : \{1,2,3\} \to \{0,1\}$ and β is the permutation of $\{1,2,3\}$ [L,1996b].

Another example of the martensitic deformation is associated with the orthorhombic to monoclinic transformations. In this case $\mathcal{Q} = \{\mathrm{I}, -\mathrm{I} + 2e_i \otimes e_i, i = 1,2,3\}$. The martensitic (monoclinic) variants are $F_i = (\mathrm{I} + \eta(-1)^i e_2 \otimes e_1)D$, where $D = \sum_{i=1}^{3} d_i e_i \otimes e_i$, $d_i > 0$, $i = 1,2,3$, $\eta > 0$ [L,1996b]. Note that

$$\{R_i F_1 R_i^T \mid R_i \in \mathcal{Q}\} = \{F_1, F_2\} \stackrel{\text{def}}{=} \mathcal{U}. \tag{2.3}$$

Since we request the martensitic deformations to be continuous vector functions the martensitic variants cannot be an arbitrary matrices. The necessary and sufficient condition that a continuous vector function can have deformation gradients given by U_1 and U_2 is the so-called Hadamard jump condition. It states that there must exist a scratch vector a and a vector n which is the normal vector to the plane of the discontinuity such that

$$U_1 = U_2 + a \otimes n. \tag{2.4}$$

We refer to this condition as the *rank-one connection*.

It is known, [BJ, 1992] or [L, 1996b], that in the above cases of the martensitic deformations none of the matrices F_i are rank-one connected to each other. Though, every F_i is rank-one connected to two distinct martensitic variants within the same set $\mathcal{V}$ or $\mathcal{U}$. This translates into the existence of the rotation matrices R and vectors a and n such that [BJ, 1987]

$$RF_2 = F_1 + a \otimes n. \tag{2.5}$$

The rotation matrix R is not unique though there exist two such matrices at the most. The above equation indicates that the regions in which the deformation gradient is constant and given by either F_1 or RF_2 are separated by the planar interfaces [BJ, 1987], called *twin planes*.

We refer to the deformations which has, upon rotation, rank-one connected martensitic variants, and, which oscillate on an arbitrary small scale as a *fine mixtures* or more frequently as *microstructures*.

The finiteness of $\mathcal{Q}$ yields existence of a Borel measurable projection $\Pi : \mathcal{M}^{3\times 3} \to \mathcal{Q}$ defined by

$$|A - \Pi A| = \min_{M \in \mathcal{K}} \|A - M\|, \qquad \mathcal{K} = \mathcal{V} \text{ or } \mathcal{U}.$$

We note, that this projection is not unique. If $\Pi_{1,2} : \mathcal{M}^{3\times 3} \to \{F_1, F_2\}$ we can find for any non-singular matrix A a matrix $B(A)$ such that

$$\Pi(A) = B(A)\Pi_{1,2}(A). \tag{2.6}$$

It is easily seen that both the matrix B and the projection $\Pi_{1,2}$ are unique for given Π.

Energetics. Some of the properties of the martensitic transformations (i.e. transitions among different variants) can be studied by minimization of the free-energy. The free-energy is constructed to have distinct local minima associated with the martensitic variants. The free-energy is the spatial sum of the energy density which describes the point-wise elastic properties of the crystal in the near-equilibrium configurations.

We require that any martensitic variant participating in the fine mixture must have the same elastic energy. Since these deformations are specified upon a possible rigid rotation by the condition

(2.5), we require that the energy density W satisfies the condition of the Galilean invariance (frame indifference) for all admissible deformations

$$W(RF) = W(F), \qquad \forall R \in \mathrm{SO}(3), \tag{2.7}$$

where $SO(3)$ is the set of the proper rotations. We note that the Galilean invariance implies that any local minimum of the associated energy density W is a sphere in the 9–dimensional space $\mathcal{M}^{3\times 3}$, and, hence, any particular matrices yielding the equilibrium variants are inseparable in this space.

Moreover, the requirement of the equal energy of the participating variants and the crystal symmetry (2.1) result in the following condition

$$W(R_i F R_i^T) = W(F), \qquad \forall R_i \in \mathcal{Q}. \tag{2.8}$$

It is easy to see that the Polar decomposition and (2.7) imply that the free-energy W has to depend on $F^T F$ instead of F. To summarize the properties of the free-energy W, it is clear from (2.5) and (2.7) that W cannot be a rank-one convex function of its argument. To accommodate this non-convexity, we allow the elastic module $D^2W(.)$ to violate the Legendre-Hadamard condition. We require only that the free-energy $W = W(p)$, $p \in \mathbb{R}^{3\times 3}$ have an analytic dependence on p. Thus there is $\beta > 0$ such that

$$W(p + \lambda q) = \sum_{|\alpha|\geq 0} W_\alpha(p, q)\lambda^\alpha \tag{2.9}$$

for $|p|$, $|q| \leq \beta$, p, $q \in \mathbb{R}^{3\times 3}$, and, for $j \geq 1$,

$$\sup_{|\lambda|<1} \left| \sum_{|\alpha|=j} W_\alpha(p, q)\lambda^\alpha \right| \leq 1, \qquad \text{for } |p|, |q| \leq \beta. \tag{2.10}$$

We assume that the energy density W is convex in the immediate neighbourhood of the equilibrium states, i.e.,

$$\frac{d^2}{dt^2} W(tp)\big|_{t=0} \geq C\ |p|^2, \qquad \text{if } |p - \Pi p| \leq 1 \tag{2.11}$$

where the constant C is independent of p, $|.|$ is the norm on the space $\mathbb{R}^{3\times 3}$, and

$$W\big|_{\mathcal{K}} = 0, \qquad \mathcal{K} = \mathcal{V} \text{ or } \mathcal{U}. \tag{2.12}$$

In connection with the real-analytic energy densities, we recall the results of Lojasiewicz [Lo] which yield for any function $F = F(p)$ which is real-analytic in a neighbourhood of $0 \in \mathbb{R}^{n\times n}$, $n \geq 1$, with $DF(0) = \frac{dF(p)}{p}(0) = 0$, some constants $\vartheta \in (0, \frac{1}{2})$, $\gamma \geq 2$ and $\delta > 0$ such that if

$$\mathcal{N} = \{v \in \mathbb{R}^{n\times n} \mid |DF(v)| = 0\} \tag{2.13}$$

then for $|v| \leq \delta$ we have

$$|DF(v)| \geq \operatorname{dist}(v, \mathcal{N})^\gamma, \tag{2.14}$$

$$|DF(v)| \geq |F(v) - F(0)|^{1-\vartheta}. \tag{2.15}$$

Non-conforming approximations. The finite element space $\mathcal{A}_h$, containing the discrete deformations, is defined to be the linear space of deformations $u_h : \Omega \to \mathbb{R}^3$ such that

$$
\begin{aligned}
&u_h\big|_{Q_h} \in \mathcal{P}\times\mathcal{P}\times\mathcal{P},\\
&-\Delta\, u_h(x) = 0, \qquad \text{in } Q_h,\\
&\partial^2_{x_i x_j} u_h = 0, \qquad \text{in } Q_h, \qquad \text{for } i \neq j.
\end{aligned}
$$

Here $\mathcal{P}$ is a polynomial space and $Q_h \in \tau_h$ is parallelepiped. We assume that the family of the partitions τ_h of Ω satisfies the following conditions

(1) $\overline{\Omega} = \bigcup_{Q_h\in\tau_h} Q_h$,
(2) any two Q_h do not overlap,
(3) there exists a positive constant C, independent of τ_h such that

$$\frac{h}{\min_{Q_h\in\tau_h} h(Q_h)} \leq C,$$

where $h(Q_h)$ is the shortest edge of $\overline{Q}_h$ and we set $h = \max_{Q_h\in\tau_h} H(Q_h)$, where $H(Q_h)$ is the longest edge in $\overline{Q}_h$.

The discrete deformations $u_h \in \mathcal{A}_h$ are required to be continuous in the sense

$$\int_{\partial Q_h^{+,-}} \left(u_h\big|_{Q_h^+} - u_h\big|_{Q_h^-}\right) dS = 0, \tag{2.16}$$

where $\partial Q_h^{+,-} = Q_h^+ \cap Q_h^-$ is the interelement face of Q_h^+ and Q_h^-.

It follows from the above construction that, in general,

$$W^{1,p}(\Omega) \subseteq \mathcal{A}_h, \qquad 1 \leq p \leq \infty.$$

In this sense, we call the space $\mathcal{A}_h$ non-conforming. The approximation properties of the non-conforming spaces cannot be better then $\mathcal{O}(h)$ since the quantities associated with the interelement boundaries are disregarded. Note, that the possibility of the reverse inclusion is not excluded by the continuity condition.

To maintain the Hilbert structure of the space $\mathcal{A}_h$ we extend the gradient operator ∇ from the space $H^1(\Omega)$ onto the algebraic sum $H^1(\Omega) \oplus \mathcal{A}_h$. The extension ∇_h is such that $\nabla_h\big|_{H^1(\Omega)} = \nabla$ and $(\nabla_h\cdot, \nabla_h\cdot)_{L^2(\Omega)}$ generates a scalar product on $\mathcal{A}_h \oplus H^1_0(\Omega)$. The extension ∇_h is understood in the piece-wise sense with respect to the decomposition τ_h. Thus, we have

$$\|w_h\|_h^2 \stackrel{\text{def}}{=} \int_\Omega \mathrm{Tr}\left((\nabla_h w_h(x))^T \nabla_h w_h(x)\right) dx = \sum_{Q_h\in\tau_h} \int_{\Omega_h} \mathrm{Tr}\left((\nabla w_h(x))^T \nabla w_h(x)\right) dx, \tag{2.17}$$

for all $w_h \in H^1_0(\Omega,\mathbb{R}^3) \oplus \mathcal{A}_h$.

Further, we assume existence of an interpolation operator $J_h : C(\bar\Omega,\mathbb{R}^3) \to \mathcal{A}_h$ defined by

$$\int_{\partial Q_h^i} J_h u(s)\, dS = \int_{\partial Q_h^i} u(s)\, dS, \qquad \forall \partial Q_h^i \in \partial Q_h, i = 1,2,\dots,6, \quad Q_h \in \tau_h, \tag{2.18}$$

for any $u \in C(\bar\Omega,\mathbb{R}^3)$ such that there exists a positive constant C, independent of u and h, such that

$$\operatorname*{ess\,sup}_{x\in\Omega} |\nabla_h J_h u(x)| \leq C \operatorname*{ess\,sup}_{x\in\Omega} |\nabla u(x)| \tag{2.19}$$

for any $u \in C(\bar{\Omega}, \mathbb{R}^3)$.

The Dirichlet set $\mathcal{A}_h^g$ is defined to be the set of functions from the space $\mathcal{A}_h$ which satisfy the Dirichlet boundary condition in the sense that for any $g \in H^{1/2}(\partial\Omega)$

$$\int_{\partial\tilde{Q}_h} u_h(s)\,dS = \int_{\partial\tilde{Q}_h} g(s)\,dS, \qquad \forall \partial\tilde{Q}_h \in \partial Q_h, \quad Q_h \cap \partial\Omega \neq \emptyset,\ Q_h \in \tau_h. \tag{2.20}$$

An example of the plausible non-conforming space $\mathcal{A}_h$ can be defined as follows. Let Q be unit parent cube. We define the triple $\{Q, \mathcal{P}, \Sigma\}$, [Ci], where

$$\begin{aligned} \mathcal{P} &= \mathrm{Span}\left\{ 1,\, x,\, y,\, z,\, x^2 - y^2,\, x^2 - z^2 \right\}, \\ \Sigma &= \left\{ \fint_{\partial Q^i} q\,dS : i = 1, \dots, 6 \right\}. \end{aligned} \tag{2.21}$$

Here, $\partial Q^i,\ i = 1, \dots, 6$, are the faces of the unit cube Q and $\fint_{\partial Q^i} \equiv \frac{1}{\mathrm{meas}(\partial Q^i)} \int_{\partial Q^i}$. The finite element is well-defined since Σ is $\mathcal{P}$-unisolvent but it is not affine. More general affine construction of the similar space can be found in [KLL]. This space was introduced in approximation of the Stokes problem [RT], and it was successful used in the approximation of the martensitic microthermodynamics in [K] and iso-thermal dynamics [KL].

Formulation of the problem. We assume, in addition to the assumptions (2.9), that the energy density W has local minima on any subsets of either $\mathcal{V}$ or $\mathcal{U}$ such that $W|_{\mathcal{V}} = W|_{\mathcal{U}} = 0$. Without loss of generality we can restrict out theory to the two-well problem. We denote $\mathcal{F}_i = SO(3)F_i$, for $i = 1, 2$ and we assume that

$$W(\mathcal{F}_i) = 0, \qquad i = 1, 2 \tag{2.22}$$

where $SO(3)$ is the space of proper rotations and $F_i \in \mathcal{V}$ or $F_i \in \mathcal{U}$, $i = 1, 2$ and we denote $\mathcal{K}_2 = \bigcup_{i=1,2} \mathcal{F}_i$.

For any $u_h \in \mathcal{A}_h$ the free-energy is given by

$$\mathcal{E}(u_h) \stackrel{\mathrm{def}}{=} \int_\Omega W(\nabla_h u_h)\,dx. \tag{2.23}$$

The Lemma 2.1 implies that the free-energy is well defined for any $u_h \in \mathcal{A}_h$ if $\|\nabla_h u_h\|_{L^p(\Omega)}$ is bounded uniformly in h for some $p > 0$. We seek approximation of

$$\mathcal{I} \stackrel{\mathrm{def}}{=} \inf\{\mathcal{E}(u) \,|\, u \in W^{1,p}(\Omega; \mathbb{R}^3);\ u = Fx \stackrel{\mathrm{def}}{=} (\lambda_1 F_1 + \lambda_2 F_2)\,x,\ x \in \partial\Omega\}, \tag{2.24}$$

where $\lambda_1 + \lambda_2 = 1$ and $F_i \in \mathcal{K}_2$, for $i = 1, 2$.

We note that there does not exist any function at which the infimum (2.24) would be attained.

Representation and approximation of the microstructures. The free-energy $\mathcal{E}$ cannot be weakly-lower semi-continuous so the weak limit of a minimizing sequence may not represent any point-wise information about the solution of (2.24). More precisely, if $|\nabla u_h| \leq C < \infty$ is a minimizing sequence in some reflexive space we have

$$\mathcal{I} = \liminf_{h \to 0} \int_\Omega W\left(\nabla u_h\right)\,dx < \int_\Omega W\left(\nabla u\right)\,dx, \tag{2.25}$$

where u represents appropriate weak limit of the sequence u_h. We can assume that there exists a function $\overline{W} \in L^1(\Omega, \mathbb{R})$ such that

$$\liminf_{h\to 0} \int_D W\left(\nabla u_h\right)\, dx = \int_D \overline{W}(x)\, dx \tag{2.26}$$

for every open measurable subset D of Ω. Moreover, it can be proven [B] that there exists a family of compactly supported Radon measures μ_x with the range $[0,1]$, depending measurably on $x \in \Omega$, such that

$$\overline{W}(x) = \int_{\mathcal{M}^{3\times 3}} W(A)\, d\mu_x(A). \tag{2.27}$$

It is known [BJ, 1992] that this probability measure, also called the gradient Young measure, associated with the problem (2.24) is unique in either $\mathcal{K} = \mathcal{V}$ or $\mathcal{K} = \mathcal{U}$. It can be shown in this case, that μ_x is discretely supported on F_i, $i = 1,2$ and that it is independent of x, i.e. $\mu_x = \delta_{F_1} + \delta_{F_2}$.

We approximate the gradient Young measure by constructing an approximate probability measure defined for any Borel subset M of $\mathcal{M}^{3\times 3}$ as follows [B]

$$\mu_{x,r,\nabla u}(M) \stackrel{\text{def}}{=} \frac{\operatorname{meas}\{y \in B_r(x) \mid \nabla u(y) \in M\}}{\operatorname{meas} B_r(x)}. \tag{2.28}$$

It is easily seen that if $u_h \rightharpoonup u$ weakly in $W^{1,p}(\Omega, \mathbb{R}^3)$ then

$$\int_{\mathbb{R}^{3\times 3}} W(A)\, d\mu_{x,r,\nabla u_h}(A) = \frac{1}{\operatorname{meas} B_r(x)} \int_{B_r(x)} W(\nabla u_h(y))\, dy \to \int_{\mathbb{R}^{3\times 3}} W(A)\, d\mu_{x,r}(A),$$

$$\mu_{x,r}(A) \stackrel{\text{def}}{=} \frac{1}{\operatorname{meas} B_r(x)} \int_{B_r(x)} \delta_{\nabla u(y)}\, dy,$$

where $B_r(x)$ is the ball centered at x with the radius r. Since the above limit pass holds true for any $W \in L^1(\Omega)$ we express this fact by writing

$$\mu_{x,r,\nabla u_h}(\mathcal{K}_2) \stackrel{*}{\rightharpoonup} \delta_{\nabla u(x)}, \qquad \text{as } r \to 0_+,\ h \to 0_+ \text{ weak-}* \text{ in the sense of measure.} \tag{2.29}$$

Thus, the approximation of the problem (2.24) reduces to showing the above limiting property of the family of the approximate probability measures $\mu_{x,r,\nabla u_h}$.

The cut-off functions. Since the domain Ω has Lipschitz boundary, there exists a function $\sigma \in W_0^{1,\infty}(\Omega) \cap C^\infty(\overline{\Omega})$, $\sigma \geq 0$, such that for some positive constants C, C_1, C_2, we have

$$\begin{gathered} C_1 \operatorname{Dist}(x, \partial\Omega) \leq \sigma(x) \leq C_2 \operatorname{Dist}(x, \partial\Omega) \\ |\nabla \sigma|_{L^\infty(\Omega)} \leq C. \end{gathered} \tag{2.30}$$

Moreover, there exists a family of positive functions $\sigma_h \in C^\infty(\Omega)$, such that

$$\begin{gathered} \operatorname{supp} \sigma_h \subset \{x \in \Omega |\ \operatorname{Dist}(x, \partial\Omega) > h\} \subset \operatorname{supp} \sigma \\ \sigma_h \stackrel{\text{uniformly}}{\longrightarrow} \sigma, \qquad \text{as } h \to 0_+, \\ \|\sigma_h\|_{2,\infty} \leq C < +\infty, \qquad \text{and } \sigma_h \leq \sigma, \qquad \text{in } \Omega. \end{gathered} \tag{2.31}$$

The existence of the functions σ and σ_h is found in [N].

Mollifiers. Let $\phi_0 \in C_0^\infty(\mathbb{R}^3)$ is such that $\phi_0(x) \geq 0$ for all $x \in \mathbb{R}^3$, supp$\phi_0 = \{x \in \mathbb{R}^3 \mid |x| = 1\}$ and $\int_{\mathbb{R}^n} \phi_0(x)\, dx = 1$. Let $\varepsilon > 0$ and $u \in L^1(\Omega)$. The mollifier is given by

$$(R_\varepsilon u)(x) = \varepsilon^{-3} \int_\Omega \phi_0\left(\frac{x-y}{\varepsilon}\right) u(y)\, dy. \tag{2.32}$$

By $(R_\varepsilon \nabla u)(x)$ we mean application of the vector function ϕ_0 on each component of ∇u separately if $u \in L^1(\Omega, \mathbb{R}^3)$. It is obvious that $R_\varepsilon u \in C^\infty(\Omega, \mathbb{R}^3)$ and that $R_\varepsilon u \to u$ in $L^p(\Omega)$, for any $u \in L^p(\Omega)$ and $1 \leq p \leq \infty$. The convergence property can be proven by using the fact that every function $u \in L^p(\Omega)$ is $p-$mean continuous [KJF]. We will use this property frequently. The function $u \in L^p(\Omega)$ is said to be $p-$mean continuous if for every $\varepsilon > 0$ there exists a $\delta = \delta(\varepsilon)$ such that

$$\int_\Omega |u(x+h) - u(x)|^p\, dx \leq \varepsilon^p, \qquad |h| < \delta(\varepsilon). \tag{2.33}$$

Throughout the paper, we assume that ϕ_0 is extended by 0 outside its domain of definition.

3. Convergence theory and the error estimates

We develop the convergence theory of the microscopic quantities such as ∇u_h separately from the minimization of the free-energy. The convergence theory is based on the observation (proven in [L, 1996a]) that the discrete deformation gradients projected into the direction of the twin planes converge strongly. The proof of this surprising property is given in the next Theorem.

Theorem 3.1. *Let $1 \leq p < \infty$, let D be any open subset of Ω with a positive Lebesgue measure, and let $u_h \in \mathcal{A}_h$. Then for any $m \in n^\perp$ there exists a positive constant C, independent of h, F, m, D and p, such that*

$$\int_D |(\nabla_h u_h(x) - F)m|^p\, dx \leq C \int_D |\nabla_h u_h(x) - \Pi \nabla_h u_h(x)|^p\, dx \tag{3.1}$$

Hence, if $\nabla_h u_h - \Pi \nabla_h u_h \to 0$ strongly in $L^p(\Omega, \mathbb{R}^{3\times 3})$ as $h \to 0_+$, then

$$(\nabla_h u_h(x) - F)\, m \to 0, \qquad \textit{strongly in } L^p(\Omega, \mathbb{R}^3).$$

Proof. Let the mapping R_ε be the mollifier and $\varepsilon > 0$ arbitrary. We have

$$\begin{gathered} C \int_D |(\nabla_h u_h(x) - F)m|^p\, dx \leq \\ \int_D |(\nabla_h u_h(x) - (R_\varepsilon \nabla_h u_h)(x))\, m|^p\, dx + \int_D |((R_\varepsilon \nabla_h u_h)(x) - F)\, m|^p\, dx. \end{gathered} \tag{3.2}$$

For any positive constant $\varepsilon_1 > 0$ there exists $\delta_1(\varepsilon_1) > 0$ such that

$$\int_D |(\nabla_h u_h(x) - (R_\varepsilon \nabla_h u_h)(x))\, m|^p\, dx \leq \varepsilon_1 \qquad \text{if } \varepsilon < \delta_1(\varepsilon_1). \tag{3.3}$$

Because for any $F_i \in \mathcal{K}_2$ we have $F_1 m = F_2 m = Fm = \Pi \nabla_h u_h(x) m$ in Ω we get for any $m \in n^\perp$

$$\int_D |(\Pi \nabla_h u_h(x) - F)\, m|^p\, dx = \int_D \left(|\Pi \nabla_h u_h(x) m|^2 - 2\Pi \nabla_h u_h(x) m \cdot Fm + |Fm|^2\right)^{\frac{p}{2}}\, dx = 0.$$

Consequently,

$$\begin{aligned}
&\int_D |R_\varepsilon((\nabla_h u_h(x) - F)m)|^p \, dx = \int_D |(R_\varepsilon(\nabla_h u_h - \Pi\nabla_h u_h)m)(x)|^p \, dx \\
&\le \int_D |(R_\varepsilon(\nabla_h u_h - \Pi\nabla_h u_h)m)(x) - (\nabla_h u_h(x) - \Pi\nabla_h u_h(x))m|^p \, dx \qquad (3.4)\\
&+ \int_D |\nabla_h u_h(x) - \Pi\nabla_h u_h(x)|^p \, dx.
\end{aligned}$$

The $p-$mean continuity yields again for any positive ε_2 some $\delta_2(\varepsilon_2) > 0$ such that

$$\int_D |(R_\varepsilon(\nabla_h u_h - \Pi\nabla_h u_h)(x) - (\nabla_h u_h - \Pi\nabla_h u_h)(x))m|^p \, dx \le \varepsilon_2, \qquad \text{if } \varepsilon < \delta_2(\varepsilon_2). \tag{3.5}$$

It follows from (3.2) and (3.5) that there exists a positive constant C, independent of h, F, m, D and p, such that

$$C \int_D |(\nabla_h u_h(x) - F)m|^p \, dx \le \varepsilon_1 + \varepsilon_2 + \int_D |\nabla_h u_h(x) - \Pi\nabla_h u_h(x)|^p \, dx.$$

The proof now follows by substituting $\varepsilon_1 \stackrel{\text{def}}{=} \varepsilon_{1,h} = \varepsilon_2 \stackrel{\text{def}}{=} \varepsilon_{2,h} = \int_D |\nabla_h u_h(x) - \Pi\nabla_h u_h(x)|^p \, dx$ and by taking ε sufficiently small. □

The first Corollary of the previous Theorem shows that the Dirichlet boundary condition $u_h(x)|_{\partial\Omega} = Fx$, which is reflected by $\nabla_h u_h - \Pi\nabla_h u_h \to 0$ strongly in $L^1(\Omega, \mathbb{R}^{3\times 3})$, is strong enough to ensure the strong convergence of the discrete deformation gradients to the variants F_1 and F_2. Similar result is obtained in the continuous case in [BJ, 1992]. The proof of this Corollary is taken from [L, 1996a].

Corollary 3.2. *Let $\Pi_{1,2} : \mathcal{M}^{3\times 3} \to \{F_1, F_2\}$ be the projection given by (2.6), and let us assume that the assumptions of the Theorem 3.1 are satisfied. Then there exists a positive constant C, independent of h, F, D and p, such that*

$$\int_D |\nabla_h u_h(x) - \Pi_{1,2}(\nabla_h u_h(x))|^p \, dx \le \int_D |\nabla_h u_h(x) - \Pi(\nabla_h u_h(x))|^p \, dx. \tag{3.6}$$

Hence, if $\nabla_h u_h - \Pi\nabla_h u_h \to 0$ strongly in $L^1(\Omega, \mathbb{R}^{3\times 3})$ as $h \to 0_+$, then

$$\nabla_h u_h \to \Pi_{1,2}\nabla_h u_h \quad \textit{strongly in} \quad L^1(\Omega, \mathbb{R}^{3\times 3}). \tag{3.7}$$

Proof. Since $\Pi\nabla_h u_h = B(\nabla_h u_h)\Pi_{1,2}\nabla_h u_h$ we get a positive constant C, independent of h, F, D and p, such that

$$\begin{aligned}
&C \int_D |\nabla_h u_h(x) - \Pi_{1,2}\nabla_h u_h(x)|^p \, dx \\
&\le \int_D |\nabla_h u_h(x) - \Pi\nabla_h u_h(x)|^p \, dx + \int_D |\Pi\nabla_h u_h(x) - \Pi_{1,2}\nabla_h u_h(x)|^p \, dx \\
&= \int_D |\nabla_h u_h(x) - \Pi\nabla_h u_h(x)|^p \, dx + \int_D |(B(\nabla_h u_h(x)) - \mathrm{I})\, \Pi_{1,2}\nabla_h u_h(x)|^p \, dx \qquad (3.8)\\
&\le \int_D |\nabla_h u_h(x) - \Pi\nabla_h u_h(x)|^p \, dx + C \int_D |B(\nabla_h u_h(x)) - \mathrm{I}|^p \, dx.
\end{aligned}$$

In order to find the estimate for the last integral in (3.8) we show that there exists a suitable constant C, independent of h, F, D and p, such that

$$\int_D |(B(\nabla_h u_h(x)) - \mathrm{I})\, j|^p \; dx \le \int_D |\nabla_h u_h(x) - \Pi \nabla_h u_h(x)|^p \; dx, \qquad j \in \{F_1 m_1, F_2 m_2, m\}. \tag{3.9}$$

Here, $m = F_1 m_1 \times F_2 m_2$, $m_1 \cdot n = m_2 \cdot n = F_1 m_1 \cdot F_2 m_2 = 0$ and n is the normal to the twin plane. We note that $\{F_1 m_1, F_2 m_2, m\}$ is a basis in $\mathbb{R}^3$ since F_1 and F_2 are linearly independent.

First, let $j \in \{F_1 m_1, F_2 m_2\}$. In this case we have for any $\tilde{m} \in n^\perp$

$$\begin{aligned}(B(\nabla_h u_h(x)) - \mathrm{I})\, F_1 \tilde{m} &= (B(\nabla_h u_h(x)) - \mathrm{I})\, \Pi_{1,2} \nabla_h u_h(x) \tilde{m} \\ &= (\Pi \nabla_h u_h(x) - \Pi_{1,2} \nabla_h u_h(x))\, \tilde{m} = (\Pi \nabla_h u_h(x) - F)\, \tilde{m} \\ &= (\Pi \nabla_h u_h(x) - \nabla_h u_h(x))\, \tilde{m} + (\nabla_h u_h(x) - F)\, \tilde{m}.\end{aligned} \tag{3.10}$$

Thus (3.9) follows from (3.10) and the Theorem 3.1.

Secondly, if $j = m$ we can use the identity

$$\begin{aligned}(B(\nabla_h u_h(x)) - \mathrm{I})\, m &= B(\nabla_h u_h(x)) F_1 m_1 \times B(\nabla_h u_h(x)) F_2 m_2 - F_1 m_1 \times F_2 m_2 \\ = (B(\nabla_h u_h(x)) - \mathrm{I})\, F_1 m_1 &\times B(\nabla_h u_h(x)) F_1 m_2 - (F_1 m_1 \times (\mathrm{I} - B(\nabla_h u_h(x)))\, F_1 m_2)\end{aligned} \tag{3.11}$$

to get (3.9) from (3.10) and the Theorem 3.1. The inequalities (3.9) and (3.8) yield (3.6) and the proof is finished. $\square$

The second Corollary of the Theorem 3.1 shows that the strong convergence of the directional derivatives is sufficient to yield the strong convergence of the deformation itself. The similar result is given in [L, 1996a] for the conforming finite element approximations.

Corollary 3.3. *Let $u_h \in \mathcal{A}_h^{Fx}$ and let as assume that the assumptions of the Theorem 3.1 are satisfied. If $\nabla_h u_h - \Pi \nabla_h u_h \to 0$ strongly in $L^p(\Omega, \mathbb{R}^{3\times 3})$ as $h \to 0_+$ then*

$$u_h \to Fx \quad \text{strongly in } L^p(\Omega, \mathbb{R}^3) \text{ as } h \to 0_+.$$

Proof. We show the strong convergence of the approximate deformations u_h to Fx in the $L^p(\Omega)$ by proving the following inequality:

There exists a positive constant C, independent of h, m and p, such that for any $m \in n^\perp$, any $w_h \in \mathcal{A}_h^{Fx}$, and $1 \le p < \infty$, we have

$$\int_\Omega |w_h(x) - Fx|^p \; dx \le C \int_\Omega |(\nabla_h w_h(x) - F) m|^p \; dx. \tag{3.12}$$

The conclusion of the Corollary then follows from (3.12) where we take u_h instead of w and from the Theorem 3.1.

We prove the inequality (3.12) by contradiction. Let us assume that there exists at least one function $w_h \in \mathcal{A}_h^{Fx}$ such that $\|w_h - Fx\|_{L^\infty(\Omega, \mathbb{R}^3)} = 1$ and for which we have

$$\int_\Omega |(\nabla_h w_h(x) - F) m|^p \; dx \le C \int_\Omega |w_h(x) - Fx|^p \; dx.$$

Without loss of generality we assume that $\Omega = (0,1)^3$. We have

$$\int_{[0,1]^3} |(\nabla_h w_h(x) - F)m|^p \, dx = \int_{[0,1]^2} \int_0^1 \left| \tfrac{d}{dt_h} \left(w_h(x+tm) - F(x+tm) \right) \right|^p \, dt \, dx,$$

where the derivative $\frac{d}{dt_h}$ is understood in the piece-wise sense corresponding to the decomposition τ_h of $[0,1]^3$. Because

$$\int_{[0,1]^3} |w_h(x) - Fx|^p \, dx = \int_{[0,1]^2} \int_0^1 |w_h(x+tm) - F(x+tm)|^p \, dt \, dx$$

it follows from the above assumption that for almost all $x \in [0,1]^2$ we have

$$\int_0^1 \left| \tfrac{d}{dt_h} \left(w_h(x+tm) - F(x+tm) \right) \right|^p \, dt \le \int_0^1 |w_h(x+tm) - F(x+tm)|^p \, dt.$$

Let ι_h be an uniform mesh on $(0,1)$ with the mesh size h. The identity mapping from $W^{1,1}(i_h)$ to $L^p(i_h)$ is bounded for any $i_h \in \iota_h$ and any $1 \le p < \infty$. Thus we have the estimate

$$\begin{aligned} \int_{i_h} |w_h(x+tm) - F(x+tm)|^p \, dt &\le \left(C \int_{i_h} \left| \tfrac{d}{dt_h} \left(w_h(x+tm) - F(x+tm) \right) \right| \, dt \right)^p \\ &\le C\, h \int_{i_h} \left| \tfrac{d}{dt_h} \left(w_h(x+tm) - F(x+tm) \right) \right|^p \, dt. \end{aligned}$$

Because

$$\begin{aligned} \int_0^1 |w_h(x+tm) - F(x+tm)|^p \, dt &= \sum_{i_h \in \iota_h} \int_{i_h} |w_h(x+tm) - F(x+tm)|^p \, dt \\ &\le C\, h \int_0^1 \left| \tfrac{d}{dt_h} \left(w_h(x+tm) - F(x+tm) \right) \right|^p \, dt \end{aligned}$$

we must have

$$\left| \tfrac{d}{dt} \left(w_h(x+tm) - F(x+tm) \right) \right| = 0, \qquad \text{for almost all } t \in [0,1] \text{ and } x \in [0,1]^2.$$

This means that $(w_h - Fx) \in \mathcal{A}_h^{Fx}$ must be piece-wise constant along the lines with the directional vector m. We finish the proof by showing that this implies $w_h(x) = Fx$ in $[0,1]^3$ which contradicts the assumption $\|w_h - Fx\|_{L^\infty(\Omega,\mathbb{R}^3)} = 1$. Since w_h may not be continuous across the inter-element boundaries except for at least one point due to (2.16), we proceed as follows.

Let $Q_h \in \tau_h$ be a "corner" boundary element, i.e. an element which has at least two boundary faces. It follows from the definition of the boundary conditions (2.20) and the fact that $(w_h - Fx)$ must be piece-wise constant along the lines with the directional vector m that there exist at least two parallel lines ℓ_1 and ℓ_2 in $\overline{Q}_h$ such that

$$w_h - Fx = 0, \qquad \text{on } \ell_1,\, \ell_2.$$

Now we define the function

$$f(t) \stackrel{\text{def}}{=} \frac{d}{dt} \left(w_h(x+tr) - F(x+tr) \right) = (\nabla w_h(x+tr) - F)r, \quad \text{for } x+tr \in Q_h,$$

where $r = (r_1, r_2, r_3)$ is a vector which is linearly independent of m and $r_i^2 = r_j^2$ for any $i, j = 1, 2, 3$. By the construction of $\mathcal{A}_h^{Fx}$ we have

$$-\Delta(w_h - Fx) = 0, \qquad \text{in } Q_h \qquad \text{and}$$
$$\partial^2_{x_i x_j}(w_h(x) - Fx) = 0, \qquad \text{in } Q_h \quad \text{if} \quad i \neq j.$$

hence

$$f'(t) = 0, \qquad \text{in } Q_h.$$

Therefore $(\nabla w_h(x + tr) - F)r$ has to be constant along the line with the directional vector n in Q_h. Let $x_i \in \ell_i$, $i = 1, 2$ and $x_2 = x_1 + tr$ for some t. Then

$$0 = (w_h(x_1) - Fx_1) - (w_h(x_2) - Fx_2) = (\nabla w_h(x + tr) - F)r.$$

The maximum principle then implies that

$$w_h - Fx = 0, \qquad \text{in the plane perpendicular to } m \times r.$$

Repeating the above computation with the vector $m \times r$ we get

$$w_h - Fx = 0, \qquad \text{in } \overline{Q}_h.$$

Next we can show that $w_h = Fx$ at the elements next to Q_h. This follows from the fact that $w_h = Fx$ on ∂Q_h and because $w_h(x + tm) - F(x + tm)$ has to be constant. Repeating this procedure we exhaust τ_h which yields $w_h = Fx$ in $[0, 1]^3$ and this leads to the contradiction. □

Remark: (i) The proof of the Corollary 3.3 indicates that the finite element approximations with the postulated property of the piecewise harmonicity behave as the conforming approximations in the case of pure twinning. This follows from the above proven fact that the boundary conditions (2.20) with $g(s) = Fs$ yield $u_h(x) = Fx$ in Ω if u_h is required to be a piecewise affine function.

(ii) The condition of the harmonicity is necessary. This can be seen from the following example. Let $\Omega = (0, 1)^2$, $m = [1, 0]^T$ and

$$\frac{\partial w(x, y)}{\partial x} = 0, \quad \text{in } (0, 1)^2, \quad w\big|_{y=0} = w\big|_{y=1} = \int_{x=0} w \, dS = \int_{x=1} w \, dS = 0.$$

We can take, e.g.

$$w = \begin{cases} x, & \text{on } (0, \frac{1}{4}) \times (0, 1), \\ -x + 1/2 & \text{on } (\frac{1}{4}, \frac{3}{4}) \times (0, 1), \\ x - 1 & \text{on } (\frac{3}{4}, 1) \times (0, 1). \end{cases}$$

Then we define $w_\varepsilon = R_\varepsilon w$, where R_ε is the mollifier. With the above definition of w we have for sufficiently small $\varepsilon > 0$ that $-\Delta w_\varepsilon = \partial^2_{y^2} w_\varepsilon < 0$ on the ε neighborhood of $x = \frac{1}{4}$ and $-\Delta w_\varepsilon > 0$ close to $x = \frac{3}{4}$ and

$$\int_{\partial(0,1)^2} w_\varepsilon \, dS = \int_{(0,1)^2} |\nabla w_\varepsilon(x, y) m| \, dx \, dy < \int_{(0,1)^2} |w_\varepsilon(x, y)| \, dx \, dy.$$

Hence, the local harmonicity of the non-conforming finite elements is a necessary condition for the Corollary 3.3 to be true.

(iii) The condition of the vanishing cross derivatives of the basis functions is also necessary. This follows from the example of the polynomial $xy(x^2 - y^2)$ considered on the square $[-1, 1]^2$.

(iv) The conditions of the local harmonicity and vanishing cross derivatives can be ommited if the construction of the finite element space guaranties pointwise satisfaction of the Dirichlet boundary condition. □

The next Theorem yields the principal error estimate of the weak convergence of the deformation gradients.

Theorem 3.4. *Let D be an arbitrary open subdomain of Ω with positive Lebesgue measure and Lipschitz boundary, let $u_h \in \mathcal{A}_h^{Fx}$, and let us assume that $\|\nabla_h u_h\|_{L^\infty(\Omega,\mathbb{R}^{3\times 3})}$ is bounded independently of h. Then there exists a positive constant C, independent of h, F, D and γ, and there exists $h_0 > 0$ such that for any h, $0 < h < h_0$, we have*

$$C\left|\int_D (\nabla_h u_h(x) - F)\, dx\right| \leq h + h^{\frac{\gamma}{2}} \|u_h(x) - Fx\|_{L^1(D,\mathbb{R}^3)}^{\gamma/2}, \qquad \text{for any } \gamma \in (0,1). \tag{3.13}$$

Hence, if $\nabla_h u_h - \Pi\nabla_h u_h \to 0$ strongly in $L^1\left(\Omega, \mathbb{R}^{3\times 3}\right)$ as $h \to 0_+$, then

$$u_h \rightharpoonup Fx \quad \text{weakly in } W^{1,1}(\Omega,\mathbb{R}^3) \quad \text{as } h \to 0_+.$$

Proof. Let D be an arbitrary open subdomain of Ω. We first extend u_h by Fx from D onto Ω. Let

$$\Omega_h^0 = \bigcup_{Q_h \in \tau_h^0} Q_h, \qquad \Omega_h^1 = \bigcup_{Q_h \in \tau_h^1} Q_h$$

where $\tau_h^0 \subset \tau_h$ and $\tau_h^1 \subset \tau_h$ are such that $\Omega_h^0 \subset \overline{D} \subset \Omega_h^1$ and $\mathrm{meas}(\Omega_h^1 \backslash \Omega_h^0) \leq \text{const.}\ h$. We assume that $\Omega_h^0 \neq \emptyset$ which is true for sufficiently small h because D has Lipschitz boundary. We construct a function $\bar{u}_h \in \mathcal{A}_h$ such that

$$\bar{u}_h(x) = \begin{cases} u_h(x), & x \in \Omega_h^0, \\ v_h(x), & x \in \Omega_h^1 \backslash \Omega_h^0, \\ Fx, & x \in \mathbb{R}^n \backslash \Omega_h^1. \end{cases}$$

The function v_h is defined as follows. If $Q_h^0 \in \Omega_h^1 \backslash \Omega_h^0$. we can find two opposite faces $\wp_h^0$, $\wp_h^1 \in \partial Q_h^0$, $\wp_h^i \cap D = \emptyset$, $i = 1, 2$, so that we have a homotopy between the values $u_h|_{\wp_h^0}$ and $Fx|_{\wp_h^1}$ given by

$$\tilde{v}_h(x + t(y - x)) \stackrel{\text{def}}{=} tFy + (1 - t)u_h(x), \qquad t \in [0,1], \quad x \in \wp_h^0, \quad y \in \wp_h^1,$$

where the directionalvector of $x - y$ is constant for any $x \in \wp_h^0$. Using the cut-off functions σ_h, with properties given by (2.31), restricted to Q_h and modified so that $\sigma_h|_{\wp_h^1} = 1$, we define

$$v_h(x + t(y - x)) = \sigma_h(x + t(y - x))\tilde{v}_h(x + t(y - x)) + (1 - \sigma_h(x + t(y - x)))u_h(x + t(y - x)).$$

We observe that v_h is defined for any $x \in Q_h^0$, that $v_h|_{\wp_h^1} = Fx$, and that v_h satisfies the integral continuity criterion (2.16). Moreover, we show that there exists a positive constant C, independent of independent of D, F and τ_h, such that

$$\int_{\Omega_h^1 \backslash D} |\nabla_h v_h(z)|\, dz + \int_{D \backslash \Omega_h^0} |\nabla_h v_h(z)|\, dz \leq C\left(h + \sqrt{h}\left(\int_D |u_h(z) - Fz|\, dz\right)^{1/2}\right).$$

To prove this inequality, we first determine a subset ι_h of τ_h such that

$$\Omega_h^1 \backslash D \subset \bigcup_{Q_h^0 \in \iota_h} Q_h^0, \qquad Q_h^0 \in \Omega_h^1 \backslash \Omega_h^0,$$

hence

$$\int_{\Omega_h^1 \backslash D} |\nabla_h v_h(z)|\, dz \leq \sum_{Q_h^0 \in \iota_h} \int_{Q_h^0} |\nabla v_h(z)|\, dz \leq \sum_{Q_h^0 \in \iota_h} \int_{Q_h^0} |\nabla \tilde{v}_h(z)|\, dz.$$

Because

$$\left|\tfrac{d}{dt}\tilde{v}_h(x+t(y-x))\right| = |F(y-x)+Fx-u_h(x)|$$

we obtain a positive constant C, independent of t and h, such that

$$C\ |\nabla\tilde{v}_h(x+t(y-x))| \le |F| + \tfrac{1}{h}\,|Fx-u_h(x)|\,, \qquad t\in[0,1],\quad x\in\wp_h^0,\quad y\in\wp_h^1.$$

This inequality yields

$$\int_{Q_h^0} |\nabla\tilde{v}_h(z)|\ dz = \int_{\wp_h^0}\int_0^1 |\nabla\tilde{v}_h(x+t(y-x))|\ dt\,dx \le h^3\,|F| + \tfrac{1}{h}\int_{\wp_h^0} |u_h(x)-Fx|\ dx.$$

The Mean Value Theorem for integrals gives for some $t_0\in(0,1]$, $t_1\in(0,t_0)$ and $t_2\in(0,t_1)$ the expression

$$\begin{aligned}
&\int_{Q_h^0} |u_h(z)-Fz|\ dz = \int_{\wp_h^0}\int_0^1 |u_h(x+t(y-x)) - F(x+t(y-x)))|\ dt\,dx\\
&= \int_{\wp_h^0} |u_h(x+t_0(y-x)) - F(x+t_0(y-x)))|\ dx\\
&= \int_{\wp_h^0} |u_h(x) - Fx + t_0\left(\nabla_h u_h(x+t_1(y-x)) - F\right)(y-x)|\ dx\\
&= \int_{\wp_h^0} \left|u_h(x) - Fx + t_0t_1\,\Delta\,u_h(x+t_2(y-x))(y-x)^T(y-x)\right|.
\end{aligned}$$

Hence, there exists a constant C, independent of h, F and Q_h^0 such that

$$C\int_{\wp_h^0} |u_h(x)-Fx|\ dx \le h^4 + \int_{Q_h^0} |u_h(z)-Fz|\ dz.$$

The inverse inequality [C, Theorem 17.2]

$$\|u_h - Fx\|_{L^\infty(\Omega,\mathbb{R}^3)} \le \frac{C}{h^{3/2}}\,\|u_h-Fx\|_{L^2(\Omega,\mathbb{R}^3)}$$

and the Hölder inequality yield a positive constant C, independent of D, u_h and F, such that

$$\begin{aligned}
&\tfrac{1}{h}\sum_{Q_h^0\in\iota_h}\int_{Q_h^0} |u_h(z)-Fz|\ dz \le C\,h^2\sum_{Q_h^0\in\iota_h}\|u_h-Fx\|_{L^\infty(Q_h^0,\mathbb{R}^3)} \le C\,h^2\,\|u_h-Fx\|_{L^\infty(D,\mathbb{R}^3)}\\
&\le C\sqrt{h}\,\|u_h-Fx\|_{L^2(D,\mathbb{R}^3)} \le C\sqrt{h}\,\|u_h-Fx\|^{1/2}_{L^\infty(D,\mathbb{R}^3)}\,\|u_h-Fx\|^{1/2}_{L^1(D,\mathbb{R}^3)}\\
&\le C\sqrt{h}\,\|u_h-Fx\|^{1/2}_{L^1(D,\mathbb{R}^3)}
\end{aligned}$$

we have

$$\begin{aligned}
C\sum_{Q_h^0\in\iota_h}|\nabla\tilde{v}_h(z)|\ dz &\le C\sum_{Q_h^0\in\iota_h} h^3 + C\tfrac{1}{h}\sum_{Q_h^0\in\iota_h}\int_{Q_h^0}|u_h(z)-Fz|\ dz\\
&\le h+\sqrt{h}\int_D |u_h(z)-Fz|\,.
\end{aligned}$$

The remaining integral over $D\backslash\Omega_h^0$ is estimated in the same way.

Let the mapping R_ε be the mollifier and $\varepsilon > 0$ arbitrary. We have

$$\left|\int_D (\nabla_h u_h(x) - F)\ dx\right| \le \left|\int_D (\nabla_h u_h(x) - R_\varepsilon \nabla_h u_h(x))\ dx\right| + \left|\int_D R_\varepsilon\,(\nabla_h u_h(x) - F)\ dx\right| + \left|\int_D (R_\varepsilon F - F)\ dx\right|. \tag{3.14}$$

We estimate each of the integrals on the right-hand side of (3.14).

First, we have

$$\begin{aligned}&\int_D (R_\varepsilon \nabla_h u_h)(x) - \nabla_h u_h(x)\, dx\\ &= \int_D (R_\varepsilon \nabla_h \bar{u}_h)(x)\, dx + \int_D R_\varepsilon(\nabla_h u_h - \nabla \bar{u}_h)(x)\, dx - \int_D \nabla_h u_h(x)\, dx.\end{aligned} \tag{3.15}$$

We write

$$\int_D (R_\varepsilon \nabla_h \bar{u}_h)(x)\, dx = \int_\Omega (R_\varepsilon \nabla_h \bar{u}_h)(x)\, dx - \int_{\Omega\setminus\Omega_h^1} (R_\varepsilon \nabla_h \bar{u}_h)(x)\, dx - \int_{\Omega_h^1\setminus D} (R_\varepsilon \nabla_h \bar{u}_h)(x)\, dx. \tag{3.16}$$

It follows from the definition of the mollifier R_ε, Fubini's theorem, integration by parts and definition of $\bar{u}_h$ that

$$\begin{aligned}&\int_\Omega (R_\varepsilon \nabla \bar{u}_h)(x)\, dx\\ &= \int_{|z|\le 1}\int_\Omega \nabla_h \bar{u}_h(x - \varepsilon\, z)\phi_0(y)\, dx\, dz = \int_{|z|\le 1} \phi_0(z) \int_{\partial\Omega} Fx \otimes n\, dS\, dz = F\,\mathrm{meas}(\Omega).\end{aligned}$$

Similarly

$$\int_{\Omega\setminus\Omega_h^1} (R_\varepsilon \nabla_h \bar{u}_h)(x)\, dx = F\,\mathrm{meas}(\Omega\setminus\Omega_h^1),$$

hence we have from (3.16) and the above two calculations

$$\int_D (R_\varepsilon \nabla_h \bar{u}_h)(x)\, dx = F\left(\mathrm{meas}(\Omega_h^1)\right) - \int_{\Omega_h^1\setminus D} (R_\varepsilon \nabla_h \bar{u}_h)(x)\, dx. \tag{3.17}$$

Because

$$\int_D (R_\varepsilon(\nabla_h u_h - \nabla_h \bar{u}_h))(x)\, dx = \int_{D\setminus\Omega_h^0} (R_\varepsilon(\nabla_h u_h - \nabla_h \bar{u}_h))(x)\, dx$$

and, similar to (3.17),

$$\begin{aligned}&-\int_D \nabla_h u_h(x)\, dx = -\int_\Omega \nabla_h u_h(x)\, dx + \int_{\Omega\setminus\Omega_h^1} \nabla_h u_h(x)\, dx + \int_{\Omega_h^1\setminus D} \nabla_h u_h(x)\, dx\\ &= -F\,\mathrm{meas}(\Omega_h^1) + \int_{\Omega_h^1\setminus D} \nabla_h u_h(x)\, dx\end{aligned}$$

we can write the first integral on the right-hand side of (3.14) in the form

$$\begin{aligned}&\int_D (\nabla_h u_h(x) - (R_\varepsilon \nabla_h u_h)(x))\ dx = -\int_{\Omega_h^1\setminus D} (R_\varepsilon \nabla_h v_h)(x)\, dx\\ &+ \int_{D\setminus\Omega_h^0} (R_\varepsilon \nabla_h u_h)(x)\, dx - \int_{D\setminus\Omega_h^0} (R_\varepsilon \nabla_h v_h)(x)\, dx + \int_{\Omega_h^1\setminus D} \nabla_h u_h(x)\, dx.\end{aligned} \tag{3.18}$$

The estimate of $\|\nabla v_h\|_{L^1(Q_h^0,\mathbb{R}^{3\times 3})}$ yields a positive constant C, which is independent of h, ε, F and D, such that

$$\left|-\int_{\Omega_h^1\setminus D}(R_\varepsilon\nabla_h v_h)(x)\,dx\right| + \left|-\int_{D\setminus\Omega_h^0}(R_\varepsilon\nabla_h v_h)(x)\,dx\right| \le C\left(h+\sqrt{h}\,\|u_h(x)-Fx\|^{1/2}_{L^1(D,\mathbb{R}^3)}\right).$$

Since meas $\left(\bigcup_{Q_h^0\in\iota_h} Q_h^0\right)\le C\,h$ and since there exists an uniform bound of $\|\nabla_h u_h\|_{L^\infty(\Omega,\mathbb{R}^{3\times 3})}$ by assumption we have

$$\left|\int_{D\setminus\Omega_h^0}(R_\varepsilon\nabla_h u_h)(x)\,dx\right| + \left|\int_{\Omega_h^1\setminus D}\nabla_h u_h)(x)\,dx\right| \le C\,h,$$

where C is a positive constant, independent of h, ε, F and D. Hence, there exists a positive constant C, independent of h, ε, F and D, such that

$$C\left|\int_D\left(\nabla_h u_h(x)-(R_\varepsilon\nabla_h u_h)(x)\right)\,dx\right| \le h+\sqrt{h}\,\|u_h-Fx\|^{1/2}_{L^1(D,R^3)}. \tag{3.19}$$

The second integral on the right-hand side of (3.14) can be estimated by using the integration by parts and the Hölder inequality. We obtain

$$\left|\int_D\left(R_\varepsilon\left(\nabla_h u_h\right)(x)-F\right)\,dx\right| \le \tfrac{1}{\varepsilon}\,\|\nabla\phi_0\|_{L^\infty(\mathbb{R},\mathbb{R}^{3\times 3})}\,\|u_h(x)-Fx\|_{L^1(D,\mathbb{R}^3)}. \tag{3.20}$$

We have $\left|\int_D\left(R_\varepsilon F-F\right)\,dx\right|=0$, therefore we obtain from (3.14), (3.19) and (3.20) existence of a positive constant C, independent of h, F, D and ε, such that

$$C\left|\int_D\left(\nabla_h u_h(x)-F\right)\,dx\right| \le h+\sqrt{h}\,\|u_h(x)-Fx\|^{1/2}_{L^1(D,\mathbb{R}^3)}+\tfrac{1}{\varepsilon}\,\|u_h(x)-Fx\|_{L^1(D,\mathbb{R}^3)}. \tag{3.21}$$

The first part of the Theorem follows from (3.14), (3.19), and (3.20) by taking

$$\varepsilon \stackrel{\text{def}}{=} \varepsilon_h = h^{-\gamma/2}\,\|u_h-Fx\|^{1-\gamma/2}_{L^1(D,\mathbb{R}^3)} \qquad \text{for any } 0<\gamma<1.$$

The Corollaries 3.3 and 3.2 yield for any $m\in n^\perp$

$$\|u_h-Fx\|_{L^1(D,\mathbb{R}^3)} \le C\,\|(\nabla_h u_h-F)\,m\|_{L^1(D,\mathbb{R}^{3\times 3})} \le C\,\|\nabla_h u_h-\Pi\nabla_h u_h\|_{L^1(D,\mathbb{R}^{3\times 3})}. \tag{3.22}$$

The second part of the Theorem can be proven as follows. The Banach-Steinhouse theorem [KJF] implies that the weak convergence of a bounded sequence x_n in $L^1(\Omega)$ is equivalent to

$$\int_\Omega x_n\chi\,dx \to \int_\Omega x\chi\,dx$$

for all χ in a dense subset of $L^\infty(\Omega)=(L^1(\Omega))^*$. Since the linear hull of the characteristic functions χ_D of the open sets with the Lipschitz boundary is a dense subset in $L^\infty(\Omega)$ the proof of the Theorem follows from the strong convergence of $\nabla_h u_h-\Pi\nabla_h u_h\to 0$ in $L^1(\Omega,\mathbb{R}^{3\times 3})$ and (3.13). $\square$

Convergence of the microscopic quantities. The approximation of the problem (2.24) reduces to the investigation of the convergence properties of the approximate probability measure $\mu_{x,r,\nabla_h u_h}$. Due to the discrete structure of the set $\mathcal{K}_2$, we can rewrite (2.25) as follows. Let $r > 0$, D be an arbitrary open subset of Ω, and let $u_h \in \mathcal{A}_h^{Fx}$. We define for $i = 1, 2$

$$D^i_{r,h} \stackrel{\text{def}}{=} \{x \in D \,|\, \Pi(\nabla_h u_h(x)) = F_i,\, |\Pi(\nabla_h u_h(x)) - (\nabla_h u_h(x))| < r\}, \tag{3.23}$$

then

$$\mu_{x,r,\nabla_h u_h}(\mathcal{F}_i) = \operatorname{meas}(D^i_{r,h}) / \operatorname{meas}(D).$$

Hence, the limit pass (2.29) reduces to

$$\lim_{r\to 0_+} \lim_{h\to 0_+} \left| \frac{\operatorname{meas}(D^i_{r,h})}{\operatorname{meas}(D)} - \lambda_i \right| = \operatorname{meas}(D) \lim_{r\to 0_+} \lim_{h\to 0_+} \left| \operatorname{meas}(D^i_{r,h}) - \lambda_i \operatorname{meas}(D) \right| = 0. \tag{3.24}$$

The next Theorem and its consequences yield sufficient and necessary condition for (3.24) to be true.

Theorem 3.5. *Let $u_h \in \mathcal{A}_h^{Fx}$. Then there exists a positive constant C, independent of h, F, D, and there exists $h_0 > 0$ such that for any $h < h_0$ we have*

$$C \left| \operatorname{meas}(D^i_{r,h}) - \lambda_i \operatorname{meas}(D) \right| \le h + \|\nabla_h u_h - \Pi \nabla_h u_h\|^{\gamma}_{L^1(D,\mathbb{R}^{3\times 3})}, \qquad \text{for any } \gamma \in (0,1). \tag{3.25}$$

Hence, if $\nabla_h u_h - \Pi \nabla_h u_h \to 0$ strongly in $L^1(\Omega, \mathbb{R}^{3\times 3})$ as $h \to 0_+$, then

$$\lim_{r\to 0_+} \lim_{h\to 0_+} \mu_{x,r,\nabla_h u_h} \stackrel{*}{\rightharpoonup} \lambda_1 \delta_{F_1} + \lambda_2 \delta_{F_2} \quad \textit{weakly-* in a sence of measure.}$$

Proof. Since F_1 and F_2 are linearly independent, and because $\lambda_1 + \lambda_2 = 1$, (3.25) is equivalent to showing that

$$\left| \left(\operatorname{meas}(D^1_{r,h}) - \lambda_1 \operatorname{meas}(D)\right) F_1 + \left(\operatorname{meas}(D^2_{r,h}) - \lambda_2 \operatorname{meas}(D)\right) F_2 \right| \le \|\nabla_h u_h - \Pi \nabla_h u_h\|^{1-\gamma}_{L^1(\Omega,\mathbb{R}^{3\times 3})},$$

for any $\gamma \in (0,1)$. Because

$$\begin{aligned}
&\left(\operatorname{meas}(D^1_{r,h}) - \lambda_1 \operatorname{meas}(D)\right) F_1 + \left(\operatorname{meas}(D^2_{r,h}) - \lambda_2 \operatorname{meas}(D)\right) F_2 \\
&= \operatorname{meas}(D^1_{r,h}) F_1 + \operatorname{meas}(D^2_{r,h}) F_2 - \operatorname{meas}(D) F \\
&= \left(\operatorname{meas}(D^1_{r,h}) + \operatorname{meas}(D^2_{r,h})\right) \Pi_{1,2}\left(\nabla_h u_h(x)\right) - \operatorname{meas}(D) F
\end{aligned}$$

we have

$$\begin{aligned}
&\left(\operatorname{meas}(D^1_{r,h}) - \lambda_1 \operatorname{meas}(D)\right) F_1 + \left(\operatorname{meas}(D^2_{r,h}) - \lambda_2 \operatorname{meas}(D)\right) F_2 = \\
&\int_D \Pi_{1,2} \nabla_h u_h - \nabla_h u_h(x)\, dx - \int_D F - \nabla_h u_h(x)\, dx - \int_{D\setminus\left(D^1_{r,h} \cup D^2_{r,h}\right)} \Pi_{1,2}(\nabla_h u_h(x))\, dx.
\end{aligned}$$

The definition of $D^i_{r,h}$, $i = 1, 2$, yields

$$\tfrac{1}{r} \left|\Pi_{1,2}(\nabla_h u_h)(x) - \nabla_h u_h(x)\right| \ge 1, \qquad \text{for all } x \in D \setminus \left(D^1_{r,h} \cup D^2_{r,h}\right).$$

Because $|\Pi_{1,2}(\nabla_h u_h(x))|_{L^\infty(\Omega)} \le C$, C independent of h, we have

$$\int_{D\setminus\left(D^1_{r,h}\cup D^2_{r,h}\right)} |\Pi_{1,2}(\nabla_h u_h(x))|\,dx \le C\operatorname{meas}\left(D\setminus\left(D^1_{r,h}\cup D^2_{r,h}\right)\right)$$
$$\le \frac{C}{r}\int_{D\setminus\left(D^1_{r,h}\cup D^2_{r,h}\right)} |\Pi_{1,2}(\nabla_h u_h)(x) - \nabla_h u_h(x)|\,dx.$$

Assuming that $h_0 > 0$ is such that for any $\gamma \in (0,1)$ we have

$$\left(\int_{D\setminus\left(D^1_{r,h}\cup D^2_{r,h}\right)} |\Pi_{1,2}(\nabla_h u_h)(x) - \nabla_h u_h(x)|\right)^{1-\gamma} < r$$

we obtain for any $h < h_0$ the following inequality

$$\left|\left(\operatorname{meas}(D^1_{r,h}) - \lambda_1\operatorname{meas}(D)\right)F_1 + \left(\operatorname{meas}(D^2_{r,h}) - \lambda_2\operatorname{meas}(D)\right)F_2\right| \le$$
$$\int_D |\Pi_{1,2}(\nabla_h u_h(x)) - \nabla_h u_h(x)|\,dx + \left|\int_D \nabla_h u_h(x) - F\,dx\right|$$
$$+\left(\int_D |\Pi_{1,2}(\nabla_h u_h(x)) - \nabla_h u_h(x)|\,dx\right)^{\gamma}.$$

The Theorem 3.1 and the inequality (3.12) yield

$$C\int_\Omega |\nabla_h u_h(x) - \Pi(\nabla_h u_h(x))|\,dx \ge C\int_\Omega |(\nabla_h u_h(x) - F)\,m|\,dx \ge C\int_\Omega |u_h(x) - Fx|\,dx.$$

The proof now follows from the Corollary 3.2 and the Theorem 3.4. □

Corollary 3.6. *Let us assume that the assumptions of Theorem 3.5 are satisfied and let us assume that $\nabla_h u_h - \Pi\nabla_h u_h \to 0$ strongly in $L^1(\Omega,\mathbb{R}^{3\times 3})$. Then there exists $h_0 > 0$ such that for any $0 < h < h_0$ we have*

$$|\nabla_h u_h(x) - F| \ge |F_1 - F_2|\,, \qquad \text{a.e. in } \Omega. \tag{3.26}$$

Proof. Let D is an arbitrary open subset of Ω. Because $D = D^1_{r,h}\cup D^2_{r,h}\cup\left(D\setminus\left(D^1_{r,h}\cup D^2_{r,h}\right)\right)$ we have

$$\int_D |\nabla_h u_h(x) - F|\,dx$$
$$= \int_{D^1_{r,h}} |\nabla_h u_h(x) - F|\,dx + \int_{D^2_{r,h}} |\nabla_h u_h(x) - F|\,dx + \int_{D\setminus\left(D^1_{r,h}\cup D^2_{r,h}\right)} |\nabla_h u_h(x) - F|\,dx$$
$$\ge \operatorname{meas}(D^1_{r,h})\,|F_1 - F| + \operatorname{meas}(D^2_{r,h})\,|F_2 - F| - \int_{D^1_{r,h}} |F_1 - \nabla_h u_h(x)|\,dx$$
$$-\int_{D^2_{r,h}} |F_2 - \nabla_h u_h(x)|\,dx.$$

It follows from the definition of D^i_r, $i = 1,2$, that

$$-\,|F_i - \nabla_h u_h(x) - F_i + \Pi_{1,2}(\nabla_h u_h(x))| = -\,|F_i - \nabla_h u_h(x)| > -r, \qquad \forall x \in D^i_r.$$

Hence, we have from (3.25)

$$\begin{aligned}&\lim_{r\to 0_+}\lim_{h\to 0_+}\int_D |\nabla_h u_h(x) - F|\, dx\\ &\geq \lim_{r\to 0_+}\lim_{h\to 0_+}\left(\operatorname{meas}(D^1_{r,h})\,|F_1 - F| + \operatorname{meas}(D^2_{r,h})\,|F_2 - F| - r\left(\operatorname{meas}(D^1_{r,h}) + \operatorname{meas}(D^2_{r,h})\right)\right.\\ &= |D|\,|F_1 - F_2|\,.\end{aligned}$$

Since D was an arbitrary open subset of Ω, we have for sufficiently small h

$$|\nabla_h u_h(x) - F| \geq |F_1 - F_2| \qquad \text{a.e. in } \Omega$$

and the proof of (3.26) follows. □

The next result indicates that the requirement of the proper limiting properties of the deformation gradients limits the order of approximation of the macroscopic quantities such as the deformation itself.

Corollary 3.7. *Let us assume that $u_h \in \mathcal{A}_h^{Fx}$ and let $\nabla_h u_h - \Pi\nabla_h u_h \to 0$ strongly in $L^1(\Omega, \mathbb{R}^{3\times 3})$. Then there exists a positive constant C, independent of h, F, and γ, and there exists $h_0 > 0$ such that for any $h < h_0$ we have*

$$h \leq C\,\|u_h - Fx\|^{2\gamma}_{L^2(\Omega,\mathbb{R}^{3\times 3})}\,, \qquad \text{for any } \gamma \in (0,1). \tag{3.27}$$

Proof. Let $\tau_h^0 \subset \tau_h$ be such that

$$\Omega_h = \bigcup_{Q_h\in\tau_h^0} Q_h \quad \text{ and } \quad \operatorname{dist}(\partial\Omega, \partial\Omega_h) \leq h.$$

Because $u_h(x) = Fx$ on $\partial\Omega$, the Corollary 3.6 implies that for any $x_0 \in \partial\Omega_h$ there exists a $\tilde{x}_0 \in \Omega\backslash\Omega_h$ such that

$$|u_h(x_0) - Fx_0| = |\nabla_h u_h(\tilde{x}_0) - F|\, h \geq |F_1 - F_2|\, h.$$

Thus we have

$$|F_1 - F_2|^2\, h^2 \leq \fint_{\partial\Omega_h} |u_h(x) - Fx|^2\, dS.$$

Now, because $\operatorname{meas}_2(\partial\Omega)/\operatorname{meas}_2(\partial\Omega_h) = \mathcal{O}(1)$, the continuous imbedding of $H^1(\Omega)$ into $L^2(\partial\Omega)$ and the Poincaré–Friedrichs inequality yield

$$\begin{aligned}C\,|F_1 - F_2|^2 \operatorname{meas}_2(\partial\Omega) h^2 &\leq \operatorname{meas}_2(\partial\Omega)\fint_{\partial\Omega_h} |u_h(x) - Fx|^2\, dS\\ &\leq \int_\Omega \left|\nabla\,|u_h(x) - Fx|^2\right|\, dx.\end{aligned} \tag{3.28}$$

Let the map R_ε be the mollifier. We have

$$\begin{aligned}&\int_\Omega \left|\nabla\,|u_h(x) - Fx|^2\right|\, dx\\ &= 2\int_\Omega |u_h(x) - Fx|\,|\nabla_h u_h(x) - F + R_\varepsilon(\nabla_h u_h(x) - F) - R_\varepsilon(\nabla_h u_h(x) - F)|\, dx\\ &\leq \tfrac{1}{\varepsilon}\int_\Omega |u_h(x) - Fx|^2\, dx + 2\sqrt{\int_\Omega |\nabla_h u_h(x) - (R_\varepsilon\nabla_h u_h)(x)|^2\, dx}\sqrt{\int_\Omega |u_h(x) - Fx|^2\, dx}.\end{aligned} \tag{3.29}$$

Now, we show that there exists a positive constant C, independent of h and ε, such that

$$\int_\Omega |\nabla_h u_h(x) - (R_\varepsilon \nabla_h u_h)(x)|^2 \, dx \le \frac{C}{\varepsilon} \int_\Omega |u_h(x) - Fx|^2 \, dx. \tag{3.30}$$

As soon as we prove (3.30), the inequality (3.27) follows from (3.28) and (3.29) by taking

$$\varepsilon \overset{\text{def}}{=} \varepsilon_h = \left(\|u_h(x) - Fx\|^2_{L^2(\Omega,\mathbb{R}^3)} \right)^{1-\gamma}$$

for any $0 < \gamma < 1$.

In order to show (3.30), we first observe that $\int_\Omega |R_\varepsilon F|^2 - |F|^2 \, dx = 0$ and thus we have

$$\begin{aligned}
&\int_\Omega |\nabla_h u_h(x) - (R_\varepsilon \nabla_h u_h)(x)|^2 \, dx = \int_\Omega |\nabla_h u_h(x)|^2 \, dx - \int_\Omega |(R_\varepsilon \nabla_h u_h)(x)|^2 \, dx \\
&- 2\int_\Omega R_\varepsilon(\nabla_h u_h - F)(x)((R_\varepsilon \nabla_h u_h)(x) - \nabla_h u_h(x))\, dx \\
&= \int_\Omega |\nabla_h u_h(x)|^2 - |F|^2 \, dx - \int_\Omega |(R_\varepsilon \nabla_h u_h)(x)|^2 - |R_\varepsilon F|^2 \, dx \\
&- 2\int_\Omega R_\varepsilon(\nabla_h u_h - F)(x)((R_\varepsilon \nabla_h u_h)(x) - \nabla_h u_h(x))\, dx \\
&= \int_\Omega (\nabla_h u_h(x) - F)(\nabla_h u_h(x) + F)\, dx \\
&- \int_\Omega ((R_\varepsilon \nabla_h u_h)(x) - R_\varepsilon F)((R_\varepsilon \nabla_h u_h)(x) + R_\varepsilon F)\, dx \\
&- 2\int_\Omega R_\varepsilon(\nabla_h u_h - F)(x))((R_\varepsilon \nabla_h u_h)(x) - \nabla_h u_h(x))\, dx.
\end{aligned} \tag{3.31}$$

It follows from the $p-$mean continuity of $(R_\varepsilon \nabla_h u_h)(x) - \nabla_h u_h)(x)$ that for sufficiently small ε we have

$$\tfrac{1}{2}\left| \int_\Omega \nabla_h u_h(x)\, dx \right| \le \sqrt{\int_\Omega |(R_\varepsilon \nabla_h u_h)(x)|^2 \, dx}.$$

Since, $\left|\int_\Omega \nabla_h u_h)(x)\, dx\right| = |F| \operatorname{meas}(\Omega)$, $|F| > 0$ by (2.1) and (2.2), and because $\nabla_h u_h$ are uniformly bounded in $L^2(\Omega, \mathbb{R}^{3\times 3})$ due to the assumed strong convergence of $\nabla_h u_h - \Pi \nabla_h u_h$ in $L^p(\Omega, \mathbb{R}^{3\times 3})$, we have a positive constant C, independent of h and ε, such that

$$C \int_\Omega |\nabla_h u_h(x)|^2 \, dx \le |F|^2 \le \int_\Omega |(R_\varepsilon \nabla_h u_h)(x)|^2 \, dx.$$

Hence,

$$\int_\Omega |\nabla_h u_h(x) - F|^2 \, dx \le \int_\Omega |(R_\varepsilon(\nabla_h u_h(x) - F)|^2 \, dx$$

and (3.30) follows from (3.31) and the above inequality by integration by parts. This concludes the proof of the second part of the Theorem. □

The next Corollary relates the measure of the macroscopic ‘smallness” with the ‘roughness” of the underlying microscopic structure.

Corollary 3.8. *Let us assume that $u_h \in \mathcal{A}_h^{Fx}$ and let $\nabla_h u_h - \Pi \nabla_h u_h \to 0$ strongly in $L^1(\Omega, \mathbb{R}^{3\times 3})$. Then there exists $h_0 > 0$ such that for any $0 < h < h_0$ there exits a continuous function $w_h \in C(\Omega, \mathbb{R}^3)$ such that*

$$\nabla w_h = \Pi_{1,2} \nabla_h u_h, \qquad \text{in } \Omega.$$

Moreover there exists a positive constant C, independent of h and F_1, F_2 such that for any $0 < h < h_0$ we have

$$\frac{\operatorname{meas}(\Omega)\,|F_1 - F_2|^2}{\|\Delta\, w_h\|_{(C(\overline{\Omega},\mathbb{R}^3))^*}} \leq C\, \|u_h - Fx\|_{L^1(\Omega,\mathbb{R}^{3\times 3})}\,. \tag{3.32}$$

Proof. The strong convergence of $\nabla_h u_h - \Pi \nabla_h u_h \to 0$, the Hadamard jump condition (2.5), Theorem 3.1 and Corollary 3.2 yield, for sufficiently small h, a continuous piece-wise linear function w_h such that

$$\nabla w_h = \Pi_{1,2} \nabla_h u_h, \qquad \text{in } \Omega.$$

Moreover, the assumed strong convergence $\nabla_h u_h - \Pi \nabla_h u_h \to 0$ implies existence of an uniform bound of $\|w_h - Fx\|_{L^\infty(\Omega,\mathbb{R}^3)}$. Let p, q be conjugate, $p > n$ and h sufficiently small. Using the Corollary 3.6 and the compact imbedding of $(C(\overline{\Omega}))^*$ into $W^{-1,p}(\Omega)$ we have

$$\begin{aligned}
&\operatorname{meas}(\Omega)\,|F_1 - F_2|^2 \leq \int_\Omega |\nabla_h u_h(x) - F|^2\, dx = \int_\Omega |\nabla_h u_h(x) - \Pi_{1,2}\nabla_h u_h(x) + \nabla w_h(x) - F|^2\, dx \\
&\leq \tfrac{1}{2} \operatorname{meas}(\Omega)\,|F_1 - F_2|^2 + \langle w_h - Fx, \Delta\, w_h\rangle_{W_0^{-1,p}(\Omega,\mathbb{R}^3),W_0^{1,p}(\Omega,\mathbb{R}^3)} \\
&\leq \|w_h - Fx\|_{L^q(\Omega,\mathbb{R}^3)}\, \|\Delta\, w_h\|_{W_0^{-1,p}(\Omega,\mathbb{R}^3)} \leq \|w_h - Fx\|_{L^q(\Omega,\mathbb{R}^3)}\, \|\Delta\, w_h\|_{(C(\overline{\Omega},\mathbb{R}^3))^*}\,,
\end{aligned}$$

for any $q \geq \frac{p}{p-1}$. Since $p > n$ is arbitrary, and because there exists a positive constant C, independent of h such that

$$\|w_h - Fx\|_{L^q(\Omega,\mathbb{R}^3)} \leq C\, \|u_h - Fx\|_{L^q(\Omega,\mathbb{R}^3)}$$

the proof follows. $\square$

Remark. Since the functions u_h cannot be discontinuous on Q_h it is possible to show [L, 1996a], [L, 1996b] that

$$\|\Delta\, w_h\|_{(C(\overline{\Omega},\mathbb{R}^3))^*} = \mathcal{O}(h^{-1/2}). \tag{3.33}$$

Thus the combination of (3.32) and (3.33) yields a stronger result then that of the Corollary 3.7, namely,

$$\operatorname{meas}(\Omega)\,|F_1 - F_2|^2\, h^{1/2} \leq C\, \|u_h - Fx\|_{L^1(\Omega)}\,. \qquad \square \tag{3.34}$$

The combination of the Theorem 3.4 with the Corollary 3.7 (or 3.34) yields a stronger version of the inequality (3.13) and (3.25).

Theorem 3.9. *Let D be an arbitrary open subdomain of Ω with positive Lebesgue measure, let $u_h \in \mathcal{A}_h^{Fx}$, and let $\nabla_h u_h - \Pi \nabla_h u_h \to 0$ strongly in $L^1\left(\Omega, \mathbb{R}^{3\times 3}\right)$. Then there exists a positive constant C, independent of h, D, F and γ, such that*

$$C \left| \int_D \left(\nabla_h u_h(x) - F\right)\, dx \right| \leq \|\nabla_h u_h(x) - \Pi \nabla_h u_h\|^\gamma_{L^1(\Omega,\mathbb{R}^{3\times 3})}\,, \tag{3.35}$$

$$C \left|\operatorname{meas}(D^i_{r,h}) - \lambda_i \operatorname{meas}(D)\right| \leq \|\nabla_h u_h - \Pi \nabla_h u_h\|^\gamma_{L^1(\Omega,\mathbb{R}^{3\times 3})}\,, \tag{3.36}$$

for any $\gamma \in (0,1)$.

Proof. The proof follows from the inequalities (3.13) and (3.55), the strong convergence of $\nabla_h u_h - \Pi \nabla_h u_h \to 0$ in $L^1\left(\Omega, \mathbb{R}^{3\times 3}\right)$, and the inequality (3.27). $\square$

4. Compactness of the conforming approximations

The previous Corollaries 3.7 and 3.8 suggest that if the approximate measures $\mu_{x,r,\nabla_h u_h}$ converge to the corresponding probability distribution $\lambda_1\delta_{F_1}+\lambda_2\delta_{F_2}$, the macroscopically measurable quantity $u_h - Fx$ converge in the norm of an arbitrary space $L^p(\Omega,\mathbb{R}^3)$ not faster then $\mathcal{O}(\sqrt{h})$ even if the conforming approximations are used. This comes as no surprise since

$$\|\nabla u_h - F\|_{L^p_{\mathrm{Loc}}(\Omega,\mathbb{R}^3)} \le \tfrac{C}{h}\,\|u_h - Fx\|_{L^p_{\mathrm{Loc}}(\Omega,\mathbb{R}^3)} \tag{4.1}$$

This inequality yields a strong convergence in $W^{1,p}_{\mathrm{Loc}}(\Omega,\mathbb{R}^3)$ if $\|u_h - Fx\|_{L^p_{\mathrm{Loc}}(\Omega,\mathbb{R}^3)} = \mathcal{O}(h^{1+\gamma})$, for some $\gamma > 0$[1].

The strong convergence of the deformation gradients ∇u_h is equivalent to the precompactness of $\Delta\, u_h$ in the space $\left(C(\overline{\Omega},\mathbb{R}^3)\right)^*$ or in $W^{-1,2}(\Omega,\mathbb{R}^3)$. This follows from the argument of L.Tartar [KM] because for some $\phi \in C^1_0(\overline{\Omega},\mathbb{R}^1)$ we have

$$\begin{aligned} -\int_\Omega \phi(x)^2\,|\nabla(u(x)-u_h(x))|^2\,dx =& 2\int_\Omega \phi(x)\nabla\phi(x)(u(x)-u_h(x))\nabla(u(x)-u_h(x))\,dx \\ &+ \langle \phi(u-u_h), \phi\,\Delta(u-u_h)\rangle_{W^{-1,2}(\Omega,\mathbb{R}^3),W^{1,2}(\Omega,\mathbb{R}^3)} \to 0 \end{aligned}$$

if there exists a subsequence of $\Delta\, u_h$ such that $\Delta\, u_{h_k} \to \Delta\, u$ strongly in $\left(C(\overline{\Omega},\mathbb{R}^3)\right)^*$. The quantity $\|\Delta\, u_h\|_{\left(C(\overline{\Omega},\mathbb{R}^3)\right)^*}$ is easily measurable. If $\nabla_h u_h - \Pi\nabla_h u_h \to 0$ then $\|\Delta\, u_h\|_{\left(C(\overline{\Omega},\mathbb{R}^3)\right)^*}$ represents the number of the twin planes.

It is known that if $u_h \to u$ in $W^{1,2}(\Omega,\mathbb{R}^3)$ but $u \in W^{1,2}(\Omega,\mathbb{R}^3)$ (and not in, say, $W^{2,2}(\Omega,\mathbb{R}^3)$), the order of convergence of ∇u_h to ∇u can be arbitrarily slow. We can measure this defect in terms of $\|\Delta\, u_h\|_{\left(C(\overline{\Omega},\mathbb{R}^3)\right)^*}$. This is proven in the following Lemma.

We assume that the finite element space $\mathcal{A}_h$ is now constructed to be the conforming approximation with restect to the second-order problems. We indicate this choice by writing $\mathcal{A}_h^{Fx} \subset W^{1,2}(\Omega,\mathbb{R}^3)$.

Lemma 4.1. *Let $u_h \in \mathcal{A}_h^{Fx} \subset W^{1,2}(\Omega,\mathbb{R}^3)$ and let $\varepsilon(h)$ be a continuous function such that $0 \le \varepsilon(h) \to 0_+$, and let h be sufficiently small. Then there there exists a continuous function $\varepsilon_1 = \varepsilon_1(h)$ such that $0 \le \varepsilon_1(h) \to 0_+$ and*

$$\tfrac{1}{2}\,\|\nabla u - \nabla u_h\|_{L^2(\Omega,\mathbb{R}^3)} \le \tfrac{1}{\varepsilon(h)}\,\|u-u_h\|_{L^1(\Omega,\mathbb{R}^3)} + \varepsilon(h)\,\|\Delta\, u_h\|_{\left(C(\bar\Omega,\mathbb{R}^{3\times 3})\right)^*} + \varepsilon_1(h). \tag{4.2}$$

Proof. Let $R_{\varepsilon(h)}$ be the mollifier. We have

$$\begin{aligned} \|\nabla u - \nabla u_h\|_{L^2(\Omega,\mathbb{R}^{3\times3})} \le& \left\|\nabla u - R_{\varepsilon(h)}\nabla u\right\|_{L^2(\Omega,\mathbb{R}^{3\times3})} \\ &+ \left\|R_{\varepsilon(h)}(\nabla u - \nabla u_h)\right\|_{L^2(\Omega,\mathbb{R}^{3\times3})} + \left\|R_{\varepsilon(h)}\nabla u_h - \nabla u_h\right\|_{L^2(\Omega,\mathbb{R}^{3\times3})}. \end{aligned} \tag{4.3}$$

---

[1] This inequality is not true if we replace $L^p_{\mathrm{Loc}}(\Omega)$ with $L^p(\Omega)$ and/or ∇u_h converges to a non-constant function. For a counterexample we can use the following argument [Ar]. Let $u : [0,1] \to [-1,1]$ be a piecewise linear function which oscillates on an uniform mesh of the size h^2 and which alternately takes values $+1$ and -1. Then u_h, the $H^1(\Omega)$ projection of u onto P_1 finite element space on a mesh of size h, is zero. Hence,

$$\|\nabla u\|_{L^2(0,1)} < \frac{C}{h}\,\|u\|_{L^2(0,1)}\,.$$

But this is obviously false since $\|\nabla u\|_{L^2(0,1)} = \mathcal{O}(1/h^2)$ and $\|u\|_{L^2(0,1)} = 1$.

No we estimate each of the terms on the right-hand side of (4.3) separately. The $p-$mean continuity of L^p functions yields a positive continuous function $\varepsilon_1(h)$ and $\delta_1 = \delta_1(\varepsilon_1(h))$ such that

$$\left\|\nabla u - R_{\varepsilon(h)}\nabla u\right\|_{L^2(\Omega,\mathbb{R}^{3\times 3})} \le \frac{\varepsilon_1(h)}{2}, \qquad \text{if } \varepsilon(h) < \delta_1(\varepsilon_1). \tag{4.4}$$

Integrating by parts in the second term on the right-hand side of (4.3) we get

$$\left\|R_{\varepsilon(h)}(\nabla u - \nabla u_h)\right\|_{L^2(\Omega,\mathbb{R}^{3\times 3})} \le \tfrac{1}{\varepsilon(h)} \left\|\nabla\phi_0\right\|_{L^\infty(\Omega,\mathbb{R}^3)} \left\|u_h(x) - Fx\right\|_{L^1(\Omega,\mathbb{R}^3)}. \tag{4.5}$$

To estimate the last term, we proceed as follows. First, we can write

$$\left\|R_{\varepsilon(h)}\nabla u_h - \nabla u_h\right\|^2_{L^2(\Omega,\mathbb{R}^{3\times 3})} = \int_\Omega \left| \int_{|z|\le 1} \phi_0(z)\left(\nabla u_h(x) - \nabla u_h(x-\varepsilon(h)z)\right)\,dz\right|^2 dx. \tag{4.6}$$

Next, we can construct a sequence $u_h^{\varepsilon_2} \in W^{2,2}(\Omega,\mathbb{R}^3)$ such that

$$\begin{aligned} &\nabla u_h^{\varepsilon_2} \to \nabla u_h, && \text{a.e. in } \Omega, \\ &\Delta\, u_h^{\varepsilon_2} \to \Delta\, u, && \text{strongly in } \left(C(\overline{\Omega},\mathbb{R}^3)\right)^*, \quad \text{as } \varepsilon_2 \to 0. \end{aligned} \tag{4.7}$$

Thus,

$$\begin{aligned} &\left\|R_{\varepsilon(h)}\nabla u_h - \nabla u_h\right\|^2_{L^2(\Omega,\mathbb{R}^{3\times 3})} \\ &= \lim_{\varepsilon_2\to 0_+} \varepsilon(h) \int_\Omega \left| \int_{|z|\le 1}\int_0^1 \phi_0(z)\,\Delta\, u_h^{\varepsilon_2}(x - \tau\varepsilon(h)z)\,d\tau\,dz\right|^2 dx. \end{aligned} \tag{4.8}$$

The function

$$x \to \int_{|z|\le 1}\int_0^1 \phi_0(z)\,\Delta\, u_h^{\varepsilon_2}(x-\tau\varepsilon(h)z)\,d\tau\,dz$$

is continuous, therefore we have[2]

$$\begin{aligned} &\left\|R_{\varepsilon(h)}\nabla u_h - \nabla u_h\right\|_{L^2(\Omega,\mathbb{R}^{3\times 3})} \\ &= \varepsilon(h) \lim_{\varepsilon_2\to 0_+} \sup_{\substack{\phi\in C(\overline{\Omega},\mathbb{R}^3) \\ \|\phi\|_{C(\overline{\Omega},\mathbb{R}^3)}\le 1}} \left| \int_\Omega \phi(x) \int_{|z|\le 1}\int_0^1 \phi_0(z)\,\Delta\, u_h^{\varepsilon_2}(x-\tau\varepsilon(h)z)\,d\tau\,dz\,dx\right| = \\ &\varepsilon(h) \lim_{\varepsilon_2\to 0_+} \left\|R_{\varepsilon(h)}\,\Delta\, u_h^{\varepsilon_2}\right\|_{\left(C(\overline{\Omega},\mathbb{R}^3)\right)^*}. \end{aligned}$$

---

[2]This can be proven as follows: Let $u \in C(\Omega,\mathbb{R}^3)$ then

$$\begin{aligned} &\sup_{\substack{\phi\in C(\overline{\Omega},\mathbb{R}^3) \\ \|\phi\|_{C(\overline{\Omega},\mathbb{R}^3)}\le 1}} \left|\int_\Omega \phi(x)u(x)\,dx\right| \le \sup_{\substack{\phi\in L^2(\overline{\Omega},\mathbb{R}^3) \\ \|\phi\|_{L(\overline{\Omega},\mathbb{R}^3)}\le 1}} \left|\int_\Omega \phi(x)u(x)\,dx\right| \le \\ &\sup_{\substack{\phi\in C(\overline{\Omega},\mathbb{R}^3) \\ \|\phi\|_{C(\overline{\Omega},\mathbb{R}^3)}\le 1}} \left|\int_\Omega \phi(x)u(x)\,dx\right| + \|u\|_{C(\overline{\Omega},\mathbb{R}^3)} \lim_{\varepsilon\to 0} \sup_{\substack{\phi\in L^2(\overline{\Omega},\mathbb{R}^3) \\ \|\phi\|_{L(\overline{\Omega},\mathbb{R}^3)}\le 1}} \int_\Omega |\phi(x) - R_\varepsilon\phi(x)|\,dx = \\ &\sup_{\substack{\phi\in C(\overline{\Omega},\mathbb{R}^3) \\ \|\phi\|_{C(\overline{\Omega},\mathbb{R}^3)}\le 1}} \left|\int_\Omega \phi(x)u(x)\,dx\right| + \|u\|_{C(\overline{\Omega},\mathbb{R}^3)} \lim_{\varepsilon\to 0} \int_\Omega \left|\hat\phi(x) - R_\varepsilon\hat\phi(x)\right|\,dx = \sup_{\substack{\phi\in C(\overline{\Omega},\mathbb{R}^3) \\ \|\phi\|_{C(\overline{\Omega},\mathbb{R}^3)}\le 1}} \left|\int_\Omega \phi(x)u(x)\,dx\right|, \end{aligned}$$

where $\hat\phi$ is some continuous function at which $\int_\Omega |\phi(x) - R_\varepsilon\phi(x)|\,dx$ attain its maximum over the set $\|\phi\|_{C(\overline{\Omega},\mathbb{R}^3)} \le 1$.

The mean continuity of $\Delta u_h^{\varepsilon_2} \in L^2(\Omega, \mathbb{R}^3)$ yields existence of $\delta_2(\varepsilon_1(h)) > 0$ such that

$$\left\| R_{\varepsilon(h)} \Delta u_h^{\varepsilon_2} - \Delta u_h^{\varepsilon_2} \right\|_{\left(C(\overline{\Omega}, \mathbb{R}^3)\right)^*} \leq \frac{\varepsilon_1(h)}{2\varepsilon(h)}, \qquad \text{if } \varepsilon(h) < \delta_2(\varepsilon_1(h)).$$

Hence,

$$\begin{aligned} &\left\| R_{\varepsilon(h)} \Delta u_h^{\varepsilon_2} \right\|_{\left(C(\overline{\Omega}, \mathbb{R}^3)\right)^*} \\ &\leq \left\| R_{\varepsilon(h)} \Delta u_h^{\varepsilon_2} - \Delta u_h^{\varepsilon_2} \right\|_{\left(C(\overline{\Omega}, \mathbb{R}^3)\right)^*} + \left\| \Delta u_h^{\varepsilon_2} - \Delta u_h \right\|_{\left(C(\overline{\Omega}, \mathbb{R}^3)\right)^*} + \left\| \Delta u_h \right\|_{C\left((\overline{\Omega}, \mathbb{R}^3)\right)^*} \\ &\leq \frac{\varepsilon_1(h)}{2\varepsilon(h)} + \left\| \Delta u_h^{\varepsilon_2} - \Delta u_h \right\|_{\left(C(\overline{\Omega}, \mathbb{R}^3)\right)^*} + \left\| \Delta u_h \right\|_{\left(C(\overline{\Omega}, \mathbb{R}^3)\right)^*}. \end{aligned} \tag{4.9}$$

The term $\| \Delta u_h^{\varepsilon_2} - \Delta u_h \|_{C(\overline{\Omega}, \mathbb{R}^3)^*}$ converges to zero as $\varepsilon_2 \to 0$ due to the construction (4.7). This finally gives

$$\left\| R_{\varepsilon(h)} \nabla u_h - \nabla u_h \right\|_{L^2(\Omega, \mathbb{R}^{3\times 3})} \leq \frac{\varepsilon_1(h)}{2} + \varepsilon(h) \left\| \Delta u_h \right\|_{\left(C(\overline{\Omega}, \mathbb{R}^3)\right)^*}. \tag{4.10}$$

The proof follows from (4.4) and (4.5), (4.10) by taking h sufficiently small so that $\varepsilon(h) \leq \min\{\delta_1, \delta_2\}$. $\square$

The above Lemma 4.1 yields the sufficient conditions for the strong convergence of the deformation gradients.

Theorem 4.2. *Let $u_h \in \mathcal{A}_h^{Fx} \subset W^{1,2}(\Omega)$ and let us assume that*

$$\begin{aligned} &u_h \rightharpoonup u, \qquad \textit{weakly in } W^{1,2}(\Omega, \mathbb{R}^3), \qquad \textit{and} \\ &\|u - u_h\|_{L^1(\Omega, \mathbb{R}^3)} < \left(\left\| \Delta u_h \right\|_{\left(C(\bar{\Omega}, \mathbb{R}^{3\times 3})\right)^*} \right)^{-1}. \end{aligned}$$

Then

$$u_h \to u, \qquad \textit{strongly in } W^{1,2}(\Omega, \mathbb{R}^3).$$

Proof. The proof follows directly from the Lemma 4.1 since the sufficient conditions for the right-hand side of (4.2) to converge to zero are

$$\begin{aligned} &\|u - u_h\|_{L^1(\Omega, \mathbb{R}^3)} < \varepsilon(h), \\ &\varepsilon(h) < \left(\left\| \Delta u_h \right\|_{\left(C(\bar{\Omega}, \mathbb{R}^{3\times 3})\right)^*} \right)^{-1}. \end{aligned}$$

The proof is finished. $\square$

The next Theorem summarizes the results of the Corollary 3.8 and Theorem 4.2 as follows.

Theorem 4.3 (The Discrete Uncertainty Principle). *Let $u_h \in \mathcal{A}_h^{Fx} \subset W^{1,2}(\Omega)$, $u_h \rightharpoonup Fx$ weakly in $W^{1,2}(\Omega, \mathbb{R}^3)$, and let the Young measure $(\mu_x)_{x \in \Omega}$ corresponding to F be such that* $\operatorname{supp} \mu_x \subset \mathcal{K}_2$. *Then*

$$\lim_{r \to 0_+} \lim_{h \to 0_+} \mu_{x, r, \nabla_h u_h} \overset{*}{\rightharpoonup} \lambda_1 \delta_{F_1} + \lambda_2 \delta_{F_2} \qquad \textit{weakly-}{*} \textit{ in a sense of measure} \tag{4.11}$$

if and only if

$$\|u_h - Fx\|_{L^1(\Omega)} \, \|\Delta\, u_h\|_{\left(C(\bar\Omega,\mathbb{R}^{3\times 3})\right)^*} \geq 1. \tag{4.12}$$

Proof. Instead of showing that (4.11) implies (4.12) we show an equivalent implication which is that if (4.12) is not true then (4.11) is not true as well. Hence, if (4.12) is not true then the Theorem 4.2 implies

$$\nabla u_h \to F, \qquad \text{a.e. in } \Omega.$$

Thus we have for any $x \in \Omega$

$$\begin{aligned}&\lim_{h\to 0_+} |\nabla u_h(x) - \Pi\nabla u_h(x)| = \lim_{h\to 0_+} |\nabla u_h(x) - F + F - \Pi\nabla u_h(x)| = \\ &\lim_{h\to 0_+} |F - \Pi\nabla u_h(x)| > 0.\end{aligned} \tag{4.13}$$

On the other hand if D is an arbitrary open subset of Ω we have the estimate

$$\begin{aligned}&\int_D |\Pi\nabla u_h(x) - \nabla u_h(x)|\, dx = \int_{D^1_{r,h}} |\Pi\nabla u_h(x) - \nabla u_h(x)|\, dx + \\ &\int_{D^2_{r,h}} |\Pi\nabla u_h(x) - \nabla u_h(x)|\, dx + \int_{D\setminus\left(D^1_{r,h}\cup D^2_{r,h}\right)} |\Pi\nabla u_h(x) - \nabla u_h(x)|\, dx \leq \\ &r\left(\text{meas}(D^1_{r,h}) + \text{meas}(D^2_{r,h})\right) + C\,\text{meas}(D\setminus(D^1_{r,h}\cup D^2_{r,h}).\end{aligned} \tag{4.14}$$

If (4.11) holds then

$$\lim_{h\to 0}\lim_{r\to 0}\left(r\left(\text{meas}(D^1_{r,h}) + \text{meas}(D^2_{r,h})\right) + \text{meas}(D\setminus(D^1_{r,h}\cup D^2_{r,h})\right) = 0. \tag{4.14}$$

thus Theorem 3.5, (4.14) and (4.15) show that

$$\begin{aligned}&\lim_{r\to 0_+}\lim_{h\to 0_+} \mu_{x,r,\nabla_h u_h} \overset{*}{\rightharpoonup} \lambda_1\delta_{F_1} + \lambda_2\delta_{F_2} \qquad \text{weakly-}*\text{ in a sense of measure} \\ &\text{if and only if} \\ &|\nabla u_h - \Pi\nabla u_h| \to 0, \qquad \text{a.e. in } \Omega.\end{aligned} \tag{4.16}$$

Therefore if (4.12) is not true, (4.16) implies that (4.11) is not true either. The remaining implication can be proven as follows.

Let (4.12) be true. The Sobolev imbeddings theorem implies that the weak convergence $\nabla u_h \to F$ in $W^{1,2}(\Omega,\mathbb{R}^{3\times 3})$ yields a strong convergence $u_h - Fx \to 0$ in $L^2(\Omega,\mathbb{R}^3)$. Hence, we have from (4.12) that

$$\lim_{h\to 0_+} \|\Delta\, u_h\|_{\left(C(\bar\Omega,\mathbb{R}^{3\times 3})\right)^*} = \infty. \tag{4.17}$$

If $\nabla u_h \to F$ a.e. in Ω then $\|\Delta\, u_h\|_{\left(C(\bar\Omega,\mathbb{R}^{3\times 3})\right)^*}$ must be uniformly bounded. Thus (4.17) implies that

$$|\nabla u_h - F| > 0, \qquad \text{a.e. in } \Omega. \tag{4.18}$$

The basic theorem of the Young measures [B] then yields the representation

$$Fx = \int_{\mathbb{R}^3} Fy\, d\mu_x(y), \qquad \text{a.e. in } \Omega.$$

The inequality (4.18) implies that μ_x has to be a non-trivial measure, i.e. μ_x cannot be a unit point mass. Then, the application of the Theorem 7.1 [BJ, 1991] for the orthorombic to monoclinic transformations and the Theorem 7.3 [BJ, 1991] for the cubic to tetragonal transformations yields

$$\mu_x = \lambda_1 \delta_{F_1} + \lambda_2 \delta_{F_2}$$

and the proof is finished. □

Remark. In the case of the double-well problem [L, 1996a] we have

$$\left(\|\Delta u_h\|_{\left(C(\bar{\Omega},\mathbb{R}^{3\times 3})\right)^*} \right)^{-1} = \mathcal{O}(\sqrt{h})$$

thus, if $u_h \rightharpoonup u$ weakly in $W^{1,2}(\Omega,\mathbb{R}^3)$, the critical order of approximation is

$$\|u_h - u\|_{L^2(\Omega)} \geq C\sqrt{h}$$

to maintain the weak convergence in this space. □

5. Relaxation of the free-energy

We have shown that the convergence theory can be developed by controling the term

$$|\nabla_h u_h - \Pi(\nabla_h u_h)|\,.$$

One of the possibilities of how to control this term is by minimization of the total energy. This is proven in the following Lemma under the constitutive assumptions (2.9)-(2.12).

Lemma 5.1. *Let $u_h \in \mathcal{A}_h^{Fx}$ be such that $\mathcal{E}(u_h)$ can be made sufficiently small and let the energy density W be a real-analytic function of its argument which is convex on the immediate neighbourhood of its equilibrium states so that (2.11) is true. Then there exists a $\gamma \geq 1$ and a positive constant C, independent of h and γ, such that*

$$\mathcal{E}(u_h) \geq C \left(\int_\Omega |\nabla_h u_h(x) - \Pi(\nabla_h u_h(x))|\; dx \right)^\gamma . \tag{5.1}$$

Proof. Since $W^{3,\infty}(\Omega,\mathbb{R}^3)$ is dense in $\mathcal{A}_h$, it is sufficient to prove (5.1) in this space. Hence, let $u \in W^{3,\infty}(\Omega,\mathbb{R}^3)$.

Applying the estimate of L. Simon [S, Theorem 3] we get a $\gamma_1 \geq 2$ such that

$$\left(\inf_{A\in\mathcal{K}} \|u - Ax\|_{L^2(\Omega,\mathbb{R}^3)} \right)^{\gamma_1} \leq \sup_{\phi\in L^2(\Omega,\mathbb{R}^3)} \left| \int_\Omega \operatorname{div} DW(\nabla u(x))\phi_\varepsilon(x)\, dx \right| .$$

Let the map R_ε be the mollifier and let $\phi_\varepsilon = R_\varepsilon \phi$. Then it follows from the mean-continuity of the L^2 functions that for any $\delta = \delta(\varepsilon)$ there exists an $\varepsilon > 0$ such that

$$\left| \int_\Omega \operatorname{div} DW(\nabla u(x))\phi(x)\, dx \right| \leq \delta(\varepsilon) + \left| \int_\Omega DW(\nabla u(x))\nabla\phi(x)\, dx \right| .$$

Because the energy density is real-analytic function of its argument, it follows from the Taylor's expansion that there exists a constant C, independent of u, and $\chi \in W^{3,\infty}(\Omega, \mathbb{R}^{3\times 3})$, such that

$$W(\nabla u+\nabla\phi_\varepsilon) = W(\nabla u)+DW(\nabla u)\nabla\phi_\varepsilon+D^2W(\chi)(\nabla\phi_\varepsilon,\nabla\phi_\varepsilon) \leq (1+C)W(\nabla u)+DW(\nabla u)\nabla\phi_\varepsilon.$$

Thus, using (2.9), we can recover a constant C, independent of u, such that

$$\begin{aligned}\left|\int_\Omega \operatorname{div} DW(\nabla u(x))\phi_\varepsilon(x)\,dx\right| &\leq \left|\int_\Omega W(\nabla u(x)+\nabla\phi_\varepsilon(x))\,dx-(1+C)\int_\Omega W(\nabla u(x))\,dx\right| \\ &\leq C\left|\int_\Omega W(\nabla u(x))\,dx\right|.\end{aligned}$$

Taking ε small enough so that there exists a $0<\varepsilon_1<1$ such that

$$\delta(\varepsilon) \leq (1-\varepsilon_1)\left(\inf_{A\in\mathcal{K}}\|u-Ax\|_{L^2(\Omega,\mathbb{R}^3)}\right)^{\gamma_1}$$

we get a $\gamma \geq 1$ such that

$$\left(\|u-Ax\|_{L^1(\Omega,\mathbb{R}^3)}\right)^\gamma \leq \frac{C}{\varepsilon_1}\left|\int_\Omega W(\nabla u(x))\,dx\right|.$$

In virtue of the definition of the projection Π, given at the second paragraph, we have

$$\inf_{A\in\mathcal{K}}\|u-Ax\|_{L^1(\Omega,\mathbb{R}^3)} = \|\nabla u-\Pi\nabla u\|_{L^1(\Omega,\mathbb{R}^{3\times 3})}.$$

The proof now follows from the density argument. □

Corollary 5.2. *Let the assumptions of the Lemma 5.2 be satisfied. Then there exists a positive constant C, independent of h, F and p, such that*

$$\mathcal{E}(u_h) \geq C\int_\Omega |u_h(x)-Fx|\,dx. \tag{5.3}$$

Proof. We have from the Lemma 5.1, Theorem 3.1 and the inequality (3.12) that there exists a constant C, independent of h and F, such that for any $m\in n^\perp$

$$\begin{aligned}&\mathcal{E}(u_h) \geq \\ &C\int_\Omega |\nabla_h u_h(x)-\Pi(\nabla_h u_h(x))|\,dx \geq C\int_\Omega |(\nabla_h u_h(x)-F)\,m|\,dx \geq C\int_\Omega |u_h(x)-Fx|\,dx.\end{aligned}$$

Thus the proof is finished. □

Now, we can combine the results of the Paragraph 3 with the Lemma 5.1 and Corollary 5.2 to obtain a summary of the results with respect to the relaxation of the free-energy.

Theorem 5.3. *Let $u_h \in \mathcal{A}_h^{Fx}$ be such that $\mathcal{E}(u_h)\to 0$ and let us assume that the energy density W is a real analytic function of its argument which is subject to the assumptions (2.9)-(2.12). Let*

D be an arbitrary open subset of Ω with a positive Lebesgue measure and Lipschitz boundary, and let $D^i_{r,h}$ be defined by (3.23). We have the following estimates

$$\int_\Omega |(\nabla_h u_h(x) - F)m| \; dx \leq C\,\mathcal{E}(u_h), \tag{5.4}$$

$$\int_\Omega |\nabla_h u_h(x) - \Pi_{1,2}(\nabla_h u_h(x))| \; dx \leq C\,\mathcal{E}(u_h), \tag{5.5}$$

$$\left|\int_D (\nabla_h u_h(x) - F) \; dx\right| \leq C\,\mathcal{E}(u_h)^\gamma, \qquad \textit{for any } \gamma \in (0,1), \tag{5.6}$$

$$\left|\frac{\text{meas}(D^i_{r,h})}{\text{meas}(D)} - \lambda_i\right| \leq C\,\mathcal{E}(u_h)^\gamma, \qquad \textit{for any } \gamma \in (0,1), \tag{5.7}$$

$$\frac{\text{meas}(\Omega)\,|F_1 - F_2|}{\|\Delta\, w_h\|_{(C(\overline{\Omega}))^*}} \leq C\,\mathcal{E}(u_h), \tag{5.8}$$

$$\int_\Omega |u_h(x) - Fx| \; dx \leq \mathcal{E}(u_h), \tag{5.9}$$

where the positive constant C is independent of h, γ, F, m, and D and the function $w_h \in C(\Omega, \mathbb{R}^3)$ is such that $\nabla w_h = \Pi_{1,2}\nabla_h u_h$ in Ω.

Proof. The proof of the inequalities follows directly from (5.1) and the inequalities (3.1), (3.6), (3.35), (3.36), (3.32) and (5.3) respectively. $\square$

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