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Heterogeneous wires made of martensitic materials

Hervé Le Dret, Nicolas Meunier

Laboratoire Jacques-Louis Lions, Université Pierre et Marie Curie, 175, rue du Chevaleret, Paris 75013, France

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Abstract

In this paper we present a direct derivation of a theory of heterogeneous wires starting from three-dimensional nonlinear hyperelasticity augmented by an interfacial energy term. The derivation involves no a priori choice of asymptotic expansion or ansatz. It yields a wire theory with two Cosserat vector fields. The theory is applied to multiwell energy functions appropriate for martensitic materials. A formal derivation of higher theories of homogeneous wires is given, which yields three additional Cosserat vector fields and an explicit form for the bending and torsion energy. *To cite this article: H. Le Dret, N. Meunier, C. R. Acad. Sci. Paris, Ser. I* 337 (2003).

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Résumé

Fils hétérogènes composés de matériaux martensitiques. On présente une méthode directe permettant d'obtenir une théorie de fils hétérogènes en partant de la théorie élastique non linéaire tridimensionnelle augmentée d'un terme d'énergie d'interface. Cette méthode ne fait intervenir ni développement asymptotique formel ni ansatz. Elle donne une théorie de fils comportant deux vecteurs de Cosserat. Cette théorie est appliquée à des fonctions d'énergie comportant plusieurs puits qui sont adaptées aux matériaux martensitiques. On fournit une méthode formelle permettant d'obtenir des théories d'ordre supérieur pour des fils homogènes, comportant trois vecteurs de Cosserat supplémentaires et une forme explicite de l'énergie de flexion et de torsion. *Pour citer cet article : H. Le Dret, N. Meunier, C. R. Acad. Sci. Paris, Ser. I 337 (2003).*

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Version française abrégée

Pour tout $\varepsilon > 0$, soit $\Omega_{\varepsilon} = \{x \in \mathbb{R}^3; (x_1, x_2) \in \omega_{\varepsilon}, x_3 \in]0, L[\}$, où $\omega_{\varepsilon} = \varepsilon \omega$, ω est un ouvert borné lipschitzien de \mathbb{R}^2 tel que $\int_{\omega} x_{\alpha} dx_1 dx_2 = \int_{\omega} x_1 x_2 dx_1 dx_2 = 0, L > 0$. Soit $W : M_3 \times \omega \times \mathbb{R} \to \mathbb{R}^+$, $(F, x_1, x_2, x_3) \to W(F, x_1, x_2, x_3)$ une fonction de Carathéodory, périodique par rapport à x_3 de période 1 satisfaisant pour presque tout $x \in \omega \times \mathbb{R}$, des hypothèses de croissance et de coercivité ainsi qu'une condition de Lipschitz. On suppose que Ω_{ε} est la configuration de référence d'un solide tridimensionnel hétérogène martensitique. Cette caractéristique mécanique est modélisée par une énergie somme d'une énergie hyperélastique dont la densité est $W(F, \frac{x_1}{\varepsilon}, \frac{x_2}{\varepsilon}, \frac{x_3}{d(\varepsilon)})$, où $d(\varepsilon)$ est un paramètre décrivant l'ordre de la taille d'un grain, et d'un terme d'énergie

E-mail addresses: ledret@ccr.jussieu.fr (H. Le Dret), meunier@ccr.jussieu.fr (N. Meunier).

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d'interface en les dérivées secondes qui pénalise les changements de phase. Comme on souhaite modéliser des matériaux martensitiques, W(F, ..., .) comporte plusieurs puits correspondant aux différentes phases. Le problème de déterminer une configuration d'équilibre peut se formuler en un problème de minimisation : Minimiser $I_{\varepsilon}(\phi_{\varepsilon})$ sur Φ_{ε} , où l'énergie totale I_{ε} est donnée par

$$I_{\varepsilon}(\phi_{\varepsilon}) = \int_{\Omega_{\varepsilon}} \left\{ \kappa^2 \| \nabla^2 \phi_{\varepsilon} \|^2 + W \left(\nabla \phi_{\varepsilon}, \frac{x_1}{\varepsilon}, \frac{x_2}{\varepsilon}, \frac{x_3}{d(\varepsilon)} \right) \right\} \mathrm{d}x, \tag{1}$$

et l'ensemble des déformations admissibles est $\Phi_{\varepsilon} = \{\phi_{\varepsilon} \in H^2(\Omega_{\varepsilon}; \mathbb{R}^3); \phi_{\varepsilon}(x) = Ax \operatorname{sur} \gamma_{\varepsilon}\}$, avec $\kappa > 0$, $A = (a_1|a_2|a_3) \in M_3$ donnée et $\gamma_{\varepsilon} = \partial \Omega_{\varepsilon} \cap \{x_3 \in \{0, L\}\}$. On cherche à décrire le comportement du fil quand $\varepsilon \to 0$ et $d(\varepsilon) \to 0$. On effectue pour cela le changement d'échelle usuel, inspiré de celui introduit par Ciarlet et Destuynder [4] : posant $\Omega = \Omega_1$ et $\gamma = \gamma_1$, on définit les déformations mises à l'échelle $\phi(\varepsilon)(x_1, x_2, x_3) = \phi_{\varepsilon}(\varepsilon x_1, \varepsilon x_2, x_3)$, les énergies mises à l'échelle

$$I(\varepsilon)(\phi(\varepsilon)) = \int_{\Omega} \left\{ \kappa^2 \left[\frac{1}{\varepsilon^4} \left(\sum_{\alpha,\beta} \left| \partial_{\alpha\beta} \phi(\varepsilon) \right|^2 \right) + \frac{2}{\varepsilon^2} \left(\sum_{\alpha} \left| \partial_{\alpha3} \phi(\varepsilon) \right|^2 \right) + \left| \partial_{33} \phi(\varepsilon) \right|^2 \right] + W\left(\left(\frac{1}{\varepsilon} \partial_1 \phi(\varepsilon) \left| \frac{1}{\varepsilon} \partial_2 \phi(\varepsilon) \right| \partial_3 \phi(\varepsilon) \right), x_1, x_2, \frac{x_3}{d(\varepsilon)} \right) \right\} dx,$$
(2)

et l'ensemble des déformations admissibles devient $\Phi(\varepsilon) = \{\phi \in H^2(\Omega; \mathbb{R}^3); \phi(x) = (\varepsilon a_1 | \varepsilon a_2 | a_3) x \text{ sur } \gamma\}.$

La présence du terme d'énergie d'interface, en garantissant des conditions de coercivité sur les dérivées secondes des déformations, permet d'éviter l'usage explicite de la Γ -convergence et de procéder directement. Il devient ainsi possible de donner des résultats de convergence variationnelle. Nous nous inspirons pour cela des travaux de Batthacharya et James [3] dans le cas des films homogènes. Nous fournissons tout d'abord un modèle de fil monodimensionnel exprimé à l'aide de la déformation de la ligne centrale et de deux vecteurs directeurs de Cosserat. Dans un deuxième temps, nous négligeons le terme d'énergie d'interface en supposant que $\kappa = 0$ et nous construisons des déformations minimisant l'énergie simplifiée qui créent une ou plusieurs variantes et une ou deux phases pour un fil homogène. Enfin toujours dans le cas homogène et en faisant des hypothèses formelles, nous donnons des théories monodimensionnelles d'ordre supérieur.

1. Preliminaries

The summation convention is assumed. Greek indices take their values in the set {1, 2} and Latin indices in the set {1, 2, 3}. For all $\varepsilon > 0$, let $\Omega_{\varepsilon} = \{x \in \mathbb{R}^3; (x_1, x_2) \in \omega_{\varepsilon}, x_3 \in]0, L[\}$, where $\omega_{\varepsilon} = \varepsilon \omega, \omega$ is a bounded open Lipschitz subset of \mathbb{R}^2 such that $\int_{\omega} x_{\alpha} dx_1 dx_2 = \int_{\omega} x_1 x_2 dx_1 dx_2 = 0$ and meas $\omega = 1$, and L > 0. Let M_3 be the space of real 3×3 matrices endowed with the usual Euclidean norm $||F|| = \sqrt{\operatorname{tr}(F^T F)}$. For all $z_i \in \mathbb{R}^3$, we denote by $(z_1|z_2|z_3)$ the matrix whose *i*-th column is z_i . Let $W: M_3 \times \omega \times \mathbb{R} \to \mathbb{R}^+$, $(F, x_1, x_2, x_3) \to W(F, x_1, x_2, x_3)$ be a Carathéodory function, periodic in x_3 with period 1. We assume that W satisfies for almost all $x \in \omega \times \mathbb{R}$ the following growth and coercivity hypotheses:

$$\exists C_1 > 0, \ \exists \alpha > 0, \ \exists \beta \ge 0, \ \exists p \text{ with } 2 \le p < 6, \ \forall F \in M_3, \ \alpha \|F\|^2 - \beta \le \left|W(F, x)\right| \le C_1 \left(1 + \|F\|^p\right),$$
(3)

and the Lipschitz condition

$$\exists C_2 > 0, \ \forall F, G \in M_3, \quad \left| W(F, x) - W(G, x) \right| \leq C_2 \left(1 + \|F\|^{p-1} + \|G\|^{p-1} \right) \|F - G\|.$$
(4)

We assume that Ω_{ε} is the reference configuration of a (sequence of) heterogeneous three-dimensional solid body made of a martensitic material. The martensitic character is modelled by assuming an energy functional in two parts. The first part is an interface energy term expressed in terms of the second derivatives of the deformation. The

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second part is a hyperelastic energy whose stored energy function is of the form $W(F, \frac{x_1}{\varepsilon}, \frac{x_2}{\varepsilon}, \frac{x_3}{d(\varepsilon)})$, where $d(\varepsilon)$ scales like the typical grain size. The dependence in x_{α} , x_3 accounts for material heterogeneity. Furthermore, in the context of martensites, W(F, ..., .) may be assumed to possess a multiwell structure. The equilibrium problem may be formulated as a minimization problem: Minimize $I_{\varepsilon}(\phi_{\varepsilon})$ over ϕ_{ε} , where the total energy I_{ε} is given by

$$I_{\varepsilon}(\phi_{\varepsilon}) = \int_{\Omega_{\varepsilon}} \left\{ \kappa^2 \| \nabla^2 \phi_{\varepsilon} \|^2 + W \left(\nabla \phi_{\varepsilon}, \frac{x_1}{\varepsilon}, \frac{x_2}{\varepsilon}, \frac{x_3}{d(\varepsilon)} \right) \right\} \mathrm{d}x,$$
(5)

and the set of admissible deformations is $\Phi_{\varepsilon} = \{\phi_{\varepsilon} \in H^2(\Omega_{\varepsilon}; \mathbb{R}^3); \phi_{\varepsilon}(x) = Ax \text{ on } \gamma_{\varepsilon} \text{ in the sense of traces}\}$, where $\kappa > 0$, $A = (a_1|a_2|a_3) \in M_3$ is a given matrix and $\gamma_{\varepsilon} = \partial \Omega_{\varepsilon} \cap \{x_3 \in \{0, L\}\}$. We are interested in describing the limit string-like behavior of the body when the thickness ε and grain size $d(\varepsilon)$ go to 0. To achieve this goal, we rescale the problem after the fashion introduced by Ciarlet and Destuynder [4]. Let $\Omega = \Omega_1$, $\gamma = \gamma_1$. We define the rescaled deformations $\phi(\varepsilon)(x_1, x_2, x_3) = \phi(\varepsilon x_1, \varepsilon x_2, x_3)$, the rescaled energies

$$I(\varepsilon)(\phi(\varepsilon)) = \int_{\Omega} \left\{ \kappa^2 \left[\frac{1}{\varepsilon^4} \left(\sum_{\alpha,\beta} \left| \partial_{\alpha\beta} \phi(\varepsilon) \right|^2 \right) + \frac{2}{\varepsilon^2} \left(\sum_{\alpha} \left| \partial_{\alpha3} \phi(\varepsilon) \right|^2 \right) + \left| \partial_{33} \phi(\varepsilon) \right|^2 \right] + W \left(\left(\frac{1}{\varepsilon} \partial_1 \phi(\varepsilon) \left| \frac{1}{\varepsilon} \partial_2 \phi(\varepsilon) \right| \partial_3 \phi(\varepsilon) \right), x_1, x_2, \frac{x_3}{d(\varepsilon)} \right) \right\} dx,$$
(6)

and the set of admissible deformations becomes $\Phi(\varepsilon) = \{\phi \in H^2(\Omega; \mathbb{R}^3); \phi(x) = (\varepsilon a_1 | \varepsilon a_2 | a_3) x \text{ on } \gamma\}.$

2. Derivation of the martensitic wire energy

First of all, due to the convexity and coercivity of the interfacial energy, it is a simple matter to prove the following existence result.

Proposition 2.1. For all $\varepsilon > 0$, there exists a minimizer $\phi(\varepsilon) \in \Phi(\varepsilon)$ of $I(\varepsilon)$.

We then let the thickness of the wire ε tend to 0, as well as the grain size $d(\varepsilon) \to 0$. The following is the main result of this section. It describes the limit behavior of the wire to leading order.

Theorem 2.1. There exists a subsequence (not relabeled) of the family of minimizers $\phi(\varepsilon)$ such that

$$\partial_{33}\phi(\varepsilon) \to \partial_{33}\phi_0, \quad \frac{1}{\varepsilon}\partial_{\alpha3}\phi(\varepsilon) \to \partial_3 b_0^{\alpha}, \quad \frac{1}{\varepsilon^2}\partial_{\alpha\beta}\phi(\varepsilon) \to 0 \quad strongly \text{ in } L^2(\Omega; \mathbb{R}^3),$$
(7)

where $(\phi_0, b_0^{\alpha}) \in \Phi_0 = \{(\phi, b^{\alpha}) \in H^2(0, L; \mathbb{R}^3) \times H^1(0, L; \mathbb{R}^3)^2; \phi(x_3) = a_3 x_3, b^{\alpha}(x_3) = a_{\alpha} \text{ on } \{0, L\}\}$ minimizes the limiting energy

$$I^{0}(\phi, b^{\alpha}) = \int_{0}^{L} \left\{ \kappa^{2} \left(|\partial_{33}\phi|^{2} + 2\sum_{\alpha} |\partial_{3}b^{\alpha}|^{2} \right) + \widetilde{W}(b^{1}|b^{2}|\partial_{3}\phi) \right\} \mathrm{d}x_{3},$$
(8)

where $\widetilde{W}(F) = \int_{\omega \times (0,1)} W(F,x) \, \mathrm{d}x$. Furthermore, $I(\varepsilon)(\phi(\varepsilon)) \to I^0(\phi_0, b_0^{\alpha})$.

The proof of Theorem 2.1 follows along the lines of [3] and [7]. It should be noted that the presence of the interfacial energy simplifies convergence questions compared with purely elastic wire or membrane energy derivation, see [1,6], by imposing coercivity conditions on the second derivatives of the deformations. It also makes it possible to easily manage the heterogeneity with respect to all variables, viz. [5].

Theorem 2.1 gives a limiting theory with three vector unknowns. The mapping ϕ_0 describes the limit deformation of the wire (i.e., of its central line). The two Cosserat vectors b_0^{α} describe the limit deformation of the cross-section of the wire. The terms involving $\partial_3 b_0^{\alpha}$ are not bending terms but appear as a contribution of the interfacial energy.

3. Energy minimizing deformations in the case of zero interfacial energy

Consider now a homogeneous martensitic wire occupying at rest the reference domain [0, L]. According to Theorem 2.1, the wire behavior is governed by the energy I^0 . However, if the wire is long enough, it can be assumed that the elastic energy is much larger than the interfacial energy. Therefore, we can formally set $\kappa = 0$ and study the resulting energy for the wire $I_*^0(\phi, b^{\alpha}) = \int_0^L W(b^1|b^2|\partial_3\phi) dx_3$. Deformations that minimize this energy are such that $(b^1, b^2, \partial_3\phi) \in SO(3)U_i$ almost everywhere, where U_i denote the positive-definite, symmetric distorsion matrices of the phases or variants, due to the multiwell structure of W. In the ensuing analysis, we ignore boundary conditions.

Let us first describe deformations that only involve one single phase U. Let U^j denote the column vectors of U. Consider any measurable SO(3)-valued mapping Q on]0, L[. Then any primitive ϕ of $Q(x_3)U^3$ defines a minimizing deformed central line. Accordingly, the minimizing Cosserat vectors are given by $b^{\alpha}(x_3) = Q(x)U^{\alpha}$. To get a better understanding of the situation, consider the case U = Id of an austenite phase. Then ϕ is any $W^{1,\infty}$ curve parametrized by arc length of total length L. The vectors b^{α} are orthogonal to the curve, but free to rotate in the normal plane. A similar picture holds for more general distortion matrices U.

We then consider deformations that consist of two phases,

$$(b^{1}|b^{2}|\partial_{3}\phi) = Q_{1}U$$
 on $]0, l[, $(b^{1}|b^{2}|\partial_{3}\phi) = Q_{2}V$ on $]l, L[.$ (9)$

For simplicity, assume that Q_1 and Q_2 are smooth on each part of the wire. The mapping ϕ must be continuous, but b^{α} and $\partial_3 \phi$ may suffer jumps across l. In fact, the deformations satisfy (9) if and only if $[\partial_3 \phi] = Q_2(l)V^3 - Q_1(l)U^3$ and $[b^{\alpha}] = Q_2(l)V^{\alpha} - Q_1(l)U^{\alpha}$, where [g] denote the jump of g across l. Since $Q_1(l)$ and $Q_2(l)$ are arbitrary rotation matrices, these compatibility conditions are very mild.

In particular, the wire case is very different from the film and bulk specimen cases for which there are much more stringent compatibility conditions (see Bhattacharya and James [3] for films and Ball and James [2] for bulk specimen).

It is of course possible to imagine more complicated phase mixtures in the wire.

4. Higher order theories

We now consider a homogeneous wire that is thicker than the wires considered in Section 2, which are governed by the energy I^0 . In this case, we expect higher order terms to become significant. We show that the first correction to I^0 is of order higher than one in the thickness ε .

Theorem 4.1. $\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} (I(\varepsilon)(\phi(\varepsilon)) - I^0(\phi_0, b_0^{\alpha})) = 0.$

Let us now turn to second order correction. Let $P_2(\varepsilon) = \frac{1}{c^2} (I(\varepsilon)(\phi(\varepsilon)) - I^0(\phi_0, b_0^{\alpha})).$

Definition 4.2. Following [3], we say that (ϕ_0, b_0^{α}) satisfy the strong variation condition if there exists $\eta > 0$ such that, for all ε small enough, for all $(f, g_1, g_2) \in H_0^2(0, L; \mathbb{R}^3) \times H_0^1(0, L; \mathbb{R}^3)^2$,

$$\frac{1}{\varepsilon^2} \left(I^0 \left(\phi_0 + \varepsilon f, b_0^{\alpha} + \varepsilon g_{\alpha} \right) - I^0 \left(\phi_0, b_0^{\alpha} \right) \right) \ge \eta \int_0^L \left(|\partial_{33} f|^2 + \sum_{\alpha} |\partial_3 g_{\alpha}|^2 \right) \mathrm{d}x_3.$$
(10)

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Theorem 4.3. We assume that W is such that $\frac{\partial W}{\partial F}$ and $\frac{\partial^2 W}{\partial F^2}$ satisfy growth conditions compatible with (3), that the minimizers (ϕ_0, b_0^{α}) given by Theorem 2.1 satisfy the strong variation condition and that $b_0^{\alpha} \in H^2(0, L; \mathbb{R}^3)$. Then, there exists $(c_0, d_0^{\alpha}) \in H^2(0, L; \mathbb{R}^3) \times H^1(0, L; \mathbb{R}^3)^2$ such that

$$\frac{1}{\varepsilon}\partial_{33}(\phi(\varepsilon) - \phi_0 - \varepsilon x_{\alpha}b_0^{\alpha}) \to \partial_{33}c_0, \qquad \frac{1}{\varepsilon}\partial_3\left(\frac{1}{\varepsilon}\partial_{\alpha}\phi(\varepsilon) - b_0^{\alpha}\right) \to \partial_3d_0^{\alpha}, \qquad \frac{1}{\varepsilon^3}\partial_{\alpha\beta}\phi(\varepsilon) \to 0$$

when $\varepsilon \to 0$ in $L^2(\Omega; \mathbb{R}^3)$. Furthermore (c_0, d_0^{α}) minimize

$$I^{2}(c, d^{\alpha}) = \int_{\Omega} \left\{ \kappa^{2} \left(|\partial_{33}c|^{2} + 2|\partial_{3}d^{1}|^{2} + 2|\partial_{3}d^{2}|^{2} + x_{\alpha}^{2}|\partial_{33}b_{0}^{\alpha}|^{2} \right) + Q\left(d^{1}|d^{2}|\partial_{3}\left(c + x_{\alpha}b_{0}^{\alpha}\right) \right) \right\} \mathrm{d}x, \tag{11}$$

among all $(c, d^{\alpha}) \in H_0^2(0, L; \mathbb{R}^3) \times H_0^1(0, L; \mathbb{R}^3)^2$, where $Q(F) = \frac{1}{2}F(\frac{\partial^2 W}{\partial F^2}|_{(b_0^1|b_0^2|\partial_3\phi_0)}) \cdot F$. In addition, we have $P_2(\varepsilon) \to I^2(c_0, d_0^{\alpha})$ when $\varepsilon \to 0$.

Again, the proof follows closely [3].

In terms of the original energy, we have $I_{\varepsilon}(\phi^{\varepsilon}) = \varepsilon^2 I^0(\phi_0, b_0^{\alpha}) + \varepsilon^4 I^2(c_0, d_0^{\alpha}) + \text{h.o.t.}$, where I^2 consists of interfacial terms plus torsion and bending terms.

According to our results, the sum $I^0 + \varepsilon^2 I^2$ is not to be minimized with respect to $(b^{\alpha}, \phi, d^{\alpha}, c)$. Instead, a twostep minimization process should be carried out. First minimize I^0 with respect to (b^{α}, ϕ) to obtain the minimizers (b_0^{α}, ϕ_0) . Then, holding (b_0^{α}, ϕ_0) fixed, minimize I^2 with respect to (d^{α}, c) . Therefore, it is clear that the vectors d_0^{α} are correctors for b_0^{α} and c_0 is a corrector for ϕ_0 .

5. Further results

The presence of interfacial energy with constant κ is the reason why a direct argument that does not resort explicitly to Γ -convergence theory is possible. However, setting $\kappa = 0$ afterwards is not very satisfactory in this respect, since this contradicts the premise upon which the limit model was obtained. To derive a more coherent macroscopic picture, we should also let $\kappa(\varepsilon) \rightarrow 0$ along with ε . This is possible using the work of Shu [7] for films. In this case, we obtain that the limiting energy depends on the ratios

$$\lim_{\varepsilon \to 0} \frac{\kappa(\varepsilon)}{d(\varepsilon)}, \quad \lim_{\varepsilon \to 0} \frac{\kappa(\varepsilon)}{\varepsilon} \quad \text{and} \quad \lim_{\varepsilon \to 0} \frac{d(\varepsilon)}{\varepsilon}.$$
(12)

The proof of these more complicated results makes use of Γ -convergence theory and will be published elsewhere.

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