Received: 26 July 2021 | Revised: 8 March 2022 | Accepted: 10 July 2022
DOI: 10.1002/mma.8581

RESEARCH ARTICLE

WILEY

Identification of microstructural information from macroscopic boundary measurements in steady-state linear elasticity

Tanja Lochner[1] | **Malte A. Peter**[1,2]

[1]Institute of Mathematics, University of Augsburg, Augsburg, Germany
[2]Centre for Advanced Analytics and Predictive Sciences, University of Augsburg, Augsburg, Germany

Correspondence
Tanja Lochner, Institute of Mathematics, University of Augsburg, 86135 Augsburg, Germany.
Email: tanja.lochner@math.uni-augsburg.de

Communicated by: M. Brokate

We consider the upscaled linear elasticity problem in the context of periodic homogenization. Based on measurements of the deformation of the (macroscopic) boundary of a body for a given forcing, it is the aim to deduce information on the geometry of the microstructure. For a parametrized microstructure, we are able to prove that there exists at least one solution of the associated minimization problem based on the L^2-difference of the measured deformation and the resulting deformation for a given parameter. To facilitate the use of gradient-based algorithms, we derive the Gâteaux derivatives using the Lagrangian method of Céa, and we present numerical experiments showcasing the functioning of the method.

KEYWORDS
linear elasticity, parameter identification, periodic homogenization, shape derivative

MSC CLASSIFICATION
35B27, 35R30, 74G75

1 | INTRODUCTION

For a given periodic microstructure, upscaling of the steady-state linear elasticity problem in three dimensions is a classical result in the context of periodic homogenization. The resulting upscaled system is of the same type, where the homogenized (effective) elasticity tensor depends on the macroscopic variable, and it is computed from solutions of auxiliary problems stated in the periodicity cell.

Here, we consider the associated inverse problem and deduce from measurements on the boundary the interior geometry of the periodicity cell. To achieve this, we combine the methods of periodic homogenization and parameter identification. Therefore, if measured data of the deformation of the exterior boundary of a two-scale composite of two solids under given forcing are available, our results allow to compute parameters characterizing the microscopic structure. Such results are of particular practical relevance if, for example, the microstructure is associated with damage (microscopic holes/domains of weak material of a certain size) and our results allow to compute the extent of the damage (size of the holes/weak domains) from macroscopic boundary measurements.

More concretely, we derive the results on the inverse problem under the assumption that the periodicity cell consists of two perfectly bonded solids, where the one part is completely contained in the cell and its geometry is described by a finite vector of real parameters τ. The aim of this paper is then to investigate the minimization problem

$$\arg\min_{\tau\in I_\kappa} \mathcal{J}(\tau) := \arg\min_{\tau\in I_\kappa} \frac{1}{2}\|u[\tau]-u_m\|^2_{[L^2(\partial\Omega)]^3},$$

where the parameter $\tau \in I_\kappa$, I_κ a compact subset, describes the geometry of the microstructure, $u[\tau] : \Omega \to \mathbb{R}^3$ is the displacement field for a given τ and u_m is the measured displacement.

There are several authors studying related parameter identification problems in the context of shape optimization and homogenization. Orlik et al.[1] optimize textile materials via homogenization and beam approximation with a similar approach as in Section 3.1 of this paper, but the result is stated for constant homogenized tensor and under different assumptions on the elasticity tensor. Another paper closely connected to our results is by Allaire et al.[2] where homogenization in connection with shape optimization for linearized elasticity in only two dimensions is studied, where the microstructure consists of a cell with a central rectangular hole (i.e., no material/void space). The aim is to find the optimal shape, that is, the length, width, and rotation of the rectangle. Michailidis[3] considers the linear elasticity equation together with some thermal stress tensor. It is also in the setting of inverse homogenization, but the method of Céa in connection with a smoothed-interface is used instead of a sharp interface as we consider here. It is also worth mentioning Allaire et al.,[4] who investigate the damage evolution in linear elasticity via shape optimization, whereby they need to compute the shape derivative. They handle the difficulty that the interface moves instead of the outer boundary, and the full strain and stress tensors are not continuous across the interface, but this work is not set in a multiscale context.

Related research fields in parameter identification in elasticity aim to identify the (microscopic) material parameters and not the shape from measurements on the boundary.[5–7] Electrical impedance tomography,[8] for example, where the aim is to find the electrical conductivity and permittivity under special structural assumptions, is another application, where related parameter identification problems arise. Some more general results in shape optimization by homogenization method can be found in the books of, for example, Allaire[9] and Delfour and Zolesio[10] and in the theory of inverse problems of, for example, Isakov[11] and Kirsch.[12]

The paper consists of two parts: the study of the direct problem (Section 2) and the study of the inverse problem (Section 3). In Section 2.1, we introduce the homogenized problem and briefly summarize existence and uniqueness of the solutions. While these results are mostly standard, we proof some more detailed properties of the homogenized elasticity tensor required in what follows in Section 2.2. In Section 3.1, we formulate the inverse problem and show the existence of at least one solution of the inverse problem. After computation of the Gâteaux derivative of the homogenized tensor in Section 3.2, we derive the Gâteaux derivative of the functional of the inverse problem in Section 3.3. Focussing on a microstructure consisting of ellipsoids, some numerical experiments showcase the functioning of the method in Section 4. Conclusions are drawn in Section 5.

2 | STATEMENT OF THE DIRECT PROBLEM

2.1 | Periodic and homogenized problem

Let Ω be an open bounded Lipschitz domain in $\mathbb{R}^3$, $\Gamma_D \subset \partial\Omega$ closed with $|\Gamma_D| > 0$, $\Gamma_N = \partial\Omega\backslash\Gamma_D$, and $Y = (0, l_1) \times (0, l_2) \times (0, l_3) \subset \mathbb{R}^3$. We consider a bounded sequence $\{A^\varepsilon\}$ of tensors of fourth order in $M(\alpha, \beta, \Omega)$, which is defined as follows:

Definition 1. Let $\alpha, \beta \in \mathbb{R}$ with $0 < \alpha < \beta$ and let $\mathcal{O}$ be an open set in $\mathbb{R}^3$. We denote by $M(\alpha, \beta, \mathcal{O})$ the set of all tensors $B = (b_{ijkh})_{1\le i,j,k,h\le 3}$ such that

(i) $b_{ijkh} \in L^\infty(\mathcal{O})$ for all $i, j, k, h \in \{1, 2, 3\}$
(ii) $b_{ijkh} = b_{jikh} = b_{khij}$ for all $i, j, k, h \in \{1, 2, 3\}$
(iii) $\alpha|m|^2 \le Bmm$ for all symmetric matrices m
(iv) $|B(x)m| \le \beta|m|$ for all matrices m

a.e. in $\mathcal{O}$, where

$$\begin{cases} Bm := \left((Bm)_{ij}\right)_{1\le i,j\le 3} = \left(\left(\sum_{k,h=1}^3 B_{ijkh} m_{kh}\right)_{ij}\right)_{1\le i,j\le 3}, \\ Bm\tilde{m} := \sum_{i,j,k,h=1}^3 b_{ijkh} m_{ij} \tilde{m}_{kh}, \\ |m| := \left(\sum_{i,j=1}^3 m_{ij}^2\right)^{\frac{1}{2}}, \end{cases}$$

for quadratic matrices $m = \left(m_{ij}\right)_{1\le i,j\le 3}$ and $\tilde{m} = \left(\tilde{m}_{ij}\right)_{1\le i,j\le 3}$.

The deformation of the domain Ω under given body load f and boundary force g can be described by the displacement field $u^\varepsilon : \Omega \to \mathbb{R}^3$, which is the solution of the steady-state linear elasticity problem

$$\begin{cases} -\mathrm{div}(A^\varepsilon e(u^\varepsilon)) = f & \text{in } \Omega, \\ u^\varepsilon = 0 & \text{on } \Gamma_\mathrm{D}, \\ A^\varepsilon e(u^\varepsilon) n = g & \text{on } \Gamma_\mathrm{N}, \end{cases} \tag{1}$$

where A^ε describes the properties of the material of the solid and n is the outer unit normal. A classical example for $\{A^\varepsilon\}$ is a sequence of tensors of the form $A^\varepsilon(x) = A\left(\frac{x}{\varepsilon}\right)$ with A Y-periodic, that is, the material properties only depend on the microstructure. The linearized strain tensor $e(u^\varepsilon)$ is given by the symmetric gradient of the displacement field, that is,

$$e(u^\varepsilon) := \frac{1}{2}(\nabla u^\varepsilon + (\nabla u^\varepsilon)^T).$$

Due to the assumptions on A^ε, there exists a unique solution u^ε for every ε.

Theorem 1. *Let $A^\varepsilon \in M(\alpha, \beta, \Omega)$, $f \in [L^2(\Omega)]^3$ and $g \in [L^2(\Gamma_\mathrm{N})]^3$. Then, there exists a unique weak solution $u^\varepsilon \in H^1_{\Gamma_\mathrm{D}}(\Omega) := \{u \in \left[H^1(\Omega)\right]^3 : u = 0 \text{ on } \Gamma_\mathrm{D}\}$ of problem (1). Moreover, u^ε is bounded in $H^1_{\Gamma_\mathrm{D}}(\Omega)$,*

$$\|u^\varepsilon\|_{[H^1(\Omega)]^3} \leq \frac{C}{\alpha}\left(\|f\|_{[L^2(\Omega)]^3} + \|g\|_{[L^2(\Gamma_\mathrm{N})]^3}\right),$$

where C is a constant only depending on Ω.

Proof. The proof can be found in Theorem 10.6.,[13] whereby we use additionally Korn's inequality for the estimate. □

We introduce the periodic unfolding operator from chapter 1.1.[14]

Definition 2. For a Lebesegue measurable function ϕ on $\Omega^\varepsilon := \text{interior} \bigcup_{\xi \in \Lambda^\varepsilon} \varepsilon(\overline{Y} + \xi)$, where $\Lambda^\varepsilon := \{\xi \in \mathbb{R}^3 : \varepsilon(Y + \xi) \subset \Omega\}$, the periodic unfolding operator $\mathcal{T}_\varepsilon : L^p(\Omega) \to L^p(\Omega \times Y)$, $p \in [1, \infty]$, is defined as follows:

$$\mathcal{T}_\varepsilon(\phi)(x, y) = \begin{cases} \phi\left(\varepsilon\left[\frac{x}{\varepsilon}\right]_Y + \varepsilon y\right) & \text{for a.e. } (x, y) \in \Omega^\varepsilon \times Y, \\ 0 & \text{for a.e. } (x, y) \in \Pi^\varepsilon \times Y, \end{cases}$$

where $\Pi^\varepsilon = \Omega \backslash \Omega^\varepsilon$ and $\left[\frac{x}{\varepsilon}\right]_Y$ is the unique linear combination of the unit vectors $e_j \in \mathbb{R}^3$ with integer coordinates $\xi_j \in \mathbb{Z}$, that is, $\left[\frac{x}{\varepsilon}\right]_Y = \sum_{j=1}^3 \xi_j e_j$, such that $x - \varepsilon\left[\frac{x}{\varepsilon}\right]_Y \in Y$.

Under an additional assumption on A^ε, we can pass to the limit $\varepsilon \to 0$ to find the homogenized solution. We denote by $H^1_{\mathrm{per},0}(Y)$ the space of all functions $u \in H^1(Y)$, which are Y-periodic and have mean value zero, that is, $\mathcal{M}_Y(u) = \frac{1}{|Y|}\int_Y u \,\mathrm{d}y = 0$.

Theorem 2. *Let $f \in [L^2(\Omega)]^3$ and $g \in [L^2(\Gamma_\mathrm{N})]^3$. Furthermore, let u^ε be the weak solution of (1) for $A^\varepsilon \in M(\alpha, \beta, \Omega)$. Suppose that*

$$B^\varepsilon := \mathcal{T}_\varepsilon(A^\varepsilon) \to B \text{ a.e. in } \Omega \times Y. \tag{2}$$

Then, $B \in M(\alpha, \beta, \Omega \times Y)$ and there exists $u \in H^1_{\Gamma_\mathrm{D}}(\Omega)$ and $\hat{u} \in [L^2(\Omega, H^1_{per,0}(Y))]^3$ such that

$$u^\varepsilon \to u \quad \text{strongly in } [L^2(\Omega)]^3, \tag{3}$$

$$\mathcal{T}_\varepsilon(u^\varepsilon) \rightharpoonup u \quad \text{weakly in } [L^2(\Omega, H^1_{per}(Y))]^3, \tag{4}$$

$$\mathcal{T}_\varepsilon(\nabla u^\varepsilon) \rightharpoonup \nabla u + \nabla_y \hat{u} \quad \text{weakly in } [L^2(\Omega \times Y)]^{3\times 3} \tag{5}$$

and $(u, \hat{u})$ is the unique solution of

$$\frac{1}{|Y|}\int_{\Omega\times Y} B(x,y)(e(u)(x) + e_y(\hat{u})(x,y))(e(v)(x) + e_y(\hat{v})(x,y))\,\mathrm{d}x\mathrm{d}y = \int_\Omega f(x)\cdot v(x)\,\mathrm{d}x + \int_{\Gamma_\mathrm{N}} g(x)\cdot v(x)\,\mathrm{d}S(x) \tag{6}$$

for all $v \in H^1_{\Gamma_\mathrm{D}}(\Omega)$ and $\hat{v} \in [L^2(\Omega, H^1_{per,0}(Y))]^3$.

Proof. The assumption (2) implies that $B \in M(\alpha, \beta, \Omega \times Y)$. Due to Theorem 1, the solutions u^ϵ are uniformly bounded in $H^1(\Omega)$ and so we can apply standard periodic unfolding results (see chapter 1.4[14]) to get convergences (3)–(5). Choosing appropriate test functions in in the weak formulation of (1) and passing to the limit, we receive (6). We can endow the space $H^1_{\Gamma_D}(\Omega) \times [L^2(\Omega, H^1_{\mathrm{per},0}(Y))]^3$ with the norm $\left(\|\nabla v\|^2_{[L^2(\Omega)]^{3\times3}} + \|\nabla_y \hat{v}\|^2_{[L^2(\Omega\times Y)]^{3\times3}} \right)^{1/2}$. Note that due to the Y-periodicity and Korn's inequality for functions with zero trace on part of the boundary and for periodic functions with zero mean value, there holds for every $(v, \hat{v}) \in H^1_{\Gamma_D}(\Omega) \times [L^2(\Omega, H^1_{\mathrm{per},0}(Y))]^3$

$$\|e(v) + e_y(\hat{v})\|^2_{[L^2(\Omega\times Y)]^{3\times3}} \geq C \left(|Y| \|\nabla v\|^2_{[L^2(\Omega)]^{3\times3}} + \|\nabla_y(\hat{v})\|^2_{[L^2(\Omega\times Y)]^{3\times3}} \right).$$

Using this inequality and the fact that $B \in M(\alpha, \beta, \Omega \times Y)$, we can apply the Lax–Milgram theorem to problem (6) to show that there exists a unique solution. □

We can split the homogenized problem into a macroscopic problem and a cell problem.

Theorem 3. *The homogenized problem (6) is of the form*

$$\begin{cases} -\mathrm{div}(A^{\mathrm{hom}} e(u)) = f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ A^{\mathrm{hom}} e(u) n = g & \text{on } \Gamma_N, \end{cases} \tag{7}$$

where $A^{\mathrm{hom}} = (A^{\mathrm{hom}}_{ijkl})_{1\leq i,j,k,l\leq 3}$ *with*

$$A^{\mathrm{hom}}_{ijkl}(x) = \frac{1}{|Y|} \int_Y B(x,y) e_{ij}(e_{kl} - e_y(w^{kl})(x,y))\,\mathrm{d}y \tag{8}$$

for a.e. $x \in \Omega$ *and* w^{kl}, $k, l \in \{1,2,3\}$, *is the unique solution in* $[L^\infty(\Omega, H^1_{per,0}(Y))]^3$ *of the cell problem*

$$\int_Y B(x,y) \left(e_y(w^{kl})(x,y) - e_{kl} \right) e_y(v)(y)\,\mathrm{d}y = 0 \tag{9}$$

for all $v \in [H^1_{per,0}(Y)]^3$. *If B is Y-periodic, we can write the cell problem in the strong form*

$$\begin{cases} -\mathrm{div}_y(B(x,\cdot)(e_y(w^{kl})(x,\cdot) - e_{kl})) = 0 & \text{in } Y, \\ w^{kl}(x,\cdot)\ Y\text{-periodic with } \mathcal{M}_Y(w^{kl}(x,\cdot)) = 0. \end{cases}$$

for a.e. $x \in \Omega$.

Proof. This result follows by standard arguments. It can be shown as in the proof of Proposition 3.7[14] for the diffusion problem. □

The variational formulation of the homogenized problem (7) is given by

$$\int_\Omega A^{\mathrm{hom}} e(u) e(v)\,\mathrm{d}x = \int_\Omega f \cdot v\,\mathrm{d}x + \int_{\Gamma_N} g \cdot v\,\mathrm{d}S(x) \tag{10}$$

for all $v \in H^1_{\Gamma_D}(\Omega)$.

2.2 | Properties of the homogenized tensor and homogenized problem

We want to show that the homogenized tensor A^{hom} (see Equation (8)) is in the set $M(\tilde{\alpha}, \tilde{\beta}, \Omega)$ for some constants $\tilde{\alpha}, \tilde{\beta} > 0$ under an additional assumption, whereby we refer to the book of Jikov, Kozlov and Oleinik[15] in the general setting of G-convergence. For the proof, we need the boundedness of the cell solutions.

Lemma 1. *The solution w^{kh} of the cell problem (9) is bounded as follows:*

$$\|e_y(w^{kh})\|_{[L^\infty(\Omega, L^2(Y))]^{3\times 3}} \leq \frac{\beta |Y|^{1/2}}{\alpha}.$$

Proof. Since $B(x, y) \in M(\alpha, \beta, \Omega \times Y)$, there holds for a.e. $x \in \Omega$

$$\alpha \|e_y(w^{kh}(x, \cdot))\|^2_{[L^2(Y)]^{3\times 3}} \leq \int_Y B(x, y) e_y(w^{kh}) e_y(w^{kh})\,\mathrm{d}y = \int_Y B(x, y) e_{kh} e_y(w^{kh})\,\mathrm{d}y \leq |Y|^{1/2} \beta \|e_y(w^{kh})(x, \cdot)\|_{[L^2(Y)]^{3\times 3}}.$$

□

We additionally need some auxiliary lemmas.

Lemma 2. *Let $v \in [H^1_{per,0}(Y)]^3$. Then, v can be extended Y-periodically to an element of $[H^1_{loc}(\mathbb{R}^3)]^3$.*

Proof. Let $v \in [H^1_{\mathrm{per},0}(Y)]^3$ be extended Y-periodically, denoted by $\tilde{v}$. We only have to prove that $\tilde{v} \in [H^1_{\mathrm{loc}}(\mathbb{R}^3)]^3$. Therefore, let K be a compact subset of $\mathbb{R}^3$. We define $\mathcal{Z} \subset \mathbb{Z}^3$ and

$$\tilde{K} := \bigcup_{\xi \in \mathcal{Z}} (Y + \xi)$$

such that

$$K \subset \tilde{K} \quad \text{and} \quad K \cap (Y + \xi) \neq \emptyset \text{ for all } \xi \in \mathcal{Z}.$$

Then, using the transformation formula,

$$\begin{aligned} \|\tilde{v}\|^2_{[L^2(K)]^3} &= \int_K |\tilde{v}(y)|^2\,\mathrm{d}y \leq \int_{\tilde{K}} |\tilde{v}(y)|^2\,\mathrm{d}y = \sum_{\xi \in \mathcal{Z}} \int_{Y+\xi} |\tilde{v}(y)|^2\,\mathrm{d}y = \sum_{\xi \in \mathcal{Z}} \int_Y |\tilde{v}(y + \xi)|^2\,\mathrm{d}y \\ &= \sum_{\xi \in \mathcal{Z}} \int_Y |v(y)|^2\,\mathrm{d}y = \|v\|^2_{[L^2(Y)]^3} \sum_{\xi \in \mathcal{Z}} \frac{1}{|Y|} \int_Y \mathrm{d}y = \frac{|\tilde{K}|}{|Y|} \|v\|^2_{[L^2(Y)]^3}, \end{aligned}$$

and analogously,

$$\|\nabla \tilde{v}\|^2_{[L^2(K)]^{3\times 3}} = \int_K |\nabla \tilde{v}(y)|^2\,\mathrm{d}y \leq \int_{\tilde{K}} |\nabla \tilde{v}(y)|^2\,\mathrm{d}y = \frac{|\tilde{K}|}{|Y|} \|\nabla v\|^2_{[L^2(Y)]^{3\times 3}}.$$

Since K was arbitrary, we get the desired result. □

Lemma 3. *Let $v \in [L^2(Y)]^{3\times 3}$ with $\int_Y v : \nabla \varphi\,\mathrm{d}y = 0$ for all $\varphi \in [H^1_{per}(Y)]^3$. Then, v can be extended Y-periodically to an element of $[L^2_{loc}(\mathbb{R}^3)]^3$, denoted again by v, such that* $-\mathrm{div}\ v = 0$ *in $[\mathcal{D}'(\mathbb{R}^3)]^3$.*

Proof. Let $v \in [L^2(Y)]^{3\times 3}$ satisfy $\int_Y v : \nabla \varphi\,\mathrm{d}y = 0$ for all $\varphi \in [H^1_{\mathrm{per}}(Y)]^3$. Then, in the sense of distributions

$$-\int_Y \mathrm{div}\ v \cdot \varphi\,\mathrm{d}y = \int_Y v : \nabla \varphi\,\mathrm{d}y = 0 = \int_Y 0 \cdot \varphi\,\mathrm{d}y$$

for all $\varphi \in [C^\infty_c(Y)]^3$. Thus, there holds for the distributional derivative $-\mathrm{div}\ v = 0 \in [L^2(Y)]^3$. So v is an element of the space $H(Y, \mathrm{div}) := \{w \in [L^2(Y)]^{3\times 3} : \mathrm{div}\ w \in [L^2(Y)]^3\}$. Using Proposition 3.47(ii),[13] there holds for all $\phi \in [H^1(Y)]^3$

$$-\int_Y \mathrm{div}\ v \cdot \phi\,\mathrm{d}y = \int_Y v : \nabla \phi\,\mathrm{d}y + \langle vn, \phi \rangle_{[H^{-1/2}(\partial Y)]^3, H^{1/2}(\partial Y)]^3}.$$

With the results from above, we get for all $\varphi \in [H^1_{\text{per}}(Y)]^3$

$$0 = \langle vn, \varphi \rangle_{[H^{-1/2}(\partial Y)]^3, H^{1/2}(\partial Y)]^3},$$

where n is the normal of ∂Y, which proves that v is Y-periodic. As in Lemma 2, we get that v can be extended Y-periodically to an element of $[L^2_{\text{loc}}(\mathbb{R}^3)]^3$, again denoted by v. It remains to prove that $-\text{div } v = 0$ in $[\mathcal{D}'(\mathbb{R}^3)]^3$. Let $\varphi \in [C_c^\infty(\mathbb{R}^3)]^3$. Then, there exists a bounded set $K \subset \mathbb{R}^3$ such that $K = \bigcup_{\xi \in \mathcal{Z}} (Y + \xi)$ for some finite set $\mathcal{Z} \subset \mathbb{Z}^3$ and $\varphi \in [C_0^\infty(K)]^3$. So we get

$$\begin{aligned} -\int_{\mathbb{R}^3} \text{div } v \cdot \varphi \, \mathrm{d}x &= \int_K v : \nabla \varphi \, \mathrm{d}x = \sum_{\xi \in \mathcal{Z}} \int_{Y+\xi} v : \nabla \varphi \, \mathrm{d}x = \sum_{\xi \in \mathcal{Z}} \int_Y v(y) : \nabla \varphi(y + \xi) \, \mathrm{d}y \\ &= \sum_{\xi \in \mathcal{Z}} \int_Y -\text{div } v(y) \cdot \varphi(y+\xi) \, \mathrm{d}y + \langle v(\cdot)n, \varphi(\cdot + \xi) \rangle_{[H^{-1/2}(\partial Y)]^3, H^{1/2}(\partial Y)]^3} \\ &= \sum_{\xi \in \mathcal{Z}} \langle v(\cdot)n, \varphi(\cdot + \xi) \rangle_{[H^{-1/2}(\partial Y)]^3, H^{1/2}(\partial Y)]^3}. \end{aligned}$$

The sum disappears since v is periodic and either φ is continuous on $\partial Y + \xi$ or already zero. So $-\text{div } v = 0$ in $[\mathcal{D}'(\mathbb{R}^3)]^3$. ☐

Let $A \in M(\alpha, \beta, \mathcal{O})$ and $m \in \mathbb{R}^{3\times 3}$ be a symmetric matrix. We introduce the Voigt notation to rewrite the tensor of fourth order as a 6×6 matrix and the symmetric matrix as a vector of $\mathbb{R}^6$:

$$A^{\text{V}} = \begin{pmatrix} A_{1111} & A_{1122} & A_{1133} & A_{1123} & A_{1113} & A_{1112} \\ A_{1122} & A_{2222} & A_{2233} & A_{2223} & A_{2213} & A_{2212} \\ A_{1133} & A_{2233} & A_{3333} & A_{3323} & A_{3313} & A_{3312} \\ A_{1123} & A_{2223} & A_{3323} & A_{2323} & A_{2313} & A_{2312} \\ A_{1113} & A_{2213} & A_{3313} & A_{2313} & A_{1313} & A_{1312} \\ A_{1112} & A_{2212} & A_{3312} & A_{2312} & A_{1312} & A_{1212} \end{pmatrix}, \quad m^{\text{V}} = \begin{pmatrix} m_{11} \\ m_{22} \\ m_{33} \\ 2m_{23} \\ 2m_{13} \\ 2m_{12} \end{pmatrix}.$$

Lemma 4. *Let $A \in M(\alpha, \beta, \mathcal{O})$. Then, the inverse of A^{V} exists and is symmetric. Furthermore, there holds*

$$A^{-1}ww \geq \frac{\alpha}{\beta^2}|w|^2$$

for all symmetric matrices $w \in \mathbb{R}^{3\times 3}$, where $A^{-1}w$ is defined by

$$\begin{pmatrix} ((A^{\text{V}})^{-1}w^{\text{V}})_1 & \frac{1}{2}((A^{\text{V}})^{-1}w^{\text{V}})_5 & \frac{1}{2}((A^{\text{V}})^{-1}w^{\text{V}})_6 \\ \frac{1}{2}((A^{\text{V}})^{-1}w^{\text{V}})_5 & ((A^{\text{V}})^{-1}w^{\text{V}})_2 & \frac{1}{2}((A^{\text{V}})^{-1}w^{\text{V}})_4 \\ \frac{1}{2}((A^{\text{V}})^{-1}w^{\text{V}})_6 & \frac{1}{2}((A^{\text{V}})^{-1}w^{\text{V}})_4 & ((A^{\text{V}})^{-1}w^{\text{V}})_3 \end{pmatrix}. \tag{11}$$

Proof. Let $A \in M(\alpha, \beta, \mathcal{O})$. Let $\lambda^{\text{V}} \in \mathbb{R}^6$. Then, the associated symmetric matrix is

$$\lambda := \begin{pmatrix} \lambda_1^{\text{V}} & \frac{1}{2}\lambda_5^{\text{V}} & \frac{1}{2}\lambda_6^{\text{V}} \\ \frac{1}{2}\lambda_5^{\text{V}} & \lambda_2^{\text{V}} & \frac{1}{2}\lambda_4^{\text{V}} \\ \frac{1}{2}\lambda_6^{\text{V}} & \frac{1}{2}\lambda_4^{\text{V}} & \lambda_3^{\text{V}} \end{pmatrix}.$$

Since A is elliptic for symmetric matrices, we get

$$(A^{\text{V}}\lambda^{\text{V}}, \lambda^{\text{V}}) = A\lambda\lambda \geq \alpha|\lambda|^2 \geq \frac{\alpha}{2}|\lambda^{\text{V}}|^2,$$

where $(\cdot, \cdot)$ denotes the standard scalar product. This shows that A^{V} is positive definite and, due to assumption, symmetric. Thus, the inverse of A^{V} exists and is symmetric. To prove the inequality, we follow the proof of Propostion

8.3,[13] where the same result is shown for tensors of second order. Let $w \in \mathbb{R}^{3\times3}$ be a symmetric matrix. Then, there holds for $m = A^{-1}w$ defined as in (11) the equation $Am = w$ and

$$A^{-1}ww = Amm \geq \alpha|m|^2 = \alpha|A^{-1}w|^2. \tag{12}$$

Since A is a linear operator, we can estimate the operator norm

$$\|A\| = \sup_{\mathbb{R}^{3\times3}\ni u\neq0} \frac{|Au|}{|u|} \leq \frac{\beta|u|}{|u|} = \beta.$$

Thus,

$$|w| = |Am| \leq |m|\|A\| \leq \beta|A^{-1}w|.$$

Together with estimate (12), we get

$$A^{-1}ww \geq \alpha|A^{-1}w|^2 \geq \frac{\alpha}{\beta^2}|w|^2.$$

□

So now we can prove the following result.

Theorem 4. *If B is additionally Y-periodic in the second argument, there holds $A^{\mathrm{hom}} \in M\left(\alpha, \frac{\beta^2}{\alpha}, \Omega\right)$.*

Proof. We prove the theorem for a.e. $\hat{x} \in \Omega$. Since $B \in M(\alpha, \beta, \Omega \times Y)$ and Lemma 1 holds, we get that $A^{\mathrm{hom}}_{ijkl} \in L^\infty(\Omega)$. Using w^{kl} as a test function in (9) for the cell solution w^{ij} (and the other way round) and the symmetry of B, we can easily compute that A^{hom} is symmetric. To prove the coercivity of A^{hom} with the coercivity constant α, we extend B Y-periodically in the second argument. So the tensor $B^\varepsilon(x) := B\left(\hat{x}, \frac{x}{\varepsilon}\right)$ is well-defined for $x \in \Omega$ and $\varepsilon > 0$ small enough. Thus, $B^\varepsilon \in M(\alpha, \beta, \Omega)$ for every ε. Let $m = (m_{kh})_{1\leq k,h\leq 3} \in \mathbb{R}^{3\times3}$ be a symmetric matrix and

$$v^\varepsilon(x) := \sum_{k,h=1}^{3} m_{kh} w^{kh}_\varepsilon(\hat{x}, x) := \sum_{k,h=1}^{3} m_{kh}\left((x_h\delta_{ik})_{1\leq i\leq3} - \varepsilon w^{kh}\left(\hat{x}, \frac{x}{\varepsilon}\right)\right)$$

with $w^{kh}(\hat{x}, \cdot)$ Y-periodically extended as in Lemma 2. Then, $v^\varepsilon \in [H^1(\Omega)]^3$ and

$$v^\varepsilon(x) \to \sum_{k,h=1}^{3} (m_{kh}x_h\delta_{ik})_{1\leq i\leq3} = \sum_{h=1}^{3} (m_{ih}x_h)_{1\leq i\leq3}$$

strongly in $[L^2(\Omega)]^3$ and since $D_y w^{kh}\left(\hat{x}, \frac{x}{\varepsilon}\right) \rightharpoonup \mathcal{M}_Y(D_y w^{kh}(\hat{x}, y)) = 0$ in $[L^2(\Omega)]^3$,

$$\partial_j v^\varepsilon(x) = \sum_{h=1}^{3} (m_{ih}\partial_j x_h)_{1\leq i\leq3} - \sum_{k,h=1}^{3} m_{kh}\partial_{y_j} w^{kh}\left(\hat{x}, \frac{x}{\varepsilon}\right) \rightharpoonup (m_{ij})_{1\leq i\leq3}$$

weakly in $[L^2(\Omega)]^3$ for $j = 1, 2, 3$. Furthermore,

$$\begin{aligned}(B^\varepsilon e(v^\varepsilon))_{ij}(x) &= \sum_{k,h=1}^{3} B_{ijkh}\left(\hat{x}, \frac{x}{\varepsilon}\right)\left(m_{kh} - \sum_{p,q=1}^{3} m_{pq} e^y_{kh}(w^{pq})\left(\hat{x}, \frac{x}{\varepsilon}\right)\right) \\ &\rightharpoonup \frac{1}{|Y|}\int_Y \sum_{k,h=1}^{3} B_{ijkh}(\hat{x}, y)\left(m_{kh} - \sum_{p,q=1}^{3} m_{pq} e^y_{kh}(w^{pq})(\hat{x}, y)\right) \mathrm{d}y = (A^{\mathrm{hom}}(\hat{x})m)_{ij}\end{aligned}$$

weakly in $L^2(\Omega)$ for all $i, j = 1, 2, 3$. In the next step, we want to prove for all $\varphi \in C^\infty_0(\Omega)$

$$\int_\Omega B^\varepsilon e(v^\varepsilon)e(v^\varepsilon)\varphi(x)\,\mathrm{d}x \to \int_\Omega A^{\mathrm{hom}}(\hat{x})mm\varphi(x)\,\mathrm{d}x.$$

We notice that

$$e_{ij}(\varphi v^{\varepsilon}) = \varphi e_{ij}(v^{\varepsilon}) + \frac{1}{2}\partial_i \varphi v_j^{\varepsilon} + \frac{1}{2}\partial_j \varphi v_i^{\varepsilon}$$

and for $\tilde{x} := \sum_{h=1}^{3} (m_{ih}x_h)_{1\le i\le 3}$

$$e_{ij}(\varphi \tilde{x}) = \frac{1}{2}\sum_{h=1}^{3} \left(\partial_i \varphi m_{jh}x_h + \partial_j \varphi m_{ih}x_h\right) + \varphi m_{ij}.$$

Using the symmetry of $B(\hat{x}, \cdot)$, we can apply Lemma 3 to $v := B(\hat{x}, \cdot)\left(e_y(w^{kl})(\hat{x}, \cdot) - e_{kl}\right)$ to get

$$-\mathrm{div}_y(B(\hat{x}, \cdot)(e(w^{pq})(\hat{x}, \cdot) - e_{pq}) = 0 \text{ in } [\mathcal{D}'(\mathbb{R}^3)]^3$$

and thus,

$$\int_\Omega B^{\varepsilon} e(v^{\varepsilon})e(\varphi v^{\varepsilon})\,\mathrm{d}x = \sum_{p,q=1}^{3} m_{pq}\left(\int_\Omega B\left(\hat{x}, \frac{x}{\varepsilon}\right)\left(e_{pq} - e_y(w^{pq})\left(\hat{x}, \frac{x}{\varepsilon}\right)\right) e(\varphi v^{\varepsilon})\,\mathrm{d}x\right) = 0,$$

since we can approximate v^{ε} by $C^{\infty}(\Omega)$ functions. Using this result and the strong and weak convergences from above,

$$\begin{aligned}\int_\Omega B^{\varepsilon} e(v^{\varepsilon})e(v^{\varepsilon})\varphi\,\mathrm{d}x &= \int_\Omega B^{\varepsilon} e(v^{\varepsilon})e(\varphi v^{\varepsilon})\,\mathrm{d}x - \int_\Omega \sum_{i,j=1}^{3}(B^{\varepsilon}e(v^{\varepsilon}))_{ij}\frac{1}{2}\left(\partial_i\varphi v_j^{\varepsilon} + \partial_j \varphi v_i^{\varepsilon}\right)\,\mathrm{d}x \\ &\to -\int_\Omega \sum_{i,j=1}^{3}(A^{\mathrm{hom}}(\hat{x})m)_{ij}\frac{1}{2}\sum_{h=1}^{3}\left(\partial_i\varphi m_{jh}x_h + \partial_j\varphi m_{ih}x_h\right)\,\mathrm{d}x = \int_\Omega A^{\mathrm{hom}}(\hat{x})mm\varphi\,\mathrm{d}x.\end{aligned}$$

The last equation holds since

$$-\int_\Omega A^{\mathrm{hom}}(\hat{x})me\left(\varphi\tilde{x}\right)\,\mathrm{d}x = -A^{\mathrm{hom}}(\hat{x})m\int_\Omega e\left(\varphi\tilde{x}\right)\,\mathrm{d}x = 0.$$

The coercivity of B^{ε} together with the weak lower semicontinuity of the L^2-norm yields for $\varepsilon \to 0$ and for all $\varphi \in C_0^{\infty}(\Omega)$ with $\varphi \ge 0$

$$\int_\Omega A^{\mathrm{hom}}(\hat{x})mm\varphi\,\mathrm{d}x = \lim_{\varepsilon\to 0}\int_\Omega B^{\varepsilon}e(v^{\varepsilon})e(v^{\varepsilon})\varphi\,\mathrm{d}x \ge \liminf_{\varepsilon\to 0}\ \alpha\int_\Omega |e(v^{\varepsilon})|^2\varphi\,\mathrm{d}x \ge \int_\Omega \alpha|m|^2\varphi\,\mathrm{d}x.$$

So

$$\int_\Omega \left(A^{\mathrm{hom}}(\hat{x})mm - \alpha|m|^2\right)\varphi\,\mathrm{d}x \ge 0,$$

which proves that $A^{\mathrm{hom}}(\hat{x})mm \ge \alpha|m|^2$. It remains to prove $|A^{\mathrm{hom}}(\hat{x})m| \le \frac{\beta^2}{\alpha}|m|$ for all matrices m. Let $m \in \mathbb{R}^{3\times 3}$. We define

$$v^{\varepsilon}(x) := \sum_{k,h=1}^{3} m_{kh}w_{\varepsilon}^{kh}(\hat{x}, x) := \sum_{k,h=1}^{3} m_{kh}\left((x_h\delta_{ik})_{1\le i\le 3} - \varepsilon w^{kh}\left(\hat{x}, \frac{x}{\varepsilon}\right)\right).$$

If we apply Lemma 4 to $w = B^{\varepsilon}e(v^{\varepsilon})$, whereby $(B^{\varepsilon})^{-1}w$ is defined as in (11), we get for all $\varphi \in C_0^{\infty}(\Omega)$ with $\varphi \ge 0$

$$\int_\Omega B^{\varepsilon}e(v^{\varepsilon})e(v^{\varepsilon})\varphi\,\mathrm{d}x = \int_\Omega w(B^{\varepsilon})^{-1}w\varphi\,\mathrm{d}x \ge \frac{\alpha}{\beta^2}\int_\Omega |w|^2\varphi\,\mathrm{d}x = \frac{\alpha}{\beta^2}\int_\Omega |B^{\varepsilon}e(v^{\varepsilon})|^2\varphi\,\mathrm{d}x.$$

Passing to the limit yields

$$\int_\Omega A^{\mathrm{hom}}(\hat{x})mm\varphi\,\mathrm{d}x \ge \frac{\alpha}{\beta^2}\int_\Omega |A^{\mathrm{hom}}(\hat{x})m|^2\varphi\,\mathrm{d}x$$

because the same convergence holds as in the proof of the coercivity due to the symmetry of B^ε and $A^{\text{hom}}(\hat{x})$. We needed the symmetry of the matrix only to get the weak convergence of $e(v^\varepsilon)$ to m. Since $\varphi \geq 0$ was arbitrary and we can apply the Cauchy–Schwarz inequality, we get

$$|A^{\text{hom}}(\hat{x})m|^2 \leq \frac{\beta^2}{\alpha} A^{\text{hom}}(\hat{x})mm \leq \frac{\beta^2}{\alpha}|A^{\text{hom}}(\hat{x})m||m|.$$

Thus,

$$|A^{\text{hom}}(\hat{x})m| \leq \frac{\beta^2}{\alpha}|m|.$$

□

Theorem 5. *For all $f \in [L^2(\Omega)]^3$, $g \in [L^2(\Gamma_{\text{N}})]^3$ there exists a unique solution $u \in H^1_{\Gamma_{\text{D}}}(\Omega)$ of problem (10). Furthermore,*

$$\|u\|_{[H^1(\Omega)]^3} \leq C\left(\|f\|_{[L^2(\Omega)]^3} + \|g\|_{[L^2(\Gamma_{\text{N}})]^3}\right) \tag{13}$$

for a constant C independent of the structure of the cell Y.

Proof. Although we have already proven in Theorem 2 the existence and uniqueness, we can use the last result to show this directly by applying the Lax–Milgram theorem. Using the properties of $A^{\text{hom}} \in M\left(\alpha, \frac{\beta^2}{\alpha}, \Omega\right)$, Korn's inequality and the trace operator, we receive the inequality (13). □

3 | INVERSE PROBLEM

For the inverse problem, we consider a reference cell $Y = (0, l_1) \times (0, l_2) \times (0, l_3)$ consisting of two parts, one of which is a Lipschitz domain Y_0 completely contained in Y, whose geometry can be described by a (finite) vector of real parameters τ. A concrete example for such a geometry is an ellipsoid of material embedded in a matrix of other material.

The following results generally hold for parametrized microstructures, but we will consider an ellipsoidal microstructure as illustrated in Figures 1 and 2 for explicit examples and computations: Let $Y_0[\tau]$ be an open ellipsoid with $\tau = (\tau_1, \tau_2, \tau_2) \in [\kappa, l_1 - \kappa] \times [\kappa, l_2 - \kappa] \times [\kappa, l_3 - \kappa] =: I_\kappa$ for some small κ, where τ_1, τ_2, and τ_3 are the lengths of the axis. Furthermore, $Y_0[\tau]$ is centered in the middle of the cuboid Y with axis in direction of the standard unit vectors, $Y_1[\tau] := Y \backslash \overline{Y_0[\tau]}$ and $\Sigma_Y[\tau] := \partial Y_0[\tau]$. Thus, $Y = Y_0 \cup Y_1 \cup \Sigma_Y$.

Since the structure in the cube Y depends on τ, we sometimes write $Y[\tau]$ instead of Y to emphasize this property. As mentioned in Section 1, we consider a perfectly bonded composite of two materials. Therefore, we define the elasticity tensor $A^\varepsilon[\tau]$ as follows:

$$A^\varepsilon[\tau](x) = A^0(x)\chi_{Y_0[\tau]}\left(\frac{x}{\varepsilon}\right) + A^1(x)\chi_{Y_1[\tau]}\left(\frac{x}{\varepsilon}\right)$$

with $\chi_{Y_0[\tau]}$ (resp. $\chi_{Y_1[\tau]}$) the characteristic function of the Y-periodically extended domain $Y_0[\tau]$ (resp. $Y_1[\tau]$) and some fourth-order tensors $A^0, A^1 \in M(\alpha, \beta, \Omega)$ such that

$$\mathcal{T}_\varepsilon(A^\varepsilon[\tau])(x, y) \to A^0(x)\chi_{Y_0[\tau]}(y) + A^1(x)\chi_{Y_1[\tau]}(y) =: B[\tau](x, y)$$

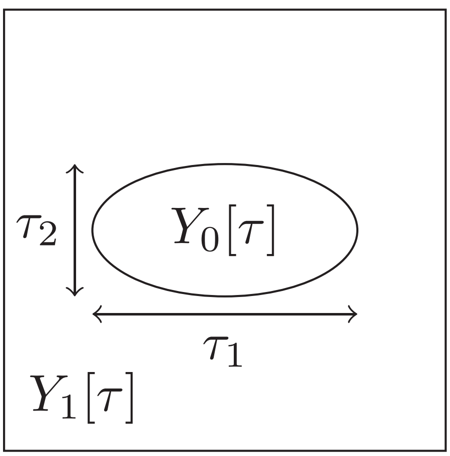

FIGURE 1 Example of a periodicity cell Y in 2D

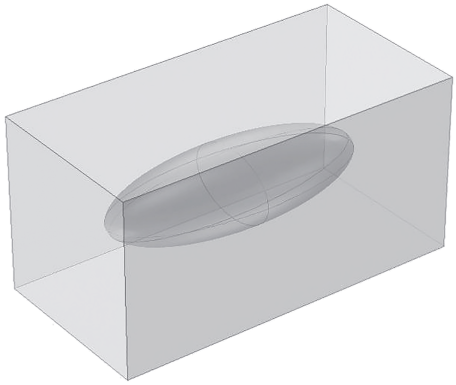

FIGURE 2 Ellipsoid Y_0 in the periodicity cell Y in 3D

for a.e. $(x, y) \in \Omega \times Y$. In this case,

$$A^{\mathrm{hom}}_{ijkl}[\tau](x) = \frac{1}{|Y|} \int\limits_{Y_0[\tau]} A^0(x) e_{ij}(e_{kl} - e_y(w^{kl})(x,y))\,\mathrm{d}y + \frac{1}{|Y|} \int\limits_{Y_1[\tau]} A^1(x) e_{ij}(e_{kl} - e_y(w^{kl})(x,y))\,\mathrm{d}y$$

and since $B[\tau]$ is Y-periodic, $A^{\mathrm{hom}}[\tau] \in M\left(\alpha, \frac{\beta^2}{\alpha}, \Omega\right)$. Since $B[\tau](x, \cdot)$ is piecewise smooth in Y, we even get that $w^{kl}(x, \cdot)$ belongs to $[C^\infty(Y_0[\tau])]^3$ and $[C^\infty(Y_1[\tau])]^3$ due to Theorem 6.2 in Chapter I.[16]

In the previous section, we were in the setting that we know the microstructure, that is, the value of τ. So if f, g are given, we can easily compute the solution $u[\tau]$. From now on, we only know f, g and some measured data u_m. With this information, we want to find the structure of the reference cell. We define the input–output operator:

Definition 3 (Input–output operator)**.** Let

$$\mathcal{L}_\tau : [L^2(\Omega)]^3 \times [L^2(\Gamma_\mathrm{N})]^3 \to [L^2(\partial\Omega)]^3, \ (f, g) \mapsto u[\tau]|_{\partial\Omega},$$

where $u[\tau]$ is the solution of the homogenized problem (10) for given τ.

The operator $\mathcal{L}_\tau$ is linear and continuous due to (13) and the properties of the trace operator. We consider the following inverse problem.

Definition 4 (Inverse problem)**.** Let $0 < \kappa < \min\{l_1, l_2, l_3\}$. Find $\tau \in I_\kappa$ such that for given measured data $u_m \in [L^2(\partial\Omega)]^3$, when forces (f, g) are applied, τ is the solution of the minimization problem

$$\arg\min_{\tau \in I_\kappa} \mathcal{J}(\tau) := \arg\min_{\tau \in I_\kappa} \frac{1}{2} \|\mathcal{L}_\tau(f, g) - u_m\|^2_{[L^2(\partial\Omega)]^3}. \tag{14}$$

Of course, other functionals than $\mathcal{J}$ could be used.

3.1 | Existence result

In this section, we want to show that there exists at least one solution of the inverse problem (14). To prove the continuity of the mapping $\mathcal{Z} : I_\kappa \to [L^2(\partial\Omega)]^3, \tau \mapsto \mathcal{L}_\tau(f, g)$ for given (f, g), we rewrite the operator as a composition of the continuous trace operator $\mathcal{T} : [H^1(\Omega)]^3 \to [L^2(\partial\Omega)]^3$ and the operator $\mathcal{H}_{f,g} : I_\kappa \to H^1_{\Gamma_\mathrm{D}}(\Omega), \tau \mapsto u[\tau]$, i.e. $\mathcal{Z}(\tau) = \mathcal{T} \circ \mathcal{H}_{f,g}(\tau)$.

Theorem 6. *The operator $\mathcal{H}_{f,g}$ is continuous.*

Proof. Let $\tau_n, \hat{\tau} \in I_\kappa$ with $\tau_n \to \hat{\tau}$ for $n \to \infty$ and $u[\tau_k]$, $u[\hat{\tau}]$ the corresponding weak solutions of the homogenized problem (10). Then, for all $\varphi \in H^1_{\Gamma_\mathrm{D}}(\Omega)$

$$a(u[\tau_n], \varphi; \tau_n) = F(\varphi), \ a(u[\hat{\tau}], \varphi; \hat{\tau}) = F(\varphi),$$

where $a : H^1_{\Gamma_D}(\Omega) \times H^1_{\Gamma_D}(\Omega) \to \mathbb{R}$ is the bilinear form of the left-hand side of (10) and $F : H^1_{\Gamma_D}(\Omega) \to \mathbb{R}$ is the τ-independent functional of the right-hand side of (10), that is,

$$a(u[\tau], \varphi; \tau) = \int_\Omega A^{\text{hom}}[\tau] e(u[\tau]) e(\varphi) \,\mathrm{d}x, \; F(\varphi) = \int_\Omega f \cdot \varphi \,\mathrm{d}x + \int_{\Gamma_N} g \cdot \varphi \,\mathrm{d}S(x).$$

The third argument of a only emphasizes that the bilinear form is considered for some given τ. Taking the difference of both equations yields

$$\int_\Omega A^{\text{hom}}[\tau_n] e(u[\tau_n] - u[\hat{\tau}]) e(\varphi) \,\mathrm{d}x = \int_\Omega (A^{\text{hom}}[\hat{\tau}] - A^{\text{hom}}[\tau_n]) e(u[\hat{\tau}]) e(\varphi) \,\mathrm{d}x.$$

Choosing the test function $\varphi = u[\tau_n] - u[\hat{\tau}]$ and using the coercivity of A^{hom}, we estimate

$$\alpha \| e(u[\tau_n] - u[\hat{\tau}]) \|^2_{[L^2(\Omega)]^{3\times3}} \le \| (A^{\text{hom}}[\hat{\tau}] - A^{\text{hom}}[\tau_n]) e(u[\hat{\tau}]) \|_{[L^2(\Omega)]^{3\times3}} \| e(u[\tau_n] - u[\hat{\tau}]) \|_{[L^2(\Omega)]^{3\times3}}.$$

Due to Korn's inequality for functions with zero value on part of the boundary, there holds

$$c \| \mathcal{H}_{f,g}(\tau_n) - \mathcal{H}_{f,g}(\hat{\tau}) \|_{[H^1(\Omega)]^3} \le \| (A^{\text{hom}}[\hat{\tau}] - A^{\text{hom}}[\tau_n]) e(u[\hat{\tau}]) \|_{[L^2(\Omega)]^{3\times3}} \tag{15}$$

for some constants $c > 0$ independent of τ. Using $B[\tau] \in M(\alpha, \beta, \Omega \times Y)$ and Lemma 1,

$$|A^{\text{hom}}_{ijkl}[\tau](x)| \le \frac{1}{|Y|} \| B[\tau](x, \cdot) e_{ij} \|_{[L^2(Y)]^{3\times3}} \| e_{kl} - e(w^{kl}[\tau](x, \cdot)) \|_{[L^2(Y)]^{3\times3}} \le \beta C \| e(w^{kl}[\tau](x, \cdot)) \|_{[L^2(Y)]^{3\times3}} \le C$$

for a.e. $x \in \Omega$ and for some constant $C > 0$ independent of τ and x. Thus, $\| A^{\text{hom}}_{ijkl}[\tau] \|_{L^\infty(\Omega)} \le C$ for all $\tau \in I_\kappa$ and $i, j, k, l \in \{1, 2, 3\}$ and

$$|(A^{\text{hom}}[\hat{\tau}](x) - A^{\text{hom}}[\tau_n](x)) e(u[\hat{\tau}(x)])|^2 \le C |e(u[\hat{\tau}](x))|^2 \in L^1(\Omega)$$

for a.e. $x \in \Omega$ and $C > 0$ independent of x. By Theorem 7,

$$|(A^{\text{hom}}_{ijkl}[\tau_n](x) - A^{\text{hom}}_{ijkl}[\hat{\tau}](x)) e(u[\hat{\tau}](x))|^2 \to 0$$

pointwise for a.e. $x \in \Omega$. So by the dominated convergence theorem, the right-hand side of (15) converges to 0 as $n \to \infty$, which proves that $\mathcal{H}_{f,g}$ is continuous. □

Theorem 7. *For a.e.* $x \in \Omega$, $A^{\text{hom}}_{ijkl}[\tau_n](x)$ *converges to* $A^{\text{hom}}_{ijkl}[\hat{\tau}](x)$ *for* $\tau_n \to \hat{\tau}$ *in* I_κ *and every* $i, j, k, l \in \{1, 2, 3\}$.

Proof. Let $x \in \Omega$ and $\tau_n \in I_\kappa$ with $\tau_n \to \hat{\tau}$. Clearly, $\hat{\tau} \in I_\kappa$ and

$$\begin{aligned} |A^{\text{hom}}_{ijkl}[\tau_n](x) - A^{\text{hom}}_{ijkl}[\hat{\tau}](x)| \le{}& \frac{1}{|Y|} \int_Y \left| (B[\tau_n](x, y) - B[\hat{\tau}](x, y)) \, e_{ij} \left(e_{kl} - e(w^{kl}[\hat{\tau}]) \right) \right| \mathrm{d}y \\ &+ \frac{1}{|Y|} \left| \int_Y B[\tau_n](x, y) e_{ij} \left(e(w^{kl}[\tau_n]) - e(w^{kl}[\hat{\tau}]) \right) \mathrm{d}y \right| =: \mathcal{I}^1_n(x) + \mathcal{I}^2_n(x). \end{aligned}$$

We consider the terms $\mathcal{I}^1_n$ and $\mathcal{I}^2_n$ separately. We estimate

$$\begin{aligned} \mathcal{I}^1_n(x) &\le \frac{1}{|Y|} \| \, (B[\tau_n](x, \cdot) - B[\hat{\tau}](x, \cdot)) \, e_{ij} \|_{[L^2(Y)]^{3\times3}} \| e_{kl} - e(w^{kl}[\hat{\tau}](x, \cdot)) \|_{[L^2(Y)]^{3\times3}} \\ &\le \frac{1}{|Y|^{1/2}} \left(1 + \frac{\beta}{\alpha} \right) \sum_{h,r=1}^{3} \| B_{ijhr}[\tau_n](x, \cdot) - B_{ijhr}[\hat{\tau}](x, \cdot) \|_{L^2(Y)}, \end{aligned}$$

where we have applied Lemma 1. Since $B_{ijhr}[\tau_n] \in L^\infty(\Omega \times Y)$ and Y is bounded, we obtain that $B_{ijhr}[\tau_n](x,\cdot) \in L^2(Y)$ for a.e. $x \in \Omega$ and

$$\|B_{ijhr}[\tau_n](x,\cdot) - B_{ijhr}[\hat{\tau}](x,\cdot)\|_{L^2(Y)} \leq |A^0_{ijhr}(x)|\,\|\chi_{Y_0[\tau_n]} - \chi_{Y_0[\hat{\tau}]}\|_{L^2(Y)} + |A^1_{ijhr}(x)|\,\|\chi_{Y_1[\tau_n]} - \chi_{Y_1[\hat{\tau}]}\|_{L^2(Y)} \to 0,$$

where we have used that $A^0, A^1 \in L^\infty(\Omega)$. The second term, $\mathcal{I}^2_n(x)$, converges to zero if we show that

$$e_{hr}(w^{kl}[\tau_n])(x,\cdot) \rightharpoonup e_{hr}(w^{kl}[\hat{\tau}])(x,\cdot) \quad \text{weakly in } \; L^2(Y)$$

for $n \to \infty$, because we already know the strong convergence

$$B_{ijhr}[\tau_n](x,\cdot) \to B_{ijhr}[\hat{\tau}](x,\cdot)$$

in $L^2(Y)$ from above. Due to Lemma 1, the solutions $w^{kl}[\tau_n]$ of the cell problem are uniformly bounded in $[L^\infty(\Omega, H^1_{\mathrm{per},0}(Y))]^3$. Thus, there exists a subsequence (again denoted by τ_n) and a function $\tilde{w} \in [H^1_{\mathrm{per},0}(Y)]^3$ such that

$$w^{kl}[\tau_n](x,\cdot) \rightharpoonup \tilde{w}(\cdot) \quad \text{weakly in } \; [H^1_{\mathrm{per},0}(Y)]^3.$$

We equate the cell problems (9) for the weak solution $w^{kl}[\tau_n]$ and $w^{kl}[\hat{\tau}]$ and pass to the limit

$$\int_Y B[\hat{\tau}](x,y)(e_{kl} - e(\tilde{w}))e(\varphi)\,\mathrm{d}y = \lim_{n\to\infty} \int_Y B[\tau_n](x,y)(e_{kl} - e(w^{kl}[\tau_n]))e(\varphi)\,\mathrm{d}y = 0 = \int_Y B[\hat{\tau}](x,y)(e_{kl} - e(w^{kl}[\hat{\tau}]))e(\varphi)\,\mathrm{d}y$$

for all $\varphi \in [C^\infty_{\mathrm{per}}(Y)]^3$. Taking $\varphi(y) = w^{kl}[\hat{\tau}](x,y) - \tilde{w}(y)$, the coercivity of B and Korn's inequality for periodic functions leads to

$$c\|w^{kl}[\hat{\tau}] - \tilde{w}\|_{[H^1(Y)]^3} \leq \alpha\|e(w^{kl}[\hat{\tau}] - \tilde{w})\|_{[L^2(Y)]^{3\times3}} \leq \int_Y B[\hat{\tau}](x,y)(e(w^{kl}[\hat{\tau}]) - e(\tilde{w}))(e(w^{kl}[\hat{\tau}]) - e(\tilde{w}))\,\mathrm{d}y = 0,$$

which shows that $\tilde{w}$ coincides with $w^{kl}[\hat{\tau}](x,\cdot)$. Since the subsequence was arbitrary and the limit function is unique, we get the convergence of the whole sequence

$$w^{kl}[\tau_n](x,\cdot) \rightharpoonup w^{kl}[\hat{\tau}](x,\cdot) \quad \text{weakly in } \; [H^1_{\mathrm{per},0}(Y)]^3$$

for a.e. $x \in \Omega$. □

With this theorem, we can easily show that there exists at least one solution of the inverse problem (14).

Theorem 8. *There exists at least one solution of the minimization problem (14).*

Proof. The operator $\mathcal{Z}(\tau) = \mathcal{T} \circ \mathcal{H}_{f,g}(\tau)$ is continuous, since the trace operator $\mathcal{T}$ and $\mathcal{H}_{f,g}$ are continuous (see Theorem 6). The set I_κ is compact, so we can apply the extreme value theorem to guarantee that there exists at least one $\hat{\tau} \in I_\kappa$, which minimizes (14). □

We even get the compactness of the solution space.

Lemma 5. *The solution space of the homogenized problem (10)*

$$\mathbb{L}_{f,g} := \left\{ u \in H^1_{\Gamma_{\mathrm{D}}}(\Omega) \,:\, u \text{ solution of (10) for some } \tau \in I_\kappa \right\}$$

for fixed (f,g) is compact.

Proof. Consider a sequence of solutions $(u_n)_n \subset \mathbb{L}_{f,g}$. Then, there exists $\tau_n \in I_\kappa$ such that $u_n = u[\tau_n]$. Since I_κ is a compact set, there exists a subsequence of $(\tau_n)_n$ (again denoted by n) such that τ_n converges to some $\hat{\tau} \in I_\kappa$. Since $\mathcal{H}_{f,g}$ is continuous (see Theorem 6), we receive the convergence of u_n to $u[\hat{\tau}]$ in $H^1_{\Gamma_D}(\Omega)$. □

In the rest of the section, we want to derive the Gâteaux derivative of $\mathcal{J}$ to facilitate the use of gradient-based optimization algorithms. As we will see later, we need the Gâteaux derivative of A^{hom} for this, which we will compute in the following section.

3.2 | Gâteaux derivative of A^{hom}

To compute the Gâteaux derivative of A^{hom}, we apply the concept of shape derivatives. More precisely, we use the Lagrangian method of Céa following the idea of Allaire et al.[4] For this, we define for all $x \in \Omega$ a Lagrangian function $\mathfrak{L}^x_{ijkl}$ which coincides with

$$\mathfrak{J}^x_{ijkl}(Y_0) := \int_Y B[Y_0](x,y)e_{ij}(e_{kl} - e(w_{kl})(x,y))\,\mathrm{d}y$$

in some special points, where $B[Y_0](x,y) := A^0(x)\chi_{Y_0}(y) + A^1(x)(1-\chi_{Y_0}(y))$ with $A^0, A^1 \in M(\alpha,\beta,\Omega)$ and $w_{kl} \in [L^\infty(\Omega, H^1_{\text{per}}(Y))]^3$ is the weak solution of

$$\begin{cases} -\operatorname{div}_y(B[Y_0](x,\cdot)(e_y(w_{kl}) - e_{kl})) = 0 \text{ in } Y, \\ \mathcal{M}_Y(w_{kl}) = 0. \end{cases} \tag{16}$$

The main advantage is that the computation of the shape derivative of $\mathfrak{L}^x_{ijkl}$ is much easier than of $\mathfrak{J}^x_{ijkl}$ since we can apply standard shape derivative results. We cannot apply these directly to $\mathfrak{J}^x_{ijkl}$ because the solutions of the cell problems also depend on Y_0. For readability, we omit the index y in the divergence $\operatorname{div}_y(\cdot)$ and in the symmetric gradient $e_y(\cdot)$ because all the computations in this section are for some fixed $x \in \Omega$. Since some spatial derivatives of w_{kl} may be discontinuous at the interface Σ_Y, we write the cell problem as a transmission problem: For a.e. $x \in \Omega$ find $(w^{x,1}_{kl}, w^{x,0}_{kl}) \in V := \{(u^1,u^0) \in [H^1(Y_1)]^3 \times [H^1(Y_0)]^3 : u^1 \text{ is Y-periodic}, \mathcal{M}_Y(u^1\chi_{Y_1} + u^0\chi_{Y_0}) = 0\}$ such that

$$\begin{cases} -\operatorname{div}(A^1_x(e(w^{x,1}_{kl}) - e_{kl})) = 0 \text{ in } Y_1, \\ w^{x,1}_{kl} = w^{x,0}_{kl} \text{ on } \Sigma_Y, \\ A^1_x(e(w^{x,1}_{kl}) - e_{kl}))n^1 + A^0_x(e(w^{x,0}_{kl}) - e_{kl}))n^0 = 0 \text{ on } \Sigma_Y \end{cases} \tag{17}$$

and

$$\begin{cases} -\operatorname{div}(A^0_x(e(w^{x,0}_{kl}) - e_{kl})) = 0 \text{ in } Y_0, \\ w^{x,0}_{kl} = w^{x,1}_{kl} \text{ on } \Sigma_Y, \\ A^1_x(e(w^{x,1}_{kl}) - e_{kl}))n^1 + A^0_x(e(w^{x,0}_{kl}) - e_{kl}))n^0 = 0 \text{ on } \Sigma_Y, \end{cases} \tag{18}$$

where $A^1_x := A^1(x)$, $A^0_x := A^0(x)$ and $n = n^0 = -n^1$ is the outward unit normal vector of the interface Σ_Y with direction from Y_0 to Y_1. It can be easily shown that the transmission problem is equivalent to (16). Clearly, the restriction of the solution $w_{kl}(x,\cdot)$ of (16) to Y_0 resp. Y_1 solves the transmission problem, that is, $w_{kl}(x,\cdot) = w^{x,1}_{kl}$ in Y_1 and $w_{kl}(x,\cdot) = w^{x,0}_{kl}$ in Y_0. Now, we define the general Lagrangian, where q^1, q^0 play the role of Lagrange multipliers,

$$\begin{aligned}
\mathfrak{L}^x_{ijkl}(v^0,v^1,q^0,q^1,Y_0) := &-\int_{Y_0} A^0_x(e(q^0)+e_{ij})(e(v^0)-e_{kl})\,\mathrm{d}y - \int_{Y_1} A^1_x(e(q^1)+e_{ij})(e(v^1)-e_{kl})\,\mathrm{d}y \\
&- \frac{1}{2}\int_{\Sigma_Y} (A^1_x(e(v^1)-e_{kl}) + A^0_x(e(v^0)-e_{kl}))n\cdot(q^1-q^0)\,\mathrm{d}S(y) \\
&- \frac{1}{2}\int_{\Sigma_Y} (A^1_x(e(q^1)+e_{ij}) + A^0_x(e(q^0)+e_{ij}))n\cdot(v^1-v^0)\,\mathrm{d}S(y)
\end{aligned}$$

for $v^0, v^1, q^0, q^1 \in [H^1_{\text{per},0}(Y)]^3$. In the next two lemmas, we compute some conditions for optimal points.

Lemma 6. *The solution* (u^1, u^0) *of the transmission problem satisfies the optimality condition*

$$0 = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial q^1}(u^0, u^1, p^0, p^1, Y_0)(\phi) = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial q^0}(u^0, u^1, p^0, p^1, Y_0)(\phi) \tag{19}$$

for all $\phi \in [H^1_{per,0}(Y)]^3$. *Therefore, the solution* $w^x_{kl} := w_{kl}(x, \cdot)$ *of (16) fulfills the condition*

$$0 = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial q^1}(w^x_{kl}, w^x_{kl}, p^0, p^1, Y_0)(\phi) = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial q^0}(w^x_{kl}, w^x_{kl}, p^0, p^1, Y_0)(\phi)$$

for all $\phi \in [H^1_{per,0}(Y)]^3$ *in particular.*

Proof. Let $\phi \in [H^1_{\mathrm{per},0}(Y)]^3$. We compute the directional derivatives by using integration by parts

$$\frac{\partial \mathfrak{L}^x_{ijkl}}{\partial q^\alpha}(v^0, v^1, q^0, q^1, Y_0)(\phi) = \int_{Y_\alpha} \operatorname{div}(A^\alpha_x(e(v^\alpha) - e_{kl}))\phi \, \mathrm{d}y + \frac{1}{2}\int_{\Sigma_Y} (A^1_x(e(v^1) - e_{kl}) - A^0_x(e(v^0) - e_{kl}))n \cdot \phi \, \mathrm{d}S(y)$$
$$- \frac{1}{2}\int_{\Sigma_Y} A^\alpha_x e(\phi)n \cdot (v^1 - v^0) \, \mathrm{d}S(y)$$

for $\alpha = 0, 1$. So (19) and the second statement of the lemma follow directly. □

We define the adjoint transmission problem:
Find $(p^1, p^0) \in V := \{(u^1, u^0) \in [H^1(Y_1)]^3 \times [H^1(Y_0)]^3 : u^1 \text{ is } Y\text{-periodic}, \mathcal{M}_Y(u^1\chi_{Y_1} + u^0\chi_{Y_0}) = 0\}$ such that

$$\begin{cases} -\operatorname{div}(A^\alpha_x(e(p^\alpha) + e_{ij})) = 0 & \text{in } Y_\alpha, \\ p^1 = p^0 & \text{on } \Sigma_Y, \\ A^1_x(e(p^1) + e_{ij}))n^1 + A^0_x(e(p^0) + e_{ij}))n^0 = 0 & \text{on } \Sigma_Y \end{cases} \tag{20}$$

for $\alpha = 0, 1$, which is equivalent to

$$\begin{cases} -\operatorname{div}(B[Y_0](x, \cdot)(e(p) + e_{ij})) = 0 & \text{in } Y, \\ \mathcal{M}_Y(p) = 0. \end{cases} \tag{21}$$

The equivalence can be proven as before.

Lemma 7. *The solution* (p^0, p^1) *of the adjoint transmission problem satisfies the optimality condition*

$$0 = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial v^1}(u^0, u^1, p^0, p^1, Y_0)(\phi) = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial v^0}(u^0, u^1, p^0, p^1, Y_0)(\phi)$$

for all $\phi \in [H^1_{per,0}(Y)]^3$. *In particular, the function* $-w^x_{ij} := -w_{ij}(x, \cdot)$, *where* w_{ij} *is the solution of (16) for* $k = i, l = j$, *is a solution of (21), and thus fulfills the condition*

$$0 = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial v^1}(u^0, u^1, -w^x_{ij}, -w^x_{ij}, Y_0)(\phi) = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial v^0}(u^0, u^1, -w^x_{ij}, -w^x_{ij}, Y_0)(\phi)$$

for all $\phi \in [H^1_{per,0}(Y)]^3$.

Proof. The proof is similar to the proof of the last lemma. □

In order to proceed, we introduce the shape derivative. The following definitions and propositions and further details can be found in Michailidis.[3]

Definition 5. Let Ω_0 be a reference domain, $\Omega = \{x + \theta(x) : x \in \Omega_0\} =: (Id + \theta)(\Omega_0)$ for some vector field $\theta : \mathbb{R}^3 \to \mathbb{R}^3$. A functional $\mathcal{F} : \Omega \to \mathbb{R}$ is said to be shape differentiable at Ω_0 if the application $\theta \mapsto \mathcal{F}((Id + \theta)(\Omega_0))$ is Fréchet differentiable at 0 in the Banach space $[W^{1,\infty}(\mathbb{R}^3)]^3$. Then, the following asymptotic expansion holds in the vicinity of 0:

$$\mathcal{F}((Id + \theta)(\Omega)) = \mathcal{F}(\Omega) + \mathcal{F}'(\Omega)(\theta) + o(\theta) \quad \text{with} \quad \lim_{\theta \to 0} \frac{|o(\theta)|}{\|\theta\|} = 0,$$

where $\mathcal{F}'(\Omega)$ is a continuous linear form on $[W^{1,\infty}(\mathbb{R}^3)]^3$.

As in the standard differentiation of functions, we can define directional derivatives.

Definition 6. The directional derivative of a functional $\mathcal{F} : \Omega \to \mathbb{R}$ at Ω in the direction $\theta \in [W^{1,\infty}(\mathbb{R}^3)]^3$ (if it exists) is defined by

$$\mathcal{F}'(\Omega)(\theta) = \lim_{\delta \to 0} \frac{\mathcal{F}((Id + \delta\theta)\Omega) - \mathcal{F}(\Omega)}{\delta}.$$

The following two propositions give the shape derivative for functionals, where the integrand does not depend on the domain.

Proposition 1. *Let $\Omega_0 \subset \mathbb{R}^3$ a smooth bounded open set. If $f \in W^{1,1}(\mathbb{R}^3)$ and $\mathcal{F} : \mathbb{C}(\Omega_0) \to \mathbb{R}$ is defined by $\mathcal{F}(\Omega) = \int_\Omega f(x)\,\mathrm{d}x$, where $\mathbb{C}(\Omega_0) := \{\Omega = (Id + \theta)(\Omega_0)$ with $\theta \in [W^{1,\infty}(\mathbb{R}^3)]^3\}$, then $\mathcal{F}$ is differentiable at Ω_0 and*

$$\mathcal{F}'(\Omega_0)(\theta) = \int_{\Omega_0} \operatorname{div}\,(\theta(x) f(x))\,\mathrm{d}x = \int_{\partial\Omega_0} \theta(x) \cdot n(x) f(x)\,\mathrm{d}S(x)$$

for all $\theta \in [W^{1,\infty}(\mathbb{R}^3)]^3$.

The proposition still holds if Ω_0 is regular enough to apply the transformation formula and Gauß's theorem.

Proposition 2. *Let $\Omega_0 \subset \mathbb{R}^3$ be a smooth bounded open set. If $f \in W^{2,1}(\mathbb{R}^3)$ and $\mathcal{F} : \mathbb{C}(\Omega_0) \to \mathbb{R}$ is defined by $\mathcal{F}(\Omega) = \int_{\partial\Omega} f(x)\,\mathrm{d}S(x)$, where $\mathbb{C}(\Omega_0) := \{\Omega = (Id + \theta)(\Omega_0)$ with $\theta \in [W^{1,\infty}(\mathbb{R}^3)]^3\}$, then $\mathcal{F}$ is differentiable at Ω_0 and for all $\theta \in [W^{1,\infty}(\mathbb{R}^3)]^3$*

$$\mathcal{F}'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \nabla f \cdot \theta + f(\operatorname{div}\,\theta - \nabla\theta n \cdot n)\,\mathrm{d}S(x) = \int_{\partial\Omega_0} \left(\frac{\partial f}{\partial n} + Hf\right) \theta \cdot n\,\mathrm{d}S(x),$$

where $H = \operatorname{div}\, n$ is the mean curvature of $\partial\Omega_0$.

The weak solution w_{kl} of the cell problem (16) is not shape differentiable. However, the next lemma shows that the restricted functions $w_{kl}^{x,0}$ and $w_{kl}^{x,1}$ are shape differentiable.

Lemma 8. *The solutions $w_{kl}^{x,1}$ of (17) and $w_{kl}^{x,0}$ of (18) are shape differentiable for a.e. $x \in \Omega$ and $\theta \in [W_0^{1,\infty}(Y)]^3$.*

Proof. The lemma can be shown as in the proof of Theorem 5.3.2.[17] The main idea is to consider the cell problem (16) on the transformed domain $Y_\theta := (Id + \theta)(Y)$ for some $\theta \in [W_0^{1,\infty}(Y)]^3$. By the change of variable theorem, the weak formulation can be rewritten as an integral over the reference cell Y. Since the integrand thus obtained is of class C^1 with respect to θ and $v \in [H^1_{\mathrm{per},0}(Y)]^3$, we can apply the implicit function theorem to get the desired result. □

In the next lemma, we prove that the Lagrangian $\mathfrak{L}^x_{ijkl}$ is equal to the functional $\mathfrak{J}^x_{ijkl}(Y_0)$ in the optimal point $(w_{kl}^{x,0}, w_{kl}^{x,1}, -w_{ij}^{x,0}, -w_{ij}^{x,1}, Y_0)$, whereby we write $w_{kl}^{x,h}, h = 0, 1$, instead of w_{kl}^x to emphasize which problem w_{kl}^x solves and that only the values in Y_h are relevant for calculation of $\mathfrak{L}^x_{ijkl}$. With this result, we can compute the shape derivative of $\mathfrak{L}^x_{ijkl}$ instead of $\mathfrak{J}^x_{ijkl}(Y_0)$, which is much easier.

Lemma 9. *The shape derivative of the objective function $\mathfrak{J}^x_{ijkl}(Y_0)$ exists and is given by*

$$(\mathfrak{J}^x_{ijkl})'(Y_0)(\theta) = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial Y_0}(w_{kl}^{x,0}, w_{kl}^{x,1}, -w_{ij}^{x,0}, -w_{ij}^{x,1}, Y_0)(\theta),$$

for all $\theta \in [W_0^{1,\infty}(Y)]^3$.

Proof. The following identity holds

$$\mathfrak{L}^x_{ijkl}(w^{x,0}_{kl}, w^{x,1}_{kl}, q^0, q^1, Y_0) = \mathfrak{J}^x_{ijkl}(Y_0) - \int_{Y_0} A^0_x(e(w^{x,0}_{kl}) - e_{kl})e(q^0)\,\mathrm{d}y - \int_{Y_1} A^1_x(e(w^{x,1}_{kl}) - e_{kl})e(q^1)\,\mathrm{d}y$$
$$+ \int_{\Sigma_Y} (A^1_x(e(w^{x,1}_{kl}) - e_{kl})n^1 \cdot q^1 + A^0_x(e(w^{x,0}_{kl}) - e_{kl}))n^0 \cdot q^0\,\mathrm{d}S(y) = \mathfrak{J}^x_{ijkl}(Y_0),$$

using the solution properties of $w^{x,1}_{kl}$ and $w^{x,0}_{kl}$. Differentiating this identity with respect to the shape yields

$$(\mathfrak{J}^x_{ijkl})'(Y_0)(\theta) = \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial Y_0}(w^{x,0}_{kl}, w^{x,1}_{kl}, q^0, q^1, Y_0)(\theta) + \sum_{\alpha=0}^{1} \frac{\partial \mathfrak{L}^x_{ijkl}}{\partial v^\alpha}(w^{x,0}_{kl}, w^{x,1}_{kl}, q^0, q^1, Y_0)\frac{\partial w^{x,\alpha}_{kl}}{\partial Y_0}(\theta).$$

In the special case where $q^0 = -w^{x,0}_{ij}$ and $q^1 = -w^{x,1}_{ij}$ the last two terms disappear, which proves the lemma. □

Since v^0, v^1, q^0, q^0 do not depend on the structure of Y_0, we can apply the standard results of Propositions 1 and 2 to compute the shape derivative of the Lagrangian $\mathfrak{L}^x_{ijkl}$:

$$\begin{aligned}
&\frac{\partial \mathfrak{L}^x_{ijkl}}{\partial Y_0}(w^{x,0}_{kl}, w^{x,1}_{kl}, -w^{x,0}_{ij}, -w^{x,1}_{ij}, Y_0)(\theta)\\
&= \int_{\Sigma_Y} A^0_x e_{ij}(e_{kl} - e(w^{x,0}_{kl}))\theta \cdot n^0\,\mathrm{d}S(y) + \int_{\Sigma_Y} A^1_x e_{ij}(e_{kl} - e(w^{x,1}_{kl}))\theta \cdot n^1\,\mathrm{d}S(y)\\
&- \int_{\Sigma_Y} A^0_x(e(w^{x,0}_{kl}) - e_{kl})e(-w^{x,0}_{ij})\theta \cdot n^0\,\mathrm{d}S(y) - \int_{\Sigma_Y} A^1_x(e(w^{x,1}_{kl}) - e_{kl})e(-w^{x,1}_{ij})\theta \cdot n^1\,\mathrm{d}S(y)\\
&- \frac{1}{2}\int_{\Sigma_Y} \left(\frac{\partial}{\partial n} + H\right)\left[(A^1_x(e(w^{x,1}_{kl}) - e_{kl}) + A^0_x(e(w^{x,0}_{kl}) - e_{kl}))n \cdot (-w^{x,1}_{ij} + w^{x,0}_{ij})\right]\theta \cdot n^0\,\mathrm{d}S(y)\\
&- \frac{1}{2}\int_{\Sigma_Y} \left(\frac{\partial}{\partial n} + H\right)\left[(A^1_x(e(-w^{x,1}_{ij}) + e_{ij}) + A^0_x(e(-w^{x,0}_{ij}) + e_{ij}))n \cdot (w^{x,1}_{kl} - w^{x,0}_{kl})\right]\theta \cdot n^0\,\mathrm{d}S(y),
\end{aligned}$$

where H is the mean curvature. The terms involving H vanish on Σ_Y, since $w^{x,1}_{kl} = w^{x,0}_{kl}$ and $w^{x,1}_{ij} = w^{x,0}_{ij}$ on Σ_Y. The same argument and the fact that $A^1_x(e(w^{x,1}_{kl}) - e_{kl})n = A^0_x(e(w^{x,0}_{kl}) - e_{kl})n$ on Σ_Y leads to

$$\begin{aligned}
&\frac{\partial \mathfrak{L}^x_{ijkl}}{\partial Y_0}(w^{x,0}_{kl}, w^{x,1}_{kl}, -w^{x,0}_{ij}, -w^{x,1}_{ij}, Y_0)(\theta)\\
&= \int_{\Sigma_Y} A^0_x(e(w^{x,0}_{kl}) - e_{kl})(e(w^{x,0}_{ij}) - e_{ij})\theta \cdot n\,\mathrm{d}S(y) - \int_{\Sigma_Y} A^1_x(e(w^{x,1}_{kl}) - e_{kl})(e(w^{x,1}_{ij}) - e_{ij})\theta \cdot n\,\mathrm{d}S(y)\\
&+ \int_{\Sigma_Y} A_x(e(w^x_{kl}) - e_{kl})n \cdot \frac{\partial(w^{x,1}_{ij} - w^{x,0}_{ij})}{\partial n}\theta \cdot n\,\mathrm{d}S(y) + \int_{\Sigma_Y} A_x(e(w^x_{ij}) - e_{ij})n \cdot \frac{\partial(w^{x,1}_{kl} - w^{x,0}_{kl})}{\partial n}\theta \cdot n\,\mathrm{d}S(y),
\end{aligned} \tag{22}$$

where we denote by $A_x(e(w^x_{kl}) - e_{kl})n$ and $A_x(e(w^x_{ij}) - e_{ij})n$ the continuous quantities through the interface.

This general formula can be simplified under additional assumptions on the materials. In what follows, we consider isotropic materials, that is, the material tensors are of the form

$$A^\alpha_x = 2\mu^\alpha_x I_4 + \lambda^\alpha_x I_2 \otimes I_2,$$

where $\alpha = 0, 1$, $\lambda^\alpha \in L^\infty(\Omega)$ and $\mu^\alpha \in L^\infty(\Omega)$ are the Lamé parameters depending on the macrovariable and I_2 and I_4 are the identity tensors of second and fourth orders. At each point of Σ_Y, we define the unit normal vector n and both unit tangential vectors as a collection t such that (t, n) is a local orthonormal basis. A 3×3 matrix in local basis can be written as follows:

$$m = \begin{pmatrix} m_{tt} & m_{tn} \\ m_{nt} & m_{nn} \end{pmatrix} \text{ with } m_{tt} \in \mathbb{R}^{2\times 2}, m_{tn} \in \mathbb{R}^2, m_{nn} \in \mathbb{R}$$

Lemma 10. *The components $A_x(e(w^x_{kl}) - e_{kl})n$ and $e(w^x_{kl})_{tt}$ are continuous across the interface Σ_Y. All other components have jumps on the interface given by*

(i) $[(e(w^x_{kl}) - e_{kl})_{nn}] = \left[\frac{1}{2\mu_x+\lambda_x}\right] (A_x(e(w^x_{kl}) - e_{kl}))_{nn} - \left[\frac{\lambda_x}{2\mu_x+\lambda_x}\right] tr(e(w^x_{kl}) - e_{kl})_{tt}$,

(ii) $[(e(w^x_{kl}) - e_{kl})_{tn}] = \left[\frac{1}{2\mu_x}\right] (A_x(e(w^x_{kl}) - e_{kl}))_{tn}$,

(iii) $[(A_x(e(w^x_{kl}) - e_{kl}))_{tt}] = [2\mu_x](e(w^x_{kl}) - e_{kl})_{tt} + \left(\left[\frac{2\mu_x\lambda_x}{2\mu_x+\lambda_x}\right] tr(e(w^x_{kl}) - e_{kl})_{tt} + \left[\frac{\lambda_x}{2\mu_x+\lambda_x}\right] (A_x(e(w^x_{kl}) - e_{kl}))_{nn}\right) I_2$,

where the square brackets denote the jump on the interface, that is, $[f] = f^1 - f^0$.

Proof. The statements follow by direct calculation using

$$I_4 = (\delta_{il}\delta_{jk})_{1\le i,j,k,l\le 3} \quad \text{and} \quad I_2 \otimes I_2 = (\delta_{ij}\delta_{kl})_{1\le i,j,k,l\le 3}$$

and the similarity invariance of the trace. □

With this lemma, we can compute

$$\begin{aligned}
&A^1_x(e(w^{x,1}_{kl}) - e_{kl})(e(w^{x,1}_{ij}) - e_{ij}) \\
&= (A^1_x(e(w^{x,1}_{kl}) - e_{kl}))_{tt}(e(w^{x,1}_{ij}) - e_{ij})_{tt} + 2(A^1_x(e(w^{x,1}_{kl}) - e_{kl}))_{tn}(e(w^{x,1}_{ij}) - e_{ij})_{tn} + (A^1_x(e(w^{x,1}_{kl}) - e_{kl}))_{nn}(e(w^{x,1}_{ij}) - e_{ij})_{nn} \\
&= 2\mu^1_x(e(w^{x,1}_{kl}) - e_{kl})_{tt}(e(w^{x,1}_{ij}) - e_{ij})_{tt} + \frac{2\mu^1_x\lambda^1_x}{2\mu^1_x + \lambda^1_x}\mathrm{tr}(e(w^{x,1}_{kl}) - e_{kl})_{tt}\mathrm{tr}(e(w^{x,1}_{ij}) - e_{ij})_{tt} \\
&\quad + \frac{1}{\mu^1_x}(A^1_x(e(w^{x,1}_{kl}) - e_{kl}))_{tn}(A^1_x(e(w^{x,1}_{ij}) - e_{ij}))_{tn} + \frac{1}{2\mu^1_x + \lambda^1_x}(A^1_x(e(w^{x,1}_{kl}) - e_{kl}))_{nn}(A^1_x(e(w^{x,1}_{ij}) - e_{ij}))_{nn}.
\end{aligned}$$

Thus,

$$\begin{aligned}
&A^1_x(e(w^{x,1}_{kl}) - e_{kl})(e(w^{x,1}_{ij}) - e_{ij}) - A^0_x(e(w^{x,0}_{kl}) - e_{kl})(e(w^{x,0}_{ij}) - e_{ij}) \\
&= [2\mu_x](e(w^x_{kl}) - e_{kl})_{tt}(e(w^x_{ij}) - e_{ij})_{tt} + \left[\frac{2\mu_x\lambda_x}{2\mu_x + \lambda_x}\right] \mathrm{tr}(e(w^x_{kl}) - e_{kl})_{tt}\mathrm{tr}(e(w^x_{ij}) - e_{ij})_{tt} \\
&\quad + \left[\frac{1}{\mu_x}\right] (A_x(e(w^x_{kl}) - e_{kl}))_{tn}(A_x(e(w^x_{ij}) - e_{ij}))_{tn} + \left[\frac{1}{2\mu_x + \lambda_x}\right] (A_x(e(w^x_{kl}) - e_{kl}))_{nn}(A_x(e(w^x_{ij}) - e_{ij}))_{nn},
\end{aligned}$$

which is an expression of only continuous functions at the interface.

Lemma 11. *For two displacements w^x_{kl} and q, there holds: if $q = 0$ on Σ_Y, then*

$$A_x(e(w^x_{kl}) - e_{kl})n \cdot \frac{\partial q}{\partial n} = 2(A_x(e(w^x_{kl}) - e_{kl})n) \cdot (e(q)n) - (A_x(e(w^x_{kl}) - e_{kl}))_{nn}e(q)_{nn}$$

on Σ_Y.

Proof. Since $q = 0$ on Σ_Y, there holds $\nabla q\, t = 0$ for all tangential vectors t. Thus, if (t_1, t_2, n) is an orthonormal basis,

$$(A_x(e(w^x_{kl}) - e_{kl}))_{nn}e(q)_{nn} = n^T(A_x(e(w^x_{kl}) - e_{kl}))(nn^T + t_1t_1^T + t_2t_2^T)(\nabla q)^T n = (A_x(e(w^x_{kl}) - e_{kl}))n \cdot (\nabla q)^T n,$$

where we have used the fact that $nn^T + t_1t_1^T + t_2t_2^T = (t_1, t_2, n)(t_1, t_2, n)^T = I_3$. The rest of the proof follows by rewritting the right-hand side of the equation. □

We apply this lemma to our problem

$$\begin{aligned}
&A_x(e(w^x_{kl}) - e_{kl})n \cdot \frac{\partial(w^{x,1}_{ij} - w^{x,0}_{ij})}{\partial n} \\
&= 2A_x(e(w^x_{kl}) - e_{kl})n \cdot (e(w^{x,1}_{ij}) - e(w^{x,0}_{ij}))n - (A_x(e(w^x_{kl}) - e_{kl}))_{nn}(e(w^{x,1}_{ij}) - e(w^{x,0}_{ij}))_{nn} \\
&= \left[\frac{1}{2\mu_x + \lambda_x}\right](A_x(e(w^x_{kl}) - e_{kl}))_{nn}(A_x(e(w^x_{ij}) - e_{ij}))_{nn} - \left[\frac{\lambda_x}{2\mu_x + \lambda_x}\right](A_x(e(w^x_{kl}) - e_{kl}))_{nn}\mathrm{tr}(e(w^x_{ij}) - e_{ij})_{tt} \\
&\quad + \left[\frac{1}{\mu_x}\right](A_x(e(w^x_{kl}) - e_{kl}))_{tn}(A_x(e(w^x_{ij}) - e_{ij}))_{tn}.
\end{aligned}$$

Summing up all the results, we obtain the shape derivative of $\mathfrak{L}^x_{ijkl}$.

Theorem 9. *The shape derivative of the Lagrangian $\mathfrak{L}^x_{ijkl}(Y_0)$ is of the form*

$$\begin{aligned}
&\frac{\partial \mathfrak{L}^x_{ijkl}}{\partial Y_0}(w^{x,0}_{kl}, w^{x,1}_{kl}, -w^{x,0}_{ij}, -w^{x,1}_{ij}, Y_0)(\theta) \\
&= \int_{\Sigma_Y} \Bigg(-[2\mu_x](e(w^x_{kl}) - e_{kl})_{tt}(e(w^x_{ij}) - e_{ij})_{tt} - \left[\frac{2\mu_x\lambda_x}{2\mu_x + \lambda_x}\right] tr(e(w^x_{kl}) - e_{kl})_{tt} tr(e(w^x_{ij}) - e_{ij})_{tt} \\
&\quad + \left[\frac{1}{\mu_x}\right](A_x(e(w^x_{kl}) - e_{kl}))_{tn}(A_x(e(w^x_{ij}) - e_{ij}))_{tn} + \left[\frac{1}{2\mu_x + \lambda_x}\right](A_x(e(w^x_{kl}) - e_{kl}))_{nn}(A_x(e(w^x_{ij}) - e_{ij}))_{nn} \\
&\quad - \left[\frac{\lambda_x}{2\mu_x + \lambda_x}\right](A_x(e(w^x_{kl}) - e_{kl}))_{nn} tr(e(w^x_{ij}) - e_{ij})_{tt} - \left[\frac{\lambda_x}{2\mu_x + \lambda_x}\right](A_x(e(w^x_{ij}) - e_{ij}))_{nn} tr(e(w^x_{kl}) - e_{kl})_{tt}\Bigg)\, \theta \cdot n\, \mathrm{d}S(y).
\end{aligned}$$

for all $\theta \in [W^{1,\infty}_0(Y)]^3$.

The idea now is to define functions Θ_α, which satisfy

$$Y_0[\tau_1 + \delta\tau_1, \tau_2 + \delta\tau_2, \tau_3 + \delta\tau_3] = (Id + \delta\tau_1\Theta_1 + \delta\tau_2\Theta_2 + \delta\tau_3\Theta_3)(Y_0[\tau])$$

and

$$Y_1[\tau_1 + \delta\tau_1, \tau_2 + \delta\tau_2, \tau_3 + \delta\tau_3] = (Id + \delta\tau_1\Theta_1 + \delta\tau_2\Theta_2 + \delta\tau_3\Theta_3)(Y_1[\tau])$$

with small increment $(\delta\tau_1, \delta\tau_2, \delta\tau_3)$. Then, using Lemma 9, we receive

$$\frac{\partial A^{\text{hom}}_{ijkl}}{\partial \tau_\alpha}[\tau](x) = \frac{1}{|Y|}(\mathfrak{J}^x_{ijkl})'(\Theta_\alpha) = \frac{1}{|Y|}\frac{\partial \mathfrak{L}^x_{ijkl}}{\partial Y_0}(\Theta_\alpha), \tag{23}$$

where the last term can be easily computed in the isotropic case by Theorem 9. Moreover, in the case of ellipsoids, we can give explicit expressions for $\Theta_\alpha \in [W^{1,\infty}_0(Y)]^3$, $\alpha = 1, 2, 3$

$$\Theta_1(y) = \begin{cases} a^{(l_1,l_2,l_3)}_{(\tau_1,\tau_2,\tau_3)}(y_2, y_3)\sin\left(\frac{2\pi}{l_1}y_1\right)e_1 & \text{, if } \frac{1}{\tau_2^2}\left(y_2 - \frac{l_2}{2}\right)^2 + \frac{1}{\tau_3^2}\left(y_3 - \frac{l_3}{2}\right)^2 < \frac{1}{4} \\ -\frac{l_1}{2\pi\tau_1}\sin\left(\frac{2\pi}{l_1}y_1\right)e_1 & \text{, if} \frac{1}{\tau_2^2}\left(y_2 - \frac{l_2}{2}\right)^2 + \frac{1}{\tau_3^2}\left(y_3 - \frac{l_3}{2}\right)^2 \geq \frac{1}{4} \end{cases} \tag{24}$$

and

$$\Theta_2(y) = \begin{cases} a^{(l_2,l_1,l_3)}_{(\tau_2,\tau_1,\tau_3)}(y_1, y_3)\sin\left(\frac{2\pi}{l_2}y_2\right)e_2 & \text{, if } \frac{1}{\tau_1^2}\left(y_1 - \frac{l_1}{2}\right)^2 + \frac{1}{\tau_3^2}\left(y_3 - \frac{l_3}{2}\right)^2 < \frac{1}{4} \\ -\frac{l_2}{2\pi\tau_2}\sin\left(\frac{2\pi}{l_2}y_2\right)e_2 & \text{, if} \frac{1}{\tau_1^2}\left(y_1 - \frac{l_1}{2}\right)^2 + \frac{1}{\tau_3^2}\left(y_3 - \frac{l_3}{2}\right)^2 \geq \frac{1}{4} \end{cases} \tag{25}$$

and

$$\Theta_3(y) = \begin{cases} a^{(l_3,l_1,l_2)}_{(\tau_3,\tau_1,\tau_2)}(y_1, y_2) \sin\left(\frac{2\pi}{l_3} y_3\right) e_3 & , \text{if } \frac{1}{\tau_1^2}\left(y_1 - \frac{l_1}{2}\right)^2 + \frac{1}{\tau_2^2}\left(y_2 - \frac{l_2}{2}\right)^2 < \frac{1}{4} \\ -\frac{l_3}{2\pi\tau_3} \sin\left(\frac{2\pi}{l_3} y_3\right) e_3 & , \text{if} \frac{1}{\tau_1^2}\left(y_1 - \frac{l_1}{2}\right)^2 + \frac{1}{\tau_2^2}\left(y_2 - \frac{l_2}{2}\right)^2 \geq \frac{1}{4} \end{cases}, \tag{26}$$

where

$$a^{(l_1,l_2,l_3)}_{(\tau_1,\tau_2,\tau_3)}(\hat{y}_2, \hat{y}_3) = -\frac{\sqrt{\frac{1}{4} - \frac{1}{\tau_2^2}\left(\hat{y}_2 - \frac{l_2}{2}\right)^2 - \frac{1}{\tau_3^2}\left(\hat{y}_3 - \frac{l_3}{2}\right)^2}}{\sin\left(\frac{2\pi}{l_1}\tau_1\sqrt{\frac{1}{4} - \frac{1}{\tau_2^2}\left(\hat{y}_2 - \frac{l_2}{2}\right)^2 - \frac{1}{\tau_3^2}\left(\hat{y}_3 - \frac{l_3}{2}\right)^2}\right)}.$$

3.3 | Gâteaux derivative of $\mathcal{J}$

In this section, we want to compute the Gâteaux derivative of (14), namely, of

$$\mathcal{J}(\tau) = \frac{1}{2}\int_{\partial\Omega} |\mathcal{L}_\tau(f, g) - u_m|^2 \, \mathrm{d}S(x).$$

We know that $u[\tau]$ is the weak solution of

$$\int_\Omega A^{\mathrm{hom}}[\tau] e(u[\tau]) e(v) \, \mathrm{d}x = \int_\Omega f \cdot v \, \mathrm{d}x + \int_{\Gamma_\mathrm{N}} g \cdot v \, \mathrm{d}S(x)$$

and $u[\tau + \varepsilon\tilde{\tau}]$ of

$$\int_\Omega A^{\mathrm{hom}}[\tau + \varepsilon\tilde{\tau}] e(u[\tau + \varepsilon\tilde{\tau}]) e(v) \, \mathrm{d}x = \int_\Omega f \cdot v \, \mathrm{d}x + \int_{\Gamma_\mathrm{N}} g \cdot v \, \mathrm{d}S(x)$$

for all $v \in H^1_{\Gamma_\mathrm{D}}(\Omega)$. Taking the difference of both equations, multiplying by $\frac{1}{\varepsilon}$ and passing to the limit yields

$$0 = \int_\Omega A^{\mathrm{hom}}[\tau] e(\delta u(\tau, \tilde{\tau})) e(v) \, \mathrm{d}x + \int_\Omega \delta A^{\mathrm{hom}}(\tau, \tilde{\tau}) e(u[\tau]) e(v) \, \mathrm{d}x. \tag{27}$$

From the last section, we know that

$$\delta A^{\mathrm{hom}}_{ijkl}(\tau, \tilde{\tau})(x) = \sum_{\alpha=1}^{3} \frac{\partial A^{\mathrm{hom}}_{ijkl}}{\partial \tau_\alpha}[\tau](x)\tilde{\tau}_\alpha.$$

Since $\frac{\partial A^{\mathrm{hom}}_{ijkl}}{\partial \tau_\alpha}[\tau] \in L^\infty(\Omega)$, problem (27) is well-defined. Additionally, $u[\tau] \in H^1_{\Gamma_\mathrm{D}}(\Omega)$ is known, so there exists due to the theorem of Lax–Milgram a unique solution $\delta u(\tau, \tilde{\tau}) \in H^1_{\Gamma_\mathrm{D}}(\Omega)$ of (27). Using the representation of the Gâteaux derivative of A^{hom}, we can rewrite the problem: Find for $\alpha = 1, 2, 3$ the functions $\frac{\partial u}{\partial \tau_\alpha} \in H^1_{\Gamma_\mathrm{D}}(\Omega)$ such that

$$\int_\Omega A^{\mathrm{hom}}[\tau] e\left(\frac{\partial u}{\partial \tau_\alpha}\right) e(v) \, \mathrm{d}x = -\int_\Omega \frac{\partial A^{\mathrm{hom}}}{\partial \tau_\alpha}[\tau] e(u[\tau]) e(v) \, \mathrm{d}x.$$

Then, due to the uniqueness of the solutions,

$$\nabla u[\tau] \cdot \tilde{\tau} := \sum_{\alpha=1}^{3} \frac{\partial u}{\partial \tau_\alpha}\tilde{\tau}_\alpha = \delta u(\tau, \tilde{\tau}).$$

We derive the first variation of $\mathcal{J}$,

$$\delta\mathcal{J}(\tau,\tilde{\tau}) = \lim_{\varepsilon\to 0}\frac{1}{2\varepsilon}\int_{\partial\Omega}|u[\tau+\varepsilon\tilde{\tau}]-u_m|^2 - |u[\tau]-u_m|^2\,\mathrm{d}S(x) = \int_{\partial\Omega}(u[\tau]-u_m)\cdot\delta u(\tau,\tilde{\tau})\,\mathrm{d}S(x).$$

Using the fact that u is Gâteaux differentiable, we can determine the Gâteaux derivative of the objective function

$$\delta\mathcal{J}(\tau,\tilde{\tau}) = \int_{\partial\Omega}(u[\tau]-u_m)\cdot\nabla u[\tau]\,\mathrm{d}S(x)\,\tilde{\tau} =: \nabla\mathcal{J}(\tau)\cdot\tilde{\tau}. \tag{28}$$

4 | SIMULATION RESULTS

We present a typical result of numerical experiments showcasing the functioning of the method. The aim is to derive the length of the axes of the ellipsoids making up the microstructure from measurements of the deformation on the boundary of a beam of 60 mm × 30 mm × 30 mm volume. We assume that the beam is made up of concrete and ellipsoidal polyvinyl chloride (PVC) aggregates arranged periodically on a microscopic scale. Due to the different scales, we nondimensionalize the cell problem, that is, we consider the (nondimensional) reference cell of side lengths $2\times 1\times 1$ with the PVC ellipsoid centered in the middle of the cuboid with axis lengths $(\tau_1,\tau_2,\tau_3)\in[0.12,1.88]\times[0.12,0.88]^2$ and the rest of the cell filled up with concrete. In our model, we assume fixed constraints on one of the small lateral faces of the beam, no volume forces, and some boundary load on part of the surface. Although we know that the PVC is of ellipsoidal structure, we want to find the exact dimension, that is, the (vector-valued) parameter τ. Therefore, we formulate the parameter identification problem

$$\arg\min_{\tau\in I_\kappa}\mathcal{J}(\tau) := \arg\min_{\tau\in I_\kappa}\frac{1}{2|\partial\Omega|^2}\int_{\partial\Omega}|u[\tau]-u_m|^2\,\mathrm{d}S, \tag{29}$$

where $I_\kappa=[0.12,1.88]\times[0.12,0.88]^2$, u_m is the deformation of the beam computed for the target value $\tau^{\text{target}}=(1.5,0.6,0.4)$ and $u[\tau]$ is the deformation for given τ. The scaling with the constant $\frac{1}{|\partial\Omega|^2}$ has no impact on the derived analytical results from the last sections apart from a scaling factor.

Our implementation is based on MATLAB® (version R2020a) and COMSOL LiveLink™ for MATLAB®. The main computation is done with the finite element simulation software COMSOL Multiphysics®,[18] that is, we solve numerically the cell problem (9) and the homogenized problem (10), whereby quadratic serendipity finite elements are used. We take these results to compute the homogenized tensor (8), the target functional (29), and its Gâteaux derivative (28). All these values are needed to apply the gradient method `fmincon` in MATLAB®, which solves the minimization problem (29).

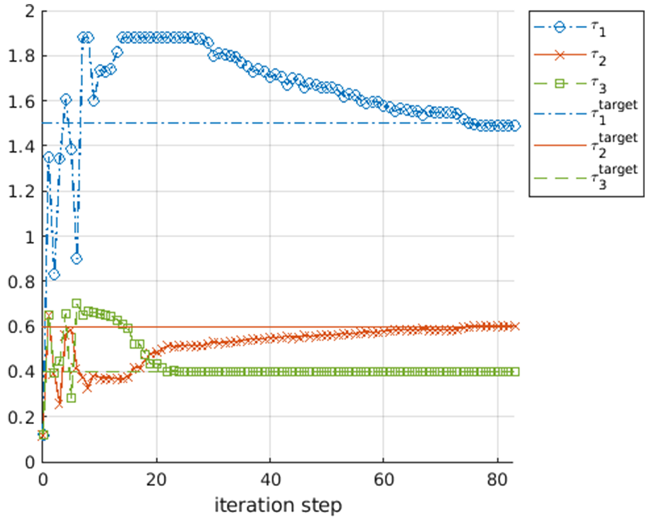

FIGURE 3 Values of τ in each iteration step [Colour figure can be viewed at wileyonlinelibrary.com]

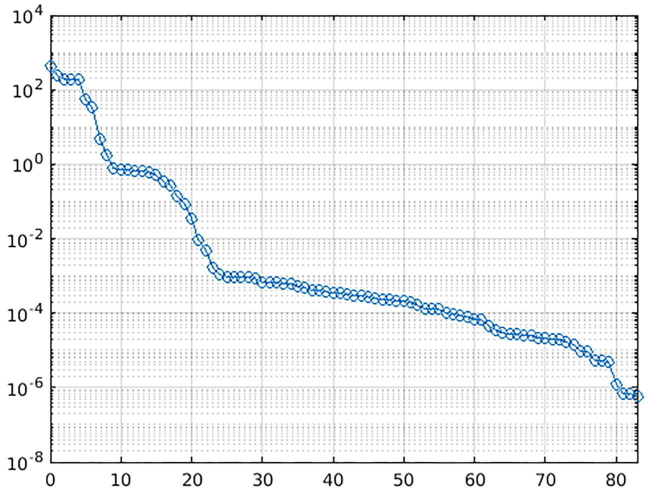

FIGURE 4 Target functional on a logarithmic scale in each iteration step [Colour figure can be viewed at wileyonlinelibrary.com]

We start the iteration with the initial guess $\tau = (0.12, 0.12, 0.12)$, which is a boundary value of I_κ. In Figure 3, the values of τ_1, τ_2, and τ_3 in every iteration step are plotted, whereby the constant function shows the value of τ_1^{target}, τ_2^{target}, and τ_3^{target}. The algorithm terminates after 84 steps when the relative changes in all elements of τ is less than the step tolerance of 10^{-6}. We obtain $\tau = (1.492, 0.602, 0.400)$. The corresponding functional values $\mathcal{J}$ in every iteration step can be seen in Figure 4.

Summing up, the simulation results show that the method works. A proper stability and sensitivity analysis, which is beyond the scope of this work, would be required to quantify this properly.

5 | CONCLUSION AND OUTLOOK

We considered the homogenized problem of linear elasticity, in which the microstructure is accounted for by the effective elasticity tensor, the elements of which are based on solutions of elliptic cell problems in the representative cell. We proved that there exists at least one solution of the corresponding inverse problem identifying the parametrised microstructure from macroscopic boundary measurements. With formula (28) for the Gâteaux derivative of $\mathcal{J}$, wherefore we have to compute the shape derivative of the homogenized tensor and solve several weak partial differential equation problems, we were able to apply generally known numerical gradient-based algorithms to get a solution of the minimization problem when measured data are given. Numerical experiments for an ellipsoidal microstructure illustrated that the length of the axes of the ellipsoids could be recovered from boundary measurements. Although we have only considered isotropic materials with ellipsoidal microstructure at the end, the results can also be applied to the anisotropic materials (using (22) instead of Theorem 9) or to more general microscopic geometries as long as there holds an equation of the form (23) for appropriate θ. In this context, it may as well be of interest to consider more advanced microscopic models, for example, linear elasticity with slip-displacement conditions.[19]

Since we only considered the case in which the microstructure is independent of the macroscopic variable, that is, the effective elasticity tensor is constant, the microstructure needs to be the same everywhere in the domain. For future work, it may be of interest to consider τ as a function of x, that is, the microscopic ellipsoids are of different sizes depending on the macroscopic variable x. While this is a classic generalization of the forward problem, the inverse problem then requires finding a vector-valued function rather than a (constant) vector, which make the optimization problem infinite-dimensional.

ACKNOWLEDGEMENT

There are no funders to report for this submission. Open Access funding enabled and organized by Projekt DEAL.

CONFLICT OF INTEREST

This work does not have any conflicts of interest.

ORCID

Tanja Lochner https://orcid.org/0000-0003-1962-5724
Malte A. Peter https://orcid.org/0000-0001-6107-9806

REFERENCES

1. Orlik J, Panasenko G, Shiryaev V. Optimization of textile-like materials via homogenization and beam approximations. *SIAM Multiscale Model Simul*. 2016;14(2):637-667.
2. Allaire G, Geoffroy-Donders P, Pantz O. Topology optimization of modulated and oriented periodic microstructures by the homogenization method. *Comput Math Appl*. 2019;78(7):2197-2229.
3. Michailidis G. Manufacturing constraints and multi-phase shape and topology optimization via a level-set method. *Theses*: Ecole Polytechnique X; 2014. https://pastel.archives-ouvertes.fr/pastel-00937306
4. Allaire G, Jouve F, Van Goethem N. Damage and fracture evolution in brittle materials by shape optimization methods. *J Comput Phys*. 2011;230(12):5010-5044.
5. Hartmann S, Gilbert RR, Marghzar AK, Leistner C, Dileep PK. Material parameter identification of unidirectional fiber-reinforced composites. *Arch Appl Mech*. 2021;91(2):687-712.
6. Schmidt U, Mergheim J, Steinmann P. Identification of elastoplastic microscopic material parameters within a homogenization scheme. *Int J Numer Methods Eng*. 2015;104(6):391-407.
7. Schmidt U, Steinmann P, Mergheim J. Two-scale elastic parameter identification from noisy macroscopic data. *Arch Appl Mech*. 2016;86(1):303-320.
8. Hintermüller M, Laurain A. Electrical impedance tomography: From topology to shape. *Control Cybern*. 2008;37(4):913-933.
9. Allaire G. *Shape Optimization by the Homogenization Method*. New York: Springer; 2002.
10. Delfour MC, Zolésio J-P. *Shapes and Geometries. Metrics, Analysis, Differential Calculus, and Optimization*. Oxford: Philadelphia, PA: Society for Industrial and Applied Mathematics (SIAM); 2011.
11. Isakov V. *Inverse Problems for Partial Differential Equations*. New York: Springer; 1998.
12. Kirsch A. *An Introduction to the Mathematical Theory of Inverse Problems*. New York: Springer; 2011.
13. Cioranescu D, Donato P. *An Introduction to Homogenization*. Oxford: Oxford Univ. Press; 1999.
14. Cioranescu D, Damlamian A, Griso G. *The Periodic Unfolding Method*. Singapore: Springer; 2018.
15. Jikov VV, Kozlov SM, Oleinik OA. *Homogenization of Differential Operators and Integral Functionals*. Berlin Heidelberg: Springer; 1994.
16. Oleinik OA, Shamaev AS, Yosifian GA. *Mathematical Problems in Elasticity and Homogenization*. Amsterdam, London, New York, Tokyo: North-Holland; 1992.
17. Henrot A, Pierre M. *Variation et Optimisation de Formes*. Berlin Heidelberg: Springer; 2005.
18. COMSOL Multiphysics®. v. 5.6, www.comsol.com. COMSOL AB, Stockholm, Sweden.
19. Lochner T, Peter MA. Homogenization of linearized elasticity in a two-component medium with slip displacement conditions. *J Math Anal Appl*. 2020;483(2):123648.

How to cite this article: Lochner T, Peter MA. Identification of microstructural information from macroscopic boundary measurements in steady-state linear elasticity. *Math Meth Appl Sci*. 2023;46(1):1295-1316. doi:10.1002/mma.8581