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# 1 TOPOLOGICAL SENSITIVITY-BASED ANALYSIS AND 2 OPTIMIZATION OF MICROSTRUCTURED INTERFACES\*

3 MARIE TOUBOUL<sup>†</sup>, RÉMI CORNAGGIA<sup>‡</sup>, AND CÉDRIC BELLIS<sup>§</sup>

4 **Abstract.** This paper concerns the optimization of microstructures when considering the prop-  
5 agation of scalar waves across a periodic row of inclusions embedded within a homogeneous matrix.  
6 The approach relies on the low-frequency homogenized model, which consists, in the present case,  
7 in some effective jump conditions. The topological derivatives of the effective parameters defining  
8 these jump conditions are computed from an asymptotic analysis. Their expressions are validated  
9 numerically and then used to study the sensitivity of the homogenized model to the geometry in  
10 case of elliptic inclusions. Finally, a topological optimization algorithm is used to minimize a given  
11 cost functional. This relies on the expression of the topological derivatives to iteratively perform  
12 phases changes in the unit cell characterizing the material, and on FFT-accelerated solvers previ-  
13 ously adapted to solve the band cell problems underlying the homogenized model. To illustrate  
14 this approach, the resulting procedure is applied to the design of a microstructure that minimizes  
15 transmitted fields along a given direction.

16 **Key words.** topological optimization, asymptotic methods, periodic media, microstructured  
17 interface, effective jump conditions

18 **1. Introduction.** The design of microstructured media allows to control wave  
19 propagation and may lead to exotic effects, e.g. negative refraction, subwavelength  
20 imaging, lensing and cloaking, to cite a few. It constitutes the paradigm of metamater-  
21 ials, which have undergone spectacular developments since the early 2000: see [17]  
22 and references therein for an overview. An active direction of research concerns the  
23 size reduction of microstructures since it is often advantageous to replace a volumic  
24 distribution by a surfacic (in 3D) or a lineic (in 2D) distribution of scatterers, often  
25 called metasurface [8] or meta-interface.

26 The two-scale homogenization method is a privileged tool to approximate wave  
27 propagation in microstructured media [10, 37]. It avoids having to mesh fine spatial  
28 scales and gives an analytical insight on the macroscopic behaviour of waves. How-  
29 ever, the usual homogenization methods fail when considering a thin row of scatterers,  
30 because of boundary effects at the transition between the scatterers and the homoge-  
31 nous medium in which it is embedded. To recover their efficiency, these methods must  
32 then be combined with matched-asymptotic expansions [24], yielding effective jump  
33 conditions on an equivalent meta-interface [19, 26, 18, 25, 36].

34 In the context of metamaterials, the optimization of the microstructures is a use-  
35 ful tool to determine designs that exhibit interesting macroscopic behaviours. To this  
36 purpose, different types of optimization can be considered: (i) the *parametric* opti-  
37 mization when the shapes are parameterised by a fixed number of variables (thickness,  
38 dimensions, etc.); (ii) the *shape* optimization when, from an initial shape, the posi-  
39 tion of the boundaries of the microstructure is changed without changing its topology;  
40 (iii) the *topological* optimization when the best possible geometry is sought, even if  
41 it means changing the topology. In this work, we are interested in topological opti-  
42 mization which leaves more freedom compared to the first two methods. The chosen

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43 mathematical tool to perform this type of optimization is the *topological derivative*  
 44 [9] which measures the sensitivity of a cost functional to infinitesimal topological  
 45 perturbations.

46 Then, different numerical methods can be employed to update the material prop-  
 47 erties based on the knowledge of the topological derivatives. One method used in  
 48 this paper is the *level-set* method. For a two-phase material distribution, it relies  
 49 on the characterization of this distribution thanks to a level-set function which is  
 50 strictly positive in one phase and strictly negative in the other phase. This has first  
 51 been introduced for *shape* optimization and is based on the fact that the interface  
 52 between phases, which corresponds to the zero level-set function, can evolve based  
 53 on the shape derivative of the cost functional with respect to a perturbation of this  
 54 interface [1, 2]. This methodology has then been adapted to topological perturbation  
 55 based on a projection algorithm [6, 7, 20, 33].

56 A strategy for microstructure optimization, in line with the homogenization con-  
 57 sidered in this paper, is to perform the optimization from the homogenized model  
 58 that describes the material. It relies on the definition of a cost function, to be mini-  
 59 mized, in terms of the effective coefficients that characterize the homogenized model.  
 60 At low frequency, this method has been used in statics [7, 21, 33], in dynamics for a  
 61 low contrast [2, 15], and a high contrast [40] of the physical properties (activating  
 62 resonances of the highly contrasted inclusions). It has also been extended to optimize  
 63 effective properties at high frequencies [32].

64 In this framework, a topological optimization procedure is presented in [15] to  
 65 optimize dynamical properties for antiplane shear waves based on homogenization.  
 66 The main ingredients are the following ones:

- 67 1. the two-scale asymptotic homogenization method is deployed,
- 68 2. a cost functional is constructed from the homogenized model,
- 69 3. its topological derivative is computed,
- 70 4. the cost functional minimization is performed thanks to a level-set algorithm,
- 71 5. the level-set is iterated by computed cell problems using FFT-accelerated  
 72 solvers.

73 Noticeably, works on the optimization in dynamics of microstructured thin lay-  
 74 ers are more scarce and recent: [27] for an optimization of slabs based on far-field  
 75 behaviour and [31] for a design of acoustic metasurfaces based on a homogenization  
 76 model. In the present paper, we perform a sensitivity analysis and the optimization  
 77 of an acoustic microstructured interface, based on the homogenized model of [25] and  
 78 following the same overall approach than [15]. Novelties compared to [31] and [15]  
 79 are (i) the derivation of topological derivatives and their use *prior to the topological*  
 80 *optimization process* to perform a sensitivity analysis of the effective properties and  
 81 to determine valuable initializations from the closed-form formula provided by the  
 82 topological derivatives for elliptical inclusions; and (ii) the use of non-conventional  
 83 FFT-based solvers to address the specific *unbounded* cell problems that arise from the  
 84 two-scale homogenization of microstructured interfaces.

85

86 The paper is organized as follows: the homogenized model is recalled in Section 2,  
 87 and an analysis of macroscopic observables is performed, so that a cost functional to  
 88 minimize is proposed. In Section 3, the topological derivatives of the effective param-  
 89 eters of the interface model are derived and validated numerically. Then, in Section  
 90 4, based on the analytical information provided by these derivatives, a topological  
 91 sensitivity-based analysis is performed for microstructures made of elliptic inclusions,  
 92 and “asymptotically optimal” ellipses are determined for the chosen cost functional.

93 Then a topological optimization scheme which relies on the topological derivatives to  
 94 update the material distribution at each iteration is presented in Section 5. We finally  
 95 summarize the results and discuss possible perspectives in Section 6.

## 96 2. Microstructured interfaces and effective model.

97 **2.1. Setting and homogenization.** Let us consider the propagation of waves  
 98 in two dimensions across a periodic row of inclusions  $\cup_i \Omega_i$  embedded within a homo-  
 99 geneous matrix  $\Omega_m$ . The thickness and the period of the row are denoted by  $e$  and  
 100  $h$ , respectively, and we assume that  $e = \mathcal{O}(h)$ . The time and the spatial coordinates  
 101 are denoted by  $t$  and  $\mathbf{X} = (X_1, X_2)$ , respectively, with  $X_2$  being the direction of  
 102 periodicity of the inclusions as shown in Figure 1. Anti-plane elastic waves are con-  
 103 sidered, and both media are assumed to be isotropic. The microstructured medium is  
 104 therefore characterized by two constitutive parameters, the mass density  $\rho_h$  and the  
 105 shear modulus  $\mu_h$ , that are piecewise constant:

$$106 \quad (2.1) \quad (\rho_h, \mu_h)(\mathbf{X}) = \begin{cases} (\rho_m, \mu_m) & \text{in the matrix,} \\ (\rho_i, \mu_i) & \text{in the inclusions,} \end{cases}$$

107 and the time-domain governing equation for the out-of-plane component  $U_h$  of the  
 108 material displacement writes:

$$109 \quad (2.2) \quad \nabla \cdot (\mu_h(\mathbf{X}) \nabla U_h(\mathbf{X}, t)) = \rho_h(\mathbf{X}) \frac{\partial^2 U_h}{\partial t^2}(\mathbf{X}, t).$$

110 Introducing the scalar velocity field  $V_h = \partial U_h / \partial t$  and the stress vector  $\Sigma_h$  gathering  
 111 the two shear components of the stress tensor, this system can be rewritten as a  
 112 first-order system in time:

$$113 \quad (2.3) \quad \begin{cases} \frac{\partial \Sigma_h}{\partial t}(\mathbf{X}, t) = \mu_h(\mathbf{X}) \nabla V_h(\mathbf{X}, t), \\ \rho_h(\mathbf{X}) \frac{\partial V_h}{\partial t}(\mathbf{X}, t) = \nabla \cdot \Sigma_h(\mathbf{X}, t), \end{cases}$$

114 with  $V_h$  and  $\Sigma_h \cdot \mathbf{n}$  being continuous at each matrix/inclusion interface  $\partial \Omega_i$ , given  
 115 that  $\mathbf{n}$  is the *inward* unit normal on each  $\partial \Omega_i$ .

116 *Remark 2.1.* The system (2.3) is also relevant to model other physical phenom-  
 117 ena, such as acoustic waves for which the fields  $\Sigma_h$ ,  $V_h$ ,  $\rho_h$  and  $1/\mu_h$  would stand  
 118 instead for in-plane particle velocity, acoustic pressure, compressibility and mass den-  
 119 sity, respectively.

120 The assumptions of the homogenization process and the results obtained in [25]  
 121 are now briefly reminded.

122 *Hypotheses of the homogenization process.* Considering an illumination by an in-  
 123 cident wave or external sources, a characteristic wavelength  $\lambda$  within the matrix is  
 124 assumed to be much larger than the period  $h$ . Defining the wavenumber within the  
 125 matrix as  $k_m = 2\pi/\lambda$ , we introduce the parameter

$$126 \quad (2.4) \quad \eta = k_m h$$

127 and we assume that  $\eta \ll 1$  for the configurations of interest.

128 Throughout this article, only the *non-resonant* case is addressed, i.e. the physical  
 129 parameters of the matrix and of inclusions are supposed to be of the same order of

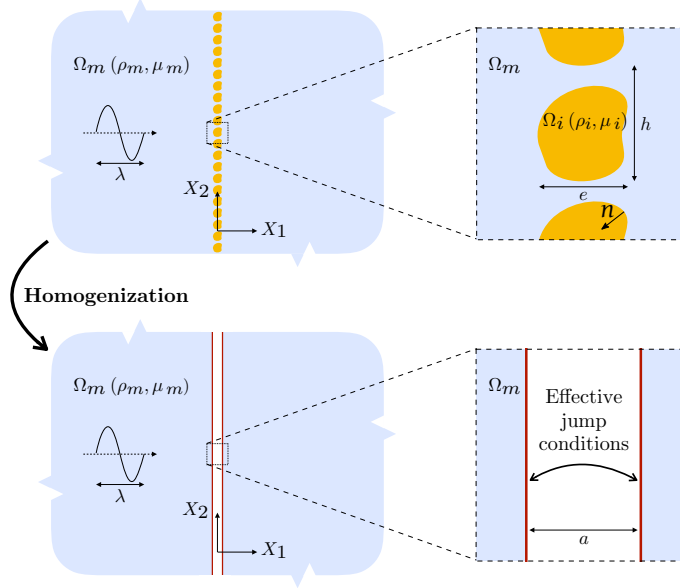


Fig. 1: Homogenization process for a single periodic array of inclusions. (*top*) Original configuration with a thin microstructured layer, (*bottom*) Homogenized interface model.

130 magnitude. For large contrasts, e.g. for very soft but dense inclusions ( $\mu_i \ll \mu_m$  and  
 131  $\rho_i \sim \rho_m$ ), the resonances of these inclusions play a key role in the transmission of  
 132 waves, and should be captured by specific homogenization methods, see e.g. [36, 39]  
 133 and the references therein.

134 These geometrical and material assumptions allows to homogenize the microstruc-  
 135 ture in the so-called long-wavelength, non-resonant regime.

136 *Notations.* The fast scale of coordinates is  $\mathbf{y} = \mathbf{X}/h = (y_1, y_2)^\top$ . The domain  $\Omega$   
 137 is the elementary cell  $\mathbb{R} \times [-1/2, 1/2]$  in  $\mathbf{y}$ -coordinates, see Figure 2, that is repeated  
 138 periodically in the  $y_2$  direction to obtain the full domain, and  $(\mathbf{e}_1, \mathbf{e}_2)$  is the canonical  
 139 basis of  $\mathbb{R}^2$ . For any function  $f(x_1)$ , we define the jump and the mean value around  
 140 the (centered) enlarged interface of thickness  $a$ :

$$141 \quad (2.5) \quad \llbracket f \rrbracket_a = f(a/2) - f(-a/2) \quad \text{and} \quad \langle f \rangle_a = \frac{1}{2}(f(a/2) + f(-a/2)).$$

142 We will also make use of the relative material constrasts  $\tau^\mu$  and  $\tau^\rho$  defined by:

$$143 \quad (2.6) \quad \tau^\mu = \frac{\mu_i - \mu_m}{\mu_m} \quad \text{and} \quad \tau^\rho = \frac{\rho_i - \rho_m}{\rho_m}.$$

144 *Cell problems.* The homogenization process requires the computation of auxil-  
 145 iary fields  $\Phi_j$  for  $j = 1, 2$  which are solutions of *elementary problems*. The problems  
 146 initially proposed by [25] were posed on the semi-infinite representative cell  $\Omega$ . For  
 147 practical implementation the authors of the present paper proposed in [16] a refor-

148 mulation on a bounded rectangular cell  $\Omega^a$  defined by:

$$149 \quad (2.7) \quad \Omega^a = \left[-\frac{a}{2h}; \frac{a}{2h}\right] \times \underbrace{\left[-\frac{1}{2}; \frac{1}{2}\right]}_I$$

150 such that

$$151 \quad (2.8) \quad \mathbf{m}(\mathbf{y}) := (\rho(\mathbf{y}), \mu(\mathbf{y})) = (\rho_m, \mu_m) \quad \forall \mathbf{y} \in \Omega \setminus \Omega^a,$$

152 as represented in Figure 2. The parameter  $a$  used in the choice of the representative  
 153 cell  $\Omega^a$  also defines the *effective interface width*, see Figure 1. It should satisfy  $a \geq e$   
 154 to ensure that the material variations are retained to  $\Omega^a$ , and for the effective model  
 155 presented below to satisfy some stability conditions [25].

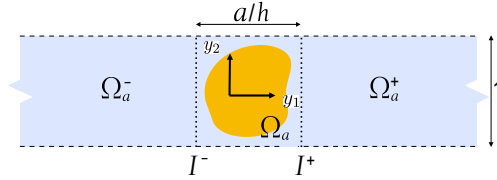


Fig. 2: Elementary cell  $\Omega$ , decomposed into the bounded cell  $\Omega^a$ , and half strips  $\Omega_a^+ = [\frac{a}{2h}, +\infty[ \times I$  and  $\Omega_a^- = ]-\infty, -\frac{a}{2h}] \times I$ .

156 Using the notation  $\Phi = (\Phi_1, \Phi_2)$  for compactness, two (uncoupled) band cell  
 157 problems are defined as:

$$158 \quad (2.9) \quad \begin{cases} \nabla \cdot (\mu(\mathbf{y}) (\nabla \Phi + \mathbf{I}_2)) = \mathbf{0} \text{ in } \Omega^a, \\ \Phi \text{ is } y_2\text{-periodic,} \\ \partial_n \Phi \left( \pm \frac{a}{2h}, \cdot \right) = \mathbf{L} \left( \Phi \left( \pm \frac{a}{2h}, \cdot \right) \right) \text{ on } I^\pm, \end{cases}$$

159 where  $\mathbf{I}_2$  is the second-order identity tensor,  $(I^-, I^+)$  are the left and right boundaries  
 160 of  $\Omega^a$  (see Figure 2) and  $\mathbf{L}$  is a nonlocal *Dirichlet-to-Neumann* (DtN) operator, whose  
 161 expression is recalled in Appendix A for completeness. In (2.9) and hereafter, the  
 162 adopted convention for the gradient components is such that  $(\nabla \Phi)_{ij} = \partial \Phi_j / \partial y_i$ .

163 These elementary solutions will serve to compute the effective parameters that  
 164 appear in the homogenized model presented now.

165 *Homogenized model.* From [25], we know that the homogenization of the problem  
 166 (2.3) at order  $\mathcal{O}(\eta)$  in such a configuration yields the following homogenized model:  
 (2.10)

$$167 \quad \begin{cases} \frac{\partial \Sigma}{\partial t} = \mu_m \nabla V & (|X_1| \geq a/2, X_2 \in \mathbb{R}), \\ \rho_m \frac{\partial V}{\partial t} = \nabla \cdot \Sigma & (|X_1| \geq a/2, X_2 \in \mathbb{R}), \\ \llbracket V \rrbracket_a = h \left\{ \mathcal{B} \left\langle \frac{\partial V}{\partial X_1} \right\rangle_a + \mathcal{B}_2 \left\langle \frac{\partial V}{\partial X_2} \right\rangle_a \right\} & (X_2 \in \mathbb{R}), \\ \llbracket \Sigma_1 \rrbracket_a = h \left\{ \mathcal{S} \langle \nabla \cdot \Sigma \rangle_a - \mathcal{C}_1 \left\langle \frac{\partial \Sigma_1}{\partial X_2} \right\rangle_a - \mathcal{C} \left\langle \frac{\partial \Sigma_2}{\partial X_2} \right\rangle_a \right\} & (X_2 \in \mathbb{R}), \end{cases}$$

168 featuring imperfect transmission conditions for the velocity  $V$  and normal component  
 169 of the stress vector  $\Sigma_1$ . The *effective coefficients* entering these conditions are the  
 170 parameter

$$171 \quad (2.11) \quad \mathcal{S} = \frac{a}{h} + \tau^\rho |\Omega_i|$$

172 where  $|\Omega_i| = \int_{\Omega_i} d\mathbf{y}$  is the surface of the inclusion phase in the rescaled coordinates;  
 173 and the four coefficients  $(\mathcal{B}, \mathcal{B}_2, \mathcal{C}_1, \mathcal{C})$  gathered in the two vector-valued parameters  
 174  $\mathcal{B} = (\mathcal{B}, \mathcal{B}_2)$  and  $\mathcal{C} = (\mathcal{C}_1, \mathcal{C})$ , which are expressed in terms of the elementary solution  
 175  $\Phi$  to (2.9) as:

$$176 \quad (2.12) \quad \mathcal{B}(\mathbf{m}) = \frac{a}{h} \mathbf{e}_1 + \int_I \left[ \Phi \left( \frac{a}{2h}, y_2 \right) - \Phi \left( -\frac{a}{2h}, y_2 \right) \right] dy_2,$$

177 and:

$$178 \quad (2.13) \quad \mathcal{C}(\mathbf{m}) = \int_{\Omega^a} \frac{\mu(\mathbf{y})}{\mu_m} \left( \frac{\partial \Phi}{\partial y_2}(\mathbf{y}) + \mathbf{e}_2 \right) d\mathbf{y}.$$

179 The effective parameters characterizing the homogenized medium are finally col-  
 180 lected in  $\mathbf{m}_{\text{eff}}$  as:

$$181 \quad (2.14) \quad \mathbf{m}_{\text{eff}} = (\mathcal{B}, \mathcal{B}_2, \mathcal{S}, \mathcal{C}_1, \mathcal{C}),$$

182 with the relation  $\mathcal{B}_2 = -\mathcal{C}_1$  that has been proven in [25].

183 **2.2. Analysis of macroscopic observables.** When the frequency-domain for-  
 184 mulation of (2.10) and an incident plane wave is considered, the expression of the  
 185 associated reflexion and transmission coefficients of the interface can be obtained  
 186 analytically [38]. For an incident plane wave at angle  $\theta_I$  with the horizontal axis,  
 187 these coefficients read respectively:

$$188 \quad (2.15) \quad \begin{cases} \mathcal{R}(\theta_I, \omega) = \frac{i\omega \mathcal{L}}{\mathcal{Z} + i\omega \mathcal{N} - \omega^2 \mathcal{M}} \exp \left( i \frac{\omega}{c_m} a \cos \theta_I \right), \\ \mathcal{T}(\theta_I, \omega) = \frac{\mathcal{Z} + i\omega \mathcal{G} + \omega^2 \mathcal{M}}{\mathcal{Z} + i\omega \mathcal{N} - \omega^2 \mathcal{M}} \exp \left( i \frac{\omega}{c_m} a \cos \theta_I \right), \end{cases}$$

189 with  $c_m = \sqrt{\mu_m / \rho_m}$  and

$$190 \quad (2.16) \quad \begin{cases} \mathcal{L} = h (\mathcal{B} \cos(\theta_I)^2 + \mathcal{C} \sin(\theta_I)^2 - \mathcal{S}), \\ \mathcal{Z} = 2c_m \cos \theta_I, \\ \mathcal{N} = h (-\mathcal{C} \sin(\theta_I)^2 + \mathcal{B} \cos(\theta_I)^2 + \mathcal{S}), \\ \mathcal{M} = \frac{h^2}{2c_m} (\mathcal{B}_2 \mathcal{C}_1 \sin(\theta_I)^2 - \mathcal{B} \mathcal{C} \sin(\theta_I)^2 + \mathcal{B} \mathcal{S}) \cos(\theta_I), \\ \mathcal{G} = -h (-\mathcal{C}_1 + \mathcal{B}_2) \cos(\theta_I) \sin(\theta_I). \end{cases}$$

191 One can notice a symmetry with respect to the normal incidence  $\theta_I = 0$  for the reflex-  
 192 ion coefficient  $\mathcal{R}(\theta_I, \omega)$  and for the modulus of the transmission coefficient  $|\mathcal{T}(\theta_I, \omega)|$ .  
 193 Consequently, only the argument of the transmission coefficient  $\arg(\mathcal{T}(\theta_I, \omega))$  is not  
 194 symmetric with respect to the normal incidence. The quantity  $\mathcal{G}$  defined in (2.16)  
 195 and proportional to  $\mathcal{B}_2 = -\mathcal{C}_1$  is responsible for this asymmetry. Therefore, one can

Table 1: Physical parameters considered for the microstructure.

$\mu_i$	$\rho_i$	$\mu_m$	$\rho_m$
78 GPa	$7800\text{kg} \cdot \text{m}^{-3}$	12 GPa	$2500\text{kg} \cdot \text{m}^{-3}$

196 wonder if a directional macroscopic effect can be obtained for geometries associated  
 197 with non-null values of this effective parameter, which corresponds to cases when the  
 198 microstructure is not symmetric with respect to the  $X_2$ -axis [25].  
 199

200 To investigate qualitatively this question, one considers a microstructure typical  
 201 of steel in concrete, for which physical parameters are given by Table 1. The peri-  
 202 odicity length is  $h = 1\text{m}$  and the examples of two geometries for the inclusion  $\Omega_i$   
 203 are investigated: one ellipse of semi-axes lengths  $(0.15, 0.5)$  tilted of  $-\pi/4$  and one  
 204 rectangle of sizes  $(1.25, 0.08)$  tilted of  $-\pi/4$ . The effective parameters associated to  
 205 these two configurations are computed and time-domain simulations are performed  
 206 in the associated effective media for  $\mathbf{X} \in [-70; 35] \times [-132; 132]$ . The excitation is a  
 207 source  $\delta(\mathbf{X} - \mathbf{X}_S)g(t)$  with  $g(t)$  defined as:

$$208 \quad (2.17) \quad g(t) = \begin{cases} A \sum_{m=1}^4 a_m \sin(\beta_m \omega_c t) & \text{if } 0 < t < \frac{1}{f_c}, \\ 0 & \text{otherwise,} \end{cases}$$

209 where  $\beta_m = 2^{m-1}$  and the coefficients  $a_m$  being  $a_1 = 1$ ,  $a_2 = -21/32$ ,  $a_3 = 63/768$ ,  
 210  $a_4 = -1/512$ . It entails that  $g \in C^6([0, +\infty[)$  and  $g(t)$  is a wide-band signal with a  
 211 central frequency  $f_c = \omega_c/2\pi$ . The source is located at  $\mathbf{X}_S = (-35, 0)$ , with  $X_1 = 0$   
 212 being the center of the enlarged effective interface. The central frequency is  $f_c = 50\text{Hz}$   
 213 which corresponds to a small parameter  $\eta = 0.14$  for which a good agreement between  
 214 the homogenized model and the microstructured configuration has been observed.  
 215 The time-domain simulations are performed thanks to Finite Differences and to the  
 216 Explicit Simplified Interface Method [23] to handle the effective enlarged interface.  
 217

218 The scattered fields are computed from time  $t = 0$  until  $t_f = 86.7\text{ms}$ . From these  
 219 data, one can compute the cumulative energy defined as:

$$220 \quad (2.18) \quad \mathcal{E}(\mathbf{X}) = \frac{1}{2} \int_0^{t_f} \left( \frac{1}{\mu_m} \Sigma(\mathbf{X}, t)^2 + \rho_m V(\mathbf{X}, t)^2 \right) dt.$$

221 This quantity is displayed for both microstructures in Figures 3a and 3b as a function  
 222 of the polar coordinates  $(r, \theta)$  centered at  $\mathbf{X}_S$ , with  $r \in [40; 60]$ , passed the inter-  
 223 face. The red crosses denote for a given value of  $r$ , the value of the critical angle  $\theta_C$   
 224 for which  $\mathcal{E}$  is minimal. One can notice that this value  $\theta_C$  seems to be independant  
 225 of  $r$ . Furthermore, the sign of  $\arg(\mathcal{T})$  is plotted in Figures 3c and 3d for the same  
 226 two microstructures directly using the analytical formula (2.16), as a function of  $\theta_I$   
 227 and  $\omega$ . It is then observed that this critical value measured on time-domain simula-  
 228 tions (denoted by the blue cross) seems to coincide with a change of sign in  $\arg(\mathcal{T})$   
 229 at low frequency.

230 To have an analytical insight into this critical value  $\theta_C$  at low frequency, one considers  
 231 a first-order approximation for  $\mathcal{T}$ . Upon introducing  $\mathcal{G} = \mathcal{G}/h$ ,  $\mathcal{M} = 2c_m \mathcal{M}/h^2$  and



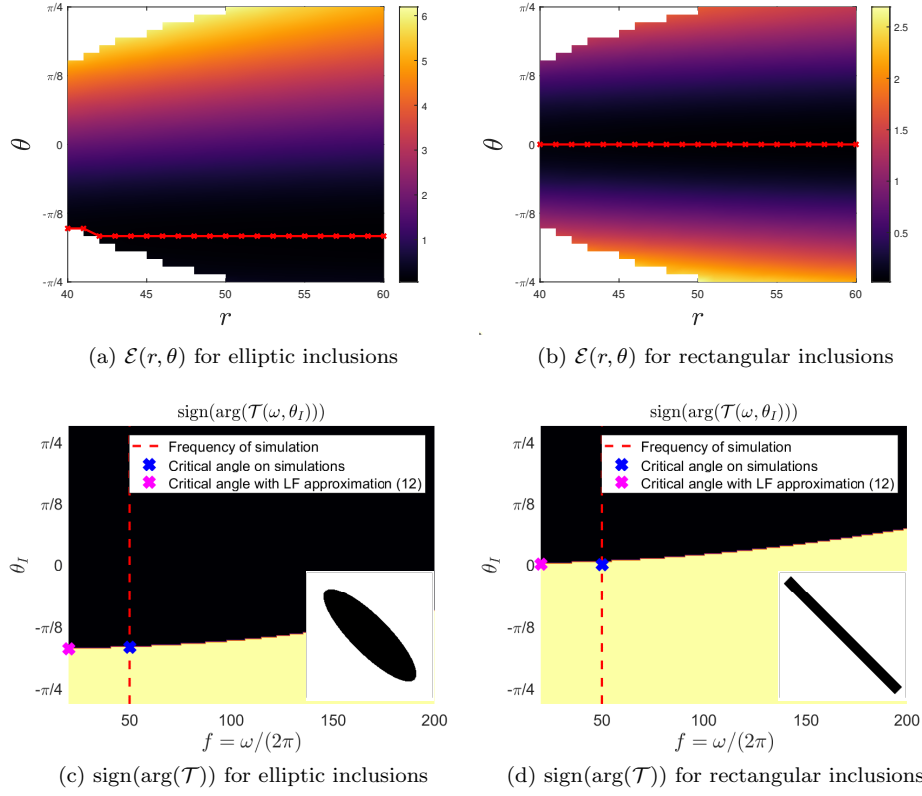


Fig. 3: Cumulative energy (first row) where the position of the minimal value for a given  $r$  is denoted by the red crosses, and study of  $\text{sign}(\arg(\mathcal{T}))$  (second row, yellow and black for positive and negative signs, respectively), computed with the effective model corresponding to elliptic (left) and rectangular (right) inclusions.

232  $\bar{\mathcal{N}} = \mathcal{N}/h$ , this leads to:

$$\begin{aligned}
 \mathcal{T}(\theta_I, \omega) &= \frac{\mathcal{L} + i\eta c_m \bar{\mathcal{G}} + \eta^2 \frac{c_m}{2} \bar{\mathcal{M}}}{\mathcal{L} + i\eta c_m \bar{\mathcal{N}} - \eta^2 \frac{c_m}{2} \bar{\mathcal{M}}} \exp\left(i\eta \frac{a}{h} \cos(\theta_I)\right) \\
 &= \frac{1 + i\eta \frac{\bar{\mathcal{G}}}{2\cos(\theta_I)} + \mathcal{O}(\eta^2)}{1 + i\eta \frac{\bar{\mathcal{N}}}{2\cos(\theta_I)} + \mathcal{O}(\eta^2)} \left(1 + i\eta \frac{a}{h} \cos(\theta_I) + \mathcal{O}(\eta^2)\right) \\
 &= 1 + i\eta \left( \frac{\bar{\mathcal{G}} - \bar{\mathcal{N}}}{2\cos(\theta_I)} + \frac{a}{h} \cos(\theta_I) \right) + \mathcal{O}(\eta^2).
 \end{aligned}$$

233 (2.19)

234 This can be summarized as

$$\mathcal{T}(\theta_I, \omega) = 1 + i\eta \mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_I) + \mathcal{O}(\eta^2)$$

235 (2.20)

236 with  $\mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_I)$  given by

$$\begin{aligned}
 237 \quad (2.21) \quad \mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_I) &= -\mathcal{B}_2 \sin(\theta_I) + \frac{\mathcal{C} \sin(\theta_I)^2 - \mathcal{B} \cos(\theta_I)^2 - \mathcal{S}}{2 \cos(\theta_I)} + \frac{a}{h} \cos(\theta_I) \\
 &= -\mathcal{B}_2 \sin(\theta_I) + \frac{\mathcal{C}^* \sin(\theta_I)^2 - \mathcal{B}^* \cos(\theta_I)^2 - \mathcal{S}^*}{2 \cos \theta_I},
 \end{aligned}$$

238 where

$$239 \quad (2.22) \quad \mathcal{B}^* = \mathcal{B} - a/h, \quad \mathcal{C}^* = \mathcal{C} - a/h, \quad \text{and} \quad \mathcal{S}^* = \mathcal{S} - a/h = \tau^\rho |\Omega_i|.$$

240 The second expression in (2.21), using the coefficients in (2.22) shows that  $\mathcal{T}_1$  does  
 241 not depend on the choice of interface thickness  $a$  and will be used in Section 4 to  
 242 slightly simplify the computations.

243 With this approximation (2.20), it is clear that, at low frequency,  $\arg(\mathcal{T})$  changes  
 244 sign when  $\mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_I)$  changes sign. This is confirmed in Figures 3c and 3d (black and  
 245 yellow maps where yellow and black stand for positive and negative sign, respectively)  
 246 where the angle for which  $\mathcal{T}_1$  changes sign is denoted by a pink cross and is observed  
 247 to be very close to both the critical angle observed in numerical simulations and the  
 248 angle for which the exact value of  $\arg(\mathcal{T})$  changes sign at low frequency.

249 This function  $\mathcal{T}_1$  then seems to be an interesting quantity to study and control  
 250 in order to get a desired macroscopic directive effect, i.e. a cumulative energy which  
 251 is minimal at a given angle  $\theta_{\text{min}}$ . Therefore, the following functional to minimize is  
 252 introduced

$$253 \quad (2.23) \quad \mathcal{J}_{\text{main}}(\mathbf{m}_{\text{eff}}) = \left( \frac{\mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_{\text{min}})}{\partial_\theta \mathcal{T}_1(\mathbf{m}_{\text{eff}}, \theta_{\text{min}})} \right)^2, \quad \text{with: } \partial_\theta \mathcal{T}_1 = \frac{\partial \mathcal{T}_1}{\partial \theta_I},$$

254 where we aim at simultaneously maximizing the derivative amplitude  $|\partial_\theta \mathcal{T}_1|$  to (i)  
 255 avoid close-to-zero local minima of  $|\mathcal{T}_1|$  without sign change and (ii) “push” the ensuing  
 256 optimization process towards “stiff” sign changes.

257 There are mainly two objectives in this paper: (i) the computation of the topolog-  
 258 ical sensitivity of the effective parameters  $\mathbf{m}_{\text{eff}}$  to changes of the microstructures and  
 259 (ii) the generation of a phase distribution  $\mathbf{m}_{\text{opt}}$  in the bounded cell  $\Omega^a$  that optimizes  
 260 an objective cost functional  $\mathcal{J}(\mathbf{m}_{\text{eff}})$  such as (2.23).

261 Regarding the second objective, additional terms will be added to the functional  
 262  $\mathcal{J}_{\text{main}}$  in (2.23) in order to reach a given surface ratio between the materials, or to  
 263 have a sufficient smoothness of the final configuration. This will be discussed through  
 264 the introduction of a total cost functional  $\mathcal{J}$  and an optimization process in Section  
 265 5.3. The topological derivatives derived in Section 3, and the optimization methods  
 266 described in Section 5.1 could however be used for any other objective.

267 **3. Topological derivatives of the effective parameters.** In this section,  
 268 one aims at describing the sensitivity of the effective parameters to periodic topo-  
 269 logical changes of the microstructure, i.e. geometric perturbations of the represen-  
 270 tative cell  $\Omega^a$ . A perturbation is defined as a small inhomogeneity  $\mathcal{P}_{\mathbf{z}, \varepsilon} = \mathbf{z} + \varepsilon \mathcal{P}$   
 271 of size  $\varepsilon$ , normalized shape  $\mathcal{P}$  and physical parameters  $(\mu + \Delta\mu, \rho + \Delta\rho)$  intro-  
 272 duced at a point  $\mathbf{z} \in \Omega^a$ . The material perturbation is  $\Delta\mathbf{m} = (\Delta\rho, \Delta\mu)$  with  
 273  $\Delta\mu > -\min_{\mathbf{y} \in \Omega^a} \mu(\mathbf{y})$  and  $\Delta\rho > -\min_{\mathbf{y} \in \Omega^a} \rho(\mathbf{y})$  to satisfy the physical constraints.  
 274 The resulting perturbed cell, denoted by  $\Omega_{\mathbf{z}, \varepsilon}^a$  and represented in Figure 4, features  
 275 the physical parameters

$$276 \quad (3.1) \quad \mathbf{m}_{\mathbf{z}, \varepsilon} = (\mu_{\mathbf{z}, \varepsilon}, \rho_{\mathbf{z}, \varepsilon}) = (\mu + \Delta\mu \chi_{\mathcal{P}_{\mathbf{z}, \varepsilon}}, \rho + \Delta\rho \chi_{\mathcal{P}_{\mathbf{z}, \varepsilon}}),$$

277 with  $\chi_{\mathcal{P}_{z,\varepsilon}}$  the characteristic function of the perturbation domain  $\mathcal{P}_{z,\varepsilon}$ . The definition  
 278 of  $\Delta\mathbf{m}$  may depend on the choice of  $\mathbf{z}$  if the unperturbed cell is heterogeneous.  
 279 However, we disregard the case where the perturbation is located at an interface  
 280 between two different materials. Consequently, we will drop any dependence of  $\Delta\mathbf{m}$  on  
 281 the space coordinate in the notations, since they don't change the integrals computed  
 282 hereafter.

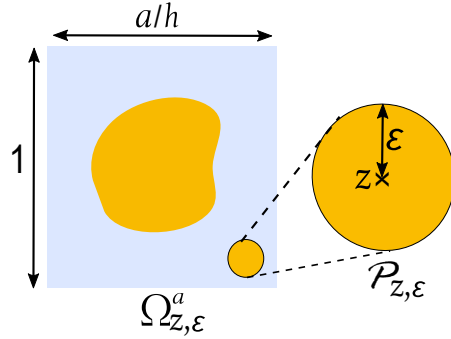


Fig. 4: Cell  $\Omega_{z,\varepsilon}^a$  perturbed by the introduction of the inhomogeneity  $\mathcal{P}_{z,\varepsilon}$ .

283 Let  $f$  be a function of the material properties. In this two-dimensional context,  
 284 the so-called *topological derivative* of a given function  $f$ , denoted by  $\mathcal{D}f$ , is defined  
 285 thanks to the following 2D asymptotic expansion:

$$286 \quad (3.2) \quad f_{z,\varepsilon} := f(\mathbf{m}_{z,\varepsilon}) \underset{\varepsilon \rightarrow 0}{=} f(\mathbf{m}) + \varepsilon^2 \mathcal{D}f(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta\mathbf{m}) + o(\varepsilon^2).$$

287 It describes the influence on the functional  $f$  of a perturbation located at  $\mathbf{z}$ , of shape  
 288  $\mathcal{P}$  and material perturbation  $\Delta\mathbf{m}$ . Therefore, the more negative  $\mathcal{D}f(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta\mathbf{m})$   
 289 is, the more efficient such a perturbation at point  $\mathbf{z}$  would be to decrease  $f$ .

290 In this section, the topological derivatives of the effective parameters collected  
 291 in (2.14) are computed. First, one looks for an expansion solution  $\Phi_{z,\varepsilon}$  to the cell  
 292 problem (2.9) in the perturbed cell  $\Omega_{z,\varepsilon}^a$  in Section 3.1. This allows the computation of  
 293 the topological sensitivities of the five effective parameters in Section 3.2.

294 **3.1. Approximation of the perturbed cell problem solution.** To compute  
 295 the topological derivatives of the homogenized coefficients, we must characterize  
 296 the asymptotic behavior of the cell function  $\Phi$  in (2.9) when the perturbation is in-  
 297 troduced. To this end, we first reformulate the cell problem (2.9) into an integral  
 298 equation, more suitable for the asymptotic analysis. This formulation will be used  
 299 formally to compute the topological derivatives, but we do not claim it is an equivalent  
 300 variational formulation of it.

301 *Weak forms of the unperturbed and perturbed cell problems.* The first step is to  
 302 write the weak form of the cell problem. To do so, we consider a function  $v \in H_{\text{per}}^1 =$   
 303  $\{u \in H^1(\Omega^a; \mathbb{R}), u \text{ } y_2\text{-periodic}\}$ . The first equation of (2.9) is then multiplied by  
 304  $v$  and integrated by parts in  $\Omega^a$ . Using the periodic condition and the boundary  
 305 condition in (2.9), one obtains after a division by  $\mu_m$ :

$$306 \quad (3.3) \quad \mathcal{A}_\mu(\Phi, v) = -\mathbf{F}_\mu(v) + \mathbf{J}(v) \quad \forall v \in H_{\text{per}}^1$$

307 where one has introduced the following functionals for  $\mathbf{u} = (u_1, u_2) \in H_{\text{per}}^1 \times H_{\text{per}}^1$   
 308 and  $v \in H_{\text{per}}^1$ :

$$309 \quad (3.4) \quad \begin{cases} \mathcal{A}_\mu(\mathbf{u}, v) = \int_{\Omega^a} \frac{\mu(\mathbf{y})}{\mu_m} \nabla \mathbf{u}(\mathbf{y})^\top \cdot \nabla v(\mathbf{y}) d\mathbf{y} + \mathcal{L}^-(\mathbf{u}, v) + \mathcal{L}^+(\mathbf{u}, v), \\ \mathbf{F}_\mu(v) = \int_{\Omega^a} \frac{\mu(\mathbf{y})}{\mu_m} \nabla v(\mathbf{y}) d\mathbf{y}, \\ \mathbf{J}(v) = \int_I \left[ v\left(\frac{a}{2h}, y_2\right) - v\left(-\frac{a}{2h}, y_2\right) \right] \mathbf{e}_1 dy_2, \end{cases}$$

310 with

$$311 \quad (3.5) \quad \mathcal{L}^\pm(\mathbf{u}, v) = - \int_I \Lambda \left[ \mathbf{u} \left( \pm \frac{a}{2h}, \cdot \right) \right] (y_2) v \left( \pm \frac{a}{2h}, y_2 \right) dy_2.$$

312 This vector-valued weak-formulation is a short-hand notation for the two uncoupled  
 313 equations satisfied by  $\Phi = (\Phi^{(1)}, \Phi^{(2)})$ .

314 Similarly, the perturbed field  $\Phi_{\mathbf{z}, \varepsilon}$  satisfies for all  $v \in H^1(\Omega^a; \mathbb{R})$ ,  $v$   $y_2$ -periodic:

$$315 \quad (3.6) \quad \mathcal{A}_{\mu_{\mathbf{z}, \varepsilon}}(\Phi_{\mathbf{z}, \varepsilon}, v) = -\mathbf{F}_\mu(v) - \delta \mathbf{F}_{\mathbf{z}, \varepsilon}(v) + \mathbf{J}(v),$$

316 with

$$317 \quad (3.7) \quad \delta \mathbf{F}_{\mathbf{z}, \varepsilon}(v) = \frac{\Delta \mu}{\mu_m} \int_{\mathcal{P}_{\mathbf{z}, \varepsilon}} \nabla v(\mathbf{y}) d\mathbf{y}.$$

318 *Integral equation.* To obtain the integral equation satisfied by  $\Phi_{\mathbf{z}, \varepsilon}$ , one then  
 319 introduces the Green's function  $G(\cdot, \mathbf{x})$  associated with a point source at  $\mathbf{x} \in \Omega^a$ , i.e.  
 320 the solution of

$$321 \quad (3.8) \quad \begin{cases} -\nabla_{\mathbf{y}} \cdot \left( \frac{\mu(\mathbf{y})}{\mu_m} \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) \right) = \delta(\mathbf{y} - \mathbf{x}) \quad \forall \mathbf{y} \in \Omega^a, \\ G(\cdot, \mathbf{x}) \text{ } y_2\text{-periodic,} \\ -\mathbf{n} \cdot \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) \Big|_{y_1 = \pm \frac{a}{2h}} = \Lambda [G(\mathbf{y}, \mathbf{x})] \Big|_{y_1 = \pm \frac{a}{2h}} \quad \forall \mathbf{y} \in I^\pm. \end{cases}$$

322 It can be decomposed as

$$323 \quad (3.9) \quad G(\mathbf{y}, \mathbf{x}) = G_\infty \left( \mathbf{y} - \mathbf{x}; \frac{\mu(\mathbf{x})}{\mu_m} \right) + G_c(\mathbf{y}, \mathbf{x}), \quad \text{with } G_\infty(\mathbf{r}; \mu_\star) = -\frac{\ln(\|\mathbf{r}\|)}{2\pi\mu_\star},$$

324 where  $G_\infty$  is the full-space Green's function solution of 2D Poisson equation that  
 325 shares the same singularity as  $G$ , and  $G_c$  is the complementary part to the Green's  
 326 function solution accounting for the heterogeneity of the cell and the boundary con-  
 327 ditions. Detail on these functions is given in Appendix B.

328 For any sufficiently smooth function  $\mathbf{w}$ , one gets from (3.8) the integral represen-  
 329 tation for all  $\mathbf{x} \in \Omega^a$ :

$$330 \quad (3.10) \quad \mathbf{w}(\mathbf{x}) = \mathcal{A}_\mu(\mathbf{w}, G(\cdot, \mathbf{x}))$$

331 with  $\mathcal{A}_\mu$  defined in (3.4).

332 Coming back to the perturbed problem, one introduces the surface integral oper-  
 333 ator  $\mathcal{N}_{\mathbf{z},\varepsilon}$  :

$$334 \quad (3.11) \quad \mathcal{N}_{\mathbf{z},\varepsilon} \mathbf{f}(\mathbf{x}) = \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}_{\mathbf{z},\varepsilon}} \nabla \mathbf{f}(\mathbf{y})^\top \cdot \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) d\mathbf{y}.$$

335 Taking  $v = G(\cdot, \mathbf{x})$  in (3.6) together with the definition (3.4) of  $\mathcal{A}_\mu$  then yields  
 336 (3.12)

$$\begin{aligned} \mathcal{A}_\mu(\Phi_{\mathbf{z},\varepsilon}, G(\cdot, \mathbf{x})) + \mathcal{N}_{\mathbf{z},\varepsilon} \Phi_{\mathbf{z},\varepsilon}(\mathbf{x}) &= -\mathbf{F}_\mu(G(\cdot, \mathbf{x})) - \delta \mathbf{F}_{\mathbf{z},\varepsilon}(G(\cdot, \mathbf{x})) + \mathbf{J}(G(\cdot, \mathbf{x})) \\ &= \mathcal{A}_\mu(\Phi, G(\cdot, \mathbf{x})) - \delta \mathbf{F}_{\mathbf{z},\varepsilon}(G(\cdot, \mathbf{x})), \end{aligned}$$

337 where in the last line we used  $v = G(\cdot, \mathbf{x})$  in (3.3). Finally, one considers  $\mathbf{w} = \Phi_{\mathbf{z},\varepsilon}$   
 338 and  $\mathbf{w} = \Phi$  in (3.10). Together with (3.12) this leads to the integral equation satisfied  
 339 by the perturbed field  $\Phi_{\mathbf{z},\varepsilon}$ :

$$340 \quad (3.13) \quad (\mathbf{I} + \mathcal{N}_{\mathbf{z},\varepsilon})(\Phi_{\mathbf{z},\varepsilon})(\mathbf{x}) = \Phi(\mathbf{x}) - \delta \mathbf{F}_{\mathbf{z},\varepsilon}(G(\cdot, \mathbf{x})),$$

341 where the integral operator  $\mathcal{N}_{\mathbf{z},\varepsilon}$  and right-hand side term  $\delta \mathbf{F}_{\mathbf{z},\varepsilon}(G(\cdot, \mathbf{x}))$  are both  
 342 supported by the perturbation domain  $\mathcal{P}_{\mathbf{z},\varepsilon}$ .

343 *Asymptotic analysis.* Aiming at reformulating the equation (3.13) onto the ref-  
 344 erence shape  $\mathcal{P}$ , let us introduce the scaled coordinates  $\mathbf{x} = \mathbf{z} + \varepsilon \bar{\mathbf{x}}$  and assume the  
 345 following expansion for all  $\mathbf{x} \in \mathcal{P}_{\mathbf{z},\varepsilon}$ :

$$346 \quad (3.14) \quad \Phi_{\mathbf{z},\varepsilon}(\mathbf{x}) = \Phi(\mathbf{z}) + \varepsilon \Phi_1(\bar{\mathbf{x}}) + o(\varepsilon).$$

347 One also writes the following Taylor expansion for the cell function

$$348 \quad (3.15) \quad \Phi(\mathbf{x}) = \Phi(\mathbf{z}) + \varepsilon \bar{\mathbf{x}} \cdot \nabla \Phi(\mathbf{z}) + o(\varepsilon).$$

349 Inserting (3.14) and (3.15) in (3.13) and keeping only the leading and first-order terms  
 350 yields, since  $\mathcal{N}_{\mathbf{z},\varepsilon} \Phi(\mathbf{z}) = \mathbf{0}$ :

$$351 \quad (3.16) \quad (\mathbf{I} + \mathcal{N}_{\mathbf{z},\varepsilon}) \left( \varepsilon \Phi_1 \left( \frac{\cdot - \mathbf{z}}{\varepsilon} \right) \right) (\mathbf{x}) = \varepsilon \bar{\mathbf{x}} \cdot \nabla \Phi(\mathbf{z}) - \delta \mathbf{F}_{\mathbf{z},\varepsilon}(G(\cdot, \mathbf{x})).$$

352 As developed in Appendix B,  $\nabla G_\infty$  is homogeneous of degree  $-1$  (see (B.1)) and  
 353  $\nabla G_c(\cdot, \mathbf{x})$  is regular in the neighborhood of  $\mathbf{z}$  (see (B.4)). The function  $G$  in (3.8)  
 354 then satisfies:

$$355 \quad (3.17) \quad \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) = \varepsilon^{-1} \nabla G_\infty \left( \bar{\mathbf{y}} - \bar{\mathbf{x}}; \frac{\mu(\mathbf{z})}{\mu_m} \right) + o(\varepsilon^{-1}).$$

356 Inserting the above expansion in (3.16), performing a change of variable to rewrite  
 357 the integral on  $\mathcal{P}$  and identifying the leading-order ( $O(\varepsilon)$ ) contributions then leads to  
 358 the scaled integral equation:

$$359 \quad (3.18) \quad (\mathbf{I} + \mathcal{M})(\tilde{\Phi}_1)(\bar{\mathbf{x}}) = \bar{\mathbf{x}} \cdot (\nabla \Phi(\mathbf{z}) + \mathbf{I}),$$

360 with  $\tilde{\Phi}_1(\bar{\mathbf{x}}) = \Phi_1(\bar{\mathbf{x}}) + \bar{\mathbf{x}}$  and  $\mathcal{M}$  defined by

$$361 \quad (3.19) \quad \mathcal{M} \mathbf{f}(\bar{\mathbf{x}}) = \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}} \nabla \mathbf{f}(\bar{\mathbf{y}})^\top \cdot \nabla G_\infty \left( \bar{\mathbf{y}} - \bar{\mathbf{x}}; \frac{\mu(\mathbf{z})}{\mu_m} \right) d\bar{\mathbf{y}}.$$

362 Consequently, introducing  $\mathbf{R}$ , the vector solution of the equation:

$$363 \quad (3.20) \quad (\mathbf{I} + \mathcal{M})\mathbf{R}(\bar{\mathbf{x}}) = \bar{\mathbf{x}}$$

364 i.e. the solution to a free-space transmission problem associated with a perturbation  
365  $(\mathcal{P}, \Delta\mu)$ , with an homogeneous background of modulus  $\mu(\mathbf{z})$ , then  $\tilde{\Phi}_1$  is given by:

$$366 \quad (3.21) \quad \tilde{\Phi}_1(\bar{\mathbf{x}}) = \mathbf{R}(\bar{\mathbf{x}}) \cdot (\nabla\Phi(\mathbf{z}) + \mathbf{I}).$$

367 Finally, one inserts this in (3.14) to get the first-order expansion:

$$368 \quad (3.22) \quad \Phi_{\mathbf{z},\varepsilon}(\mathbf{x}) = \Phi(\mathbf{z}) + \varepsilon(\mathbf{R}(\bar{\mathbf{x}}) \cdot (\nabla\Phi(\mathbf{z}) + \mathbf{I}) - \bar{\mathbf{x}}) + o(\varepsilon).$$

369 **3.2. Calculation of the topological derivatives.** The results of this section  
370 are summarized in the following proposition:

371 *Proposition 3.1.* The topological derivatives of the effective coefficients  $\mathcal{S}, \mathcal{B}, \mathcal{C}$ ,  
372 for a material perturbation  $(\Delta\mu, \Delta\rho)$  supported by the domain  $\mathcal{P}_{\mathbf{z},\varepsilon} = \mathbf{z} + \varepsilon\mathcal{P}$ , are  
373 given by :

$$374 \quad (3.23) \quad \mathcal{D}\mathcal{S}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta\mathbf{m}) = \frac{\Delta\rho}{\rho_m} |\mathcal{P}|,$$

$$375 \quad (3.24) \quad \mathcal{D}\mathcal{B}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta\mathbf{m}) = -(\nabla\Phi_1(\mathbf{z}) + \mathbf{e}_1) \cdot \mathbf{A}(\mathcal{P}, \mu(\mathbf{z}), \Delta\mu) \cdot (\nabla\Phi(\mathbf{z}) + \mathbf{I}),$$

$$376 \quad (3.25) \quad \mathcal{D}\mathcal{C}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta\mathbf{m}) = (\nabla\Phi_2(\mathbf{z}) + \mathbf{e}_2) \cdot \mathbf{A}(\mathcal{P}, \mu(\mathbf{z}), \Delta\mu) \cdot (\nabla\Phi(\mathbf{z}) + \mathbf{I}),$$

377 where the so-called polarization second-order tensor  $\mathbf{A}$  is defined from the solution  $\mathbf{R}$   
378 of the problem (3.20) as

$$379 \quad (3.26) \quad \mathbf{A}(\mathcal{P}, \mu(\mathbf{z}), \Delta\mu) = \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}} \nabla_{\bar{\mathbf{y}}} \mathbf{R}(\bar{\mathbf{y}}) d\bar{\mathbf{y}}.$$

380 *Remark 3.2.* The polarization tensor  $\mathbf{A}$  (also called concentration or localization  
381 tensor [34]) has been used in previous studies [14, 3, 12]. It is symmetric and is known  
382 analytically for a variety of inclusion shapes  $\mathcal{P}$ , see [34]. In particular, for an elliptic  
383 perturbation of semiaxes lengths  $(1, \gamma)$  along directions  $(\mathbf{a}_1, \mathbf{a}_2)$ , it is given by:  
384

$$385 \quad (3.27) \quad \mathbf{A}(\mathcal{P}, \mu(\mathbf{z}), \Delta\mu) = \pi\gamma(\gamma + 1) \frac{\Delta\mu}{\mu_m} \left( \frac{\mathbf{a}_1 \otimes \mathbf{a}_1}{1 + \gamma + \gamma \frac{\Delta\mu}{\mu(\mathbf{z})}} + \frac{\mathbf{a}_2 \otimes \mathbf{a}_2}{1 + \gamma + \frac{\Delta\mu}{\mu(\mathbf{z})}} \right).$$

386 The steps leading to the expressions above are now given.

387 **3.2.1. Computation of  $\mathcal{D}\mathcal{S}$ .** We first notice that, owing to the definition of  $\mathcal{S}$   
388 in (2.11), one has

$$389 \quad (3.28) \quad \mathcal{S}(\mathbf{m}) = \int_{\Omega^a} \frac{\rho(\mathbf{y})}{\rho_m} d\mathbf{y}.$$

390 Consequently, one gets

$$391 \quad (3.29) \quad \mathcal{S}_{\mathbf{z},\varepsilon} = \mathcal{S}(\mathbf{m}) + \int_{\mathcal{P}_{\mathbf{z},\varepsilon}} \frac{\Delta\rho}{\rho_m} d\mathbf{y} = \mathcal{S}(\mathbf{m}) + \varepsilon^2 \frac{\Delta\rho}{\rho_m} |\mathcal{P}|$$

392 which yields by identification with (3.2) the following result

$$393 \quad (3.30) \quad \mathcal{D}\mathcal{S}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta\mathbf{m}) = \frac{\Delta\rho}{\rho_m} |\mathcal{P}|.$$

394 **3.2.2. Computation of  $\mathcal{DB}$ .** From the expression (2.12), the effective parame-  
 395 ter  $\mathcal{B}_{\mathbf{z},\varepsilon}$  associated with the perturbed cell writes

$$396 \quad (3.31) \quad \mathcal{B}_{\mathbf{z},\varepsilon} = \mathcal{B}(\mathbf{m}) + \int_I \left[ \delta\Phi_{\mathbf{z},\varepsilon} \left( \frac{a}{2h}, y_2 \right) - \delta\Phi_{\mathbf{z},\varepsilon} \left( -\frac{a}{2h}, y_2 \right) \right] dy_2,$$

397 with the perturbation for the solution of the cell problem  $\delta\Phi_{\mathbf{z},\varepsilon}$  defined by

$$398 \quad (3.32) \quad \delta\Phi_{\mathbf{z},\varepsilon} = \Phi_{\mathbf{z},\varepsilon} - \Phi.$$

399 The left-hand side of (3.6) writes

$$400 \quad (3.33) \quad \mathcal{A}_{\mu_{\mathbf{z},\varepsilon}}(\Phi_{\mathbf{z},\varepsilon}, v) = \mathcal{A}_\mu(\Phi, v) + \mathcal{A}_\mu(\delta\Phi_{\mathbf{z},\varepsilon}, v) + \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}_{\mathbf{z},\varepsilon}} \nabla\Phi_{\mathbf{z},\varepsilon}(\mathbf{y})^\top \cdot \nabla v(\mathbf{y}) d\mathbf{y}.$$

401 Inserting this equation in (3.6) and using (3.3), one gets for all  $v \in H_{\text{per}}^1$ :

$$402 \quad (3.34) \quad \mathcal{A}_\mu(\delta\Phi_{\mathbf{z},\varepsilon}, v) + \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}_{\mathbf{z},\varepsilon}} \nabla\Phi_{\mathbf{z},\varepsilon}(\mathbf{y})^\top \cdot \nabla v(\mathbf{y}) d\mathbf{y} = -\delta\mathbf{F}_{\mathbf{z},\varepsilon}(v).$$

403 Furthermore,  $\beta = \Phi^{(1)} + y_1$  satisfies for all  $\mathbf{w} \in H^1(\Omega^a; \mathbb{R}^2)$ ,  $\mathbf{w}$   $y_2$ -periodic

$$404 \quad (3.35) \quad \mathcal{A}_\mu(\mathbf{w}, \beta) = \int_I \left[ \mathbf{w} \left( \frac{a}{2h}, y_2 \right) - \mathbf{w} \left( -\frac{a}{2h}, y_2 \right) \right] dy_2.$$

405 Taking  $v = \beta$  in (3.34) and  $\mathbf{w} = \delta\Phi_{\mathbf{z},\varepsilon}$  in (3.35), the expansion (3.31) writes

$$406 \quad (3.36) \quad \mathcal{B}_{\mathbf{z},\varepsilon} = \mathcal{B}(\mathbf{m}) - \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}_{\mathbf{z},\varepsilon}} \nabla\beta(\mathbf{y}) \cdot (\nabla\Phi_{\mathbf{z},\varepsilon}(\mathbf{y}) + \mathbf{I}) d\mathbf{y}.$$

407 Consequently, one looks for an asymptotic expansion for  $\nabla\Phi_{\mathbf{z},\varepsilon}$ . For this purpose, one  
 408 uses the final expansion (3.22) of the previous section. One also writes the expansion  
 409  $\nabla\beta(\mathbf{y}) = \nabla\beta(\mathbf{z}) + o(1)$  for all  $\mathbf{y} \in \mathcal{P}_{\mathbf{z},\varepsilon}$  and expresses the integral in the scaled  
 410 coordinates as

$$411 \quad (3.37) \quad \mathcal{B}_{\mathbf{z},\varepsilon} = \mathcal{B}(\mathbf{m}) - \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}} \nabla\beta(\mathbf{z}) \cdot \left( \frac{1}{\varepsilon} \nabla\Phi_{\mathbf{z},\varepsilon}(\bar{\mathbf{y}}) + \mathbf{I} \right) \varepsilon^2 d\bar{\mathbf{y}} + o(\varepsilon^2).$$

412 Inserting the expansion (3.22) in the above equation yields

$$413 \quad (3.38) \quad \mathcal{B}_{\mathbf{z},\varepsilon} = \mathcal{B}(\mathbf{m}) - \varepsilon^2 \frac{\Delta\mu}{\mu_m} \nabla\beta(\mathbf{z}) \cdot \int_{\mathcal{P}} \nabla\mathbf{R}(\bar{\mathbf{y}}) d\bar{\mathbf{y}} \cdot (\nabla\Phi(\mathbf{z}) + \mathbf{I}) + o(\varepsilon^2).$$

414 Using the definition the definition  $\beta = \Phi_1 + y_1$  and the polarization tensor  $\mathbf{A}$   
 415 defined by (3.26), the topological derivative of  $\mathcal{B}$  writes

$$416 \quad (3.39) \quad \mathcal{DB}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta\mathbf{m}) = -(\nabla\Phi_1(\mathbf{z}) + \mathbf{e}_1) \cdot \mathbf{A}(\mathcal{P}, \mu(\mathbf{z}), \Delta\mu) \cdot (\nabla\Phi(\mathbf{z}) + \mathbf{I}).$$

417 **3.2.3. Computation of  $\mathcal{DC}$ .** From the expression (2.13), the effective parame-  
 418 ter  $\mathcal{C}_{\mathbf{z},\varepsilon}$  associated with the perturbed cell writes

$$419 \quad (3.40) \quad \mathcal{C}_{\mathbf{z},\varepsilon} = \mathcal{C}(\mathbf{m}) + \int_{\Omega^a} \frac{\mu(\mathbf{y})}{\mu_m} \frac{\partial\delta\Phi_{\mathbf{z},\varepsilon}}{\partial y_2}(\mathbf{y}) d\mathbf{y} + \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}_{\mathbf{z},\varepsilon}} \left( \frac{\partial\Phi_{\mathbf{z},\varepsilon}}{\partial y_2}(\mathbf{y}) + \mathbf{e}_2 \right) d\mathbf{y} + o(\varepsilon^2).$$

420 We know that  $\Phi_2$  satisfies for all  $\mathbf{w} \in H_{\text{per}}^1$

$$421 \quad (3.41) \quad \mathcal{A}_\mu(\mathbf{w}, \Phi_2) = - \int_{\Omega^a} \frac{\mu(\mathbf{y})}{\mu_m} \frac{\partial \mathbf{w}}{\partial y_2}(\mathbf{y}) d\mathbf{y}.$$

422 One takes  $v = \Phi_2$  in (3.34) and  $\mathbf{w} = \delta\Phi_{\mathbf{z},\varepsilon}$  in (3.41) and gets

$$423 \quad (3.42) \quad \int_{\Omega^a} \frac{\mu(\mathbf{y})}{\mu_m} \frac{\partial \delta\Phi_{\mathbf{z},\varepsilon}}{\partial y_2}(\mathbf{y}) d\mathbf{y} = \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}_{\mathbf{z},\varepsilon}} \nabla\Phi_2(\mathbf{y}) \cdot (\nabla\Phi_{\mathbf{z},\varepsilon}(\mathbf{y}) + \mathbf{I}) d\mathbf{y},$$

424 which yields

$$425 \quad (3.43) \quad \mathcal{C}_{\mathbf{z},\varepsilon} = \mathcal{C}(\mathbf{m}) + \frac{\Delta\mu}{\mu_m} \int_{\mathcal{P}_{\mathbf{z},\varepsilon}} (\nabla\Phi_2(\mathbf{y}) + \mathbf{e}_2) \cdot (\nabla\Phi_{\mathbf{z},\varepsilon}(\mathbf{y}) + \mathbf{I}) d\mathbf{y} + o(\varepsilon^2).$$

426 Once again, we use the Taylor expansion  $\nabla\Phi_2(\mathbf{y}) = \nabla\Phi_2(\mathbf{z}) + o(1)$  for all  $\mathbf{y}$  in  $\mathcal{P}_{\mathbf{z},\varepsilon}$ ,  
 427 the expression of the integral in the scaled coordinates and the expansion (3.22) to  
 428 get the final expression for the topological derivative

$$429 \quad (3.44) \quad \mathcal{DC}(\mathbf{m}, \mathbf{z}, \mathcal{P}, \Delta\mathbf{m}) = (\nabla\Phi_2(\mathbf{z}) + \mathbf{e}_2) \cdot \mathbf{A}(\mathcal{P}, \mu(\mathbf{z}), \Delta\mu) \cdot (\nabla\Phi(\mathbf{z}) + \mathbf{I}).$$

430 **3.3. Numerical validation.** To validate numerically the found expressions of  
 431 the topological derivatives, we can compute the error made by the approximation of  
 432  $\mathcal{B}_{\mathbf{z},\varepsilon}$  and  $\mathcal{C}_{\mathbf{z},\varepsilon}$  by  $\mathcal{B} + \varepsilon^2\mathcal{DB}$  and  $\mathcal{C} + \varepsilon^2\mathcal{DC}$ , respectively. Indeed, due to (3.38) and  
 433 (3.43), this error should be of order  $\varepsilon^3$  at least.

434 One starts with an initial reference configuration ( $\varepsilon = 0$ ), computes numerically  
 435 the solutions of the cell problems (2.9) (their computation will be briefly described  
 436 in Section 5.1.1), and thus the value of  $\mathcal{B}$  and  $\mathcal{C}$  from (2.12) and (2.13). The initial  
 437 configuration is chosen to be heterogenous in order to avoid simplifications than can  
 438 occur with a homogeneous medium as reference. More precisely, we choose a homoge-  
 439 nous medium containing an ellipsoidal inclusion of center  $(0, 0)$  and semixes lengths  
 440  $(0.32 \text{ m}, 0.1 \text{ m})$ , tilted of  $45^\circ$ . The physical parameters are again given by Table 1.  
 Then one inserts a perturbation in the background matrix at  $\mathbf{z} = (-0.26 \text{ m}, 0.24 \text{ m})$ .

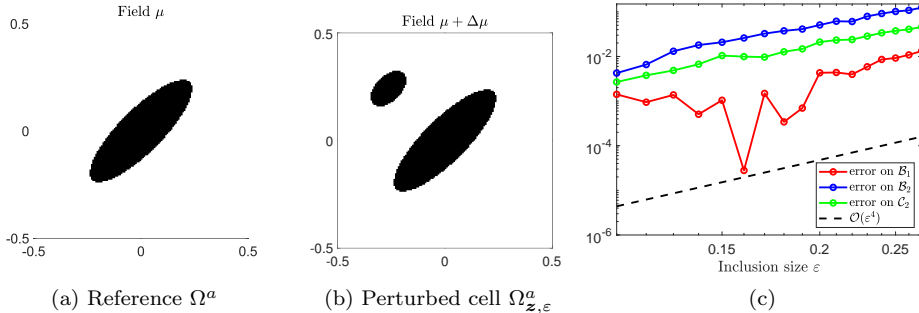


Fig. 5: Test case for an ellipsoidal perturbation: (a) Reference configuration (b) Perturbed onfiguration for  $\varepsilon = 0.1$ . (c) Relative error between the exact and approximated effectives parameters as a function of  $\varepsilon$  in a log-log scale.

441



442 Its physical parameters are the ones of the ellipsoidal inclusion  $(\rho_i, \mu_i)$ . Its shape is an  
 443 ellipse of semiaxes lengths  $(\varepsilon, 0.6\varepsilon)$  and tilted of  $45^\circ$ . For  $\varepsilon = 0.1$ , the configuration is  
 444 plotted in Figure 5b. For a given value of  $\varepsilon$ , one computes the perturbed cell solutions  
 445 and thus the exact effective parameters  $\mathcal{B}_{\mathbf{z},\varepsilon}$  and  $\mathcal{C}_{\mathbf{z},\varepsilon}$  from (2.12) and (2.13). Their  
 446 first-order approximations  $\mathcal{B} + \varepsilon^2 \mathcal{D}\mathcal{B}$  and  $\mathcal{C} + \varepsilon^2 \mathcal{D}\mathcal{C}$  are computed from (3.24) and  
 447 (3.25) using (3.27).

448 The relative errors (e.g.  $|(\mathcal{B}^*)_{\mathbf{z},\varepsilon} - \mathcal{B}^* - \varepsilon^2 \mathcal{D}\mathcal{B}_1|/|(\mathcal{B}^*)_{\mathbf{z},\varepsilon}|$ ) between both the exact  
 449 and approximated values are plotted as functions of perturbation size  $\varepsilon$  in log-log  
 450 scale in Figure 5c. Since  $\mathcal{B}_2 = \mathcal{C}_1$ , only one of the corresponding misfit is represented.  
 451 The dashed line stands for an error of  $\mathcal{O}(\varepsilon^4)$ . It seems that this is the actual order  
 452 of approximation of the effective parameters, the small variations for low values  
 453 of  $\varepsilon$  being probably due to numerical errors in the computation of the coefficients.  
 454 This underlines the fact that the leading order term and consequently the topological  
 455 derivatives are well accounted for and that the terms of order  $\varepsilon^3$  in the expansions  
 456 (3.38) and (3.43) are probably equal to zero for this type of perturbations with a  
 457 central symmetry. This was already observed for the volumic case in [11, 12], with  
 458 the intuition that it occurs for perturbations with a central symmetry. This remains  
 459 however to be proved.

460

461 **4. Topological sensitivity-based analysis of the effective parameters for**  
**462 elliptic inclusions.** In this section, the topological derivatives are used as tools to  
 463 analyse the case of cells made of a unique *elliptic* inclusion  $\Omega_i$  in a homogenous  
 464 material. First, the quality of the approximation of the effective parameters in this  
 465 case is investigated. Then, we show that “asymptotically optimal” elliptic shapes can  
 466 be determined for our choice of cost functional, i.e. shapes for which the leading-order  
 467 contribution to the cost functionnal, given by the topological derivative, vanishes.

468 **4.1. Approximation of the effective parameters.** Consider a unique inclu-  
 469 sion in an otherwise homogeneous cell, a configuration which can be seen as a single  
 470 perturbation in a homogeneous reference cell. In this case, the effective coefficient  
 471  $\mathcal{S}^* = \mathcal{S} - a/h$  in (2.22) is given by the exact expression:

$$472 \quad (4.1) \quad \mathcal{S}^* = \varepsilon^2 |\mathcal{P}| \tau^\rho,$$

473 where the topological derivatives formula provide the following approximations:

$$474 \quad (4.2) \quad \mathcal{B}^* = -\varepsilon^2 A_{11} + o(\varepsilon^2), \quad \mathcal{B}_2 = -\varepsilon^2 A_{12} + o(\varepsilon^2), \quad \mathcal{C}^* = \varepsilon^2 A_{22} + o(\varepsilon^2).$$

475 Computing these approximations only requires the knowledge of the polarization  
 476 tensor (3.27) for the perturbation shape  $\mathcal{P}$ , and the scaling of the result by  $\varepsilon^2$ . This  
 477 is much less costly than computing numerically the cell solutions and the associated  
 478 effective parameters for each choice of inclusion, especially for elliptic inclusions for  
 479 which the polarization tensor is known analytically.

480 As an example of the quality of these approximations, we consider an ellipse, lo-  
 481 cated at  $\mathbf{z} = (0, 0)$ , of tilted angle  $40^\circ$ , and semiaxes lengths  $(\varepsilon, 0.2\varepsilon)$ . In Figure 6b,  
 482 the relative errors between the numerically computed value of the effective parameters  
 483 through (2.12-2.13) and their approximations given above are represented for an in-  
 484 creasing value of  $\varepsilon$ . We first note that the order of convergence of the *relative* error is  
 485 of  $\mathcal{O}(\varepsilon^2)$  in this case because the zeroth-order term in the denominator vanishes when  
 486 the reference configuration is homogeneous. We also observe that a good agreement  
 487 is obtained even for high values of  $\varepsilon$  (i.e. even outside of the asymptotic regime).

488 Indeed, for  $\varepsilon = 0.5$  (illustrated in Figure 6a) the major axis length is equal to the size  
 489 of the unit cell and the relative errors remain below 15%.

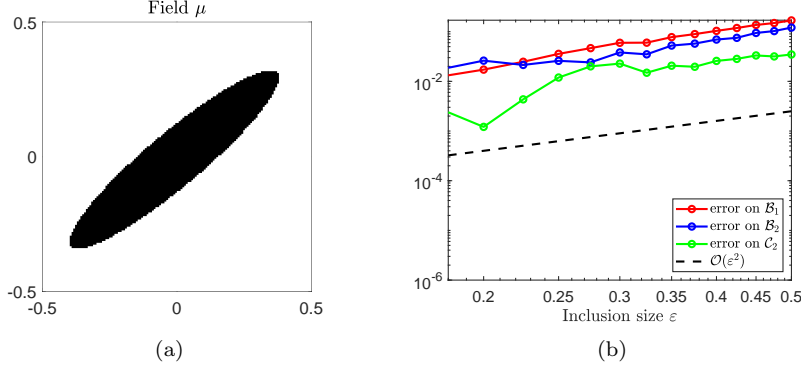


Fig. 6: Test case for an ellipsoidal inclusion: (a) Configuration for  $\varepsilon = 0.5$ . (b) Relative errors between the exact and approximated effective parameters as functions of inclusion size  $\varepsilon$  in a log-log scale.

489

490 *Remark 4.1.* The approximation (4.2), using only the polarization tensor com-  
 491 puted from the free-space transmission problem (3.20), is well-known in the domain  
 492 of micromechanics as the “dilute” or “Eshelby” approximation (see for instance [34]  
 493 and the numerous references therein). It does not account for interactions between  
 494 inclusions, and is therefore supposedly restricted to very low concentrations of inclu-  
 495 sions, but provides surprisingly accurate results in the present context.

496 Consequently, we propose to use the expressions (4.2) to obtain “optimal” ellipses  
 497 that minimize the chosen functional (2.23).

498 **4.2. Normal incidence: explicit formula and analysis.** When the case  
 499 of interest is normal incidence of waves, i.e. when  $\theta_1 = 0$ , closed-form results are  
 500 available, that are used in this section as a first example of minimization of a cost  
 501 functional finding an optimal ellipse. Indeed, the expression (2.20) of the function of  
 502 interest  $\mathcal{T}_1$  is considerably simplified:

$$503 \quad (4.3) \quad \mathcal{T}_1(\theta_1 = 0) = -\frac{1}{2} (\mathcal{B}^* + \mathcal{S}^*) = -\frac{\varepsilon^2}{2} (-A_{11} + \pi\gamma\tau^\rho) + o(\varepsilon^2).$$

504 Then, couples  $(\theta, \gamma)$  for which  $\mathcal{T}_1 = o(\varepsilon^2)$  can be found analytically for given material  
 505 contrasts  $(\tau^\rho, \tau^\mu)$ . Indeed, canceling the leading-order term above and introducing  
 506 the expression (3.27) of the polarization tensor gives:

$$507 \quad (4.4) \quad \pi\gamma\tau^\rho = A_{11} \Leftrightarrow \tau^\rho = (1 + \gamma)\tau^\mu \left( \frac{\cos^2(\theta)}{1 + \gamma + \gamma\tau^\mu} + \frac{\sin^2(\theta)}{1 + \gamma + \tau^\mu} \right)$$

508 which leads to

$$509 \quad (4.5) \quad \tau^\rho(1 + \gamma + \gamma\tau^\mu)(1 + \gamma + \tau^\mu) - \tau^\mu(1 + \gamma)^2 - (\tau^\mu)^2(1 + \gamma)(\gamma + (1 - \gamma)\cos^2(\theta)) = 0.$$

510 Therefore, we eventually get

511 (4.6) 
$$\begin{cases} \theta = \arccos \sqrt{\beta} & \text{if } \beta \geq 0 \\ \text{no solution} & \text{if } \beta < 0 \end{cases}, \quad \text{with } \beta = \frac{[\tau^\rho(1 + \gamma + \tau^\mu) - \tau^\mu(1 + \gamma)](1 + \gamma + \gamma\tau^\mu)}{(\tau^\mu)^2(1 - \gamma^2)}.$$

512 This particular solution can be used to check the numerical implementation of  
513  $\mathcal{T}_1$ .

514 To find an optimal couple  $(\theta^{\text{opt}}, \gamma^{\text{opt}})$  with respect to the cost functional (2.23)  
515 we furthermore look for the maximal absolute value of the derivative,  $|\partial_\theta \mathcal{T}_1(\theta_I = 0)|$ ,  
516 along the curve defined by the function (4.6) above. To do so, we rely again on the  
517 simplified expression of the function  $\partial_\theta \mathcal{T}_1$  for normal incidence ( $\theta_I = 0$ ) and on the  
518 approximations (4.2) of the effective coefficients, and use the approximation:

519 (4.7) 
$$\begin{aligned} \partial_\theta \mathcal{T}_1(\theta_I = 0) &= -\mathcal{B}_2 = \varepsilon^2 A_{12} + o(\varepsilon^2) \\ &= \frac{\varepsilon^2 \sin(2\theta)}{2} \frac{\pi\gamma(1 - \gamma^2)(\tau^\mu)^2}{[1 + \gamma(1 + \tau^\mu)][1 + \gamma + \tau^\mu]} + o(\varepsilon^2). \end{aligned}$$

520 Then plugging the expression (4.6) of  $\theta$ , one obtains an expression for the leading-  
521 order contribution of  $\partial_\theta \mathcal{T}_1$  as a function of  $\gamma$  only, whose maximum is easily found  
522 numerically, as represented in Figure 7.

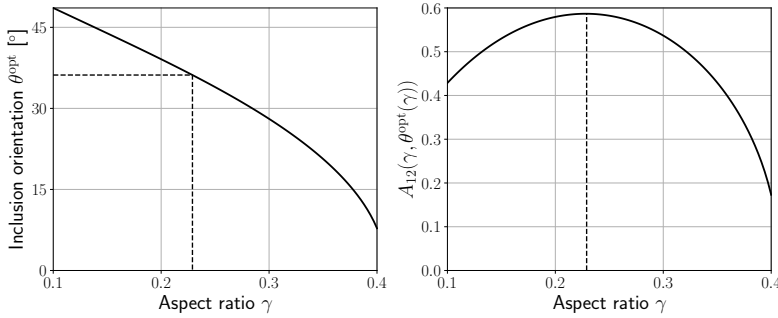


Fig. 7: Left: Curve  $\theta(\gamma)$  corresponding to  $\mathcal{T}_1(\theta_I = 0) = o(\varepsilon^2)$ . Right: coefficient  $A_{12}$ , i.e. leading-order contribution of  $\partial_\theta \mathcal{T}_1(\theta_I = 0)$ , along this curve. Positions of the optimal parameters  $(\theta^{\text{opt}}, \gamma^{\text{opt}})$  are given in dashed lines.

523 Finally, the numerical “true” values of the homogenized coefficients and functions  
524  $\mathcal{T}_1$ ,  $\partial_\theta \mathcal{T}_1$  and  $\mathcal{J}_{\text{main}}$  are computed for non-vanishing inclusions, of increasing finite size  
525  $\varepsilon$ , as plotted in Figure 8. As expected, the value of  $\mathcal{T}_1$  and therefore the cost functional  
526  $\mathcal{J}_{\text{main}}$  (2.23) diverge from their asymptotic values. Nevertheless, as summarized in  
527 Table 2, the ellipse parametrized by  $(\theta^{\text{opt}}, \gamma^{\text{opt}})$  gives significantly better results (lower  
528 values of  $\mathcal{T}_1$  and  $\mathcal{J}_{\text{main}}$ ) than a disk or an arbitrarily chosen ellipse with equal surface  
529 ratio, also represented in Figure 8.

530 This asymptotic analysis therefore provides good “first guess” that can be used  
531 as initial guess for topological optimization procedures as seen in the next section.

532 **4.3. Arbitrary incidence: numerical optimum.** For an arbitrary incidence  
533 angle  $\theta_I$ , closed-form expressions for an optimal couple such as (4.6) and (4.7) would be  
534 too tedious to obtain. However, the asymptotic approximation of  $\mathcal{T}_1(\theta_I)$  as a function  
535 of  $(\theta, \gamma)$  can easily be computed numerically.

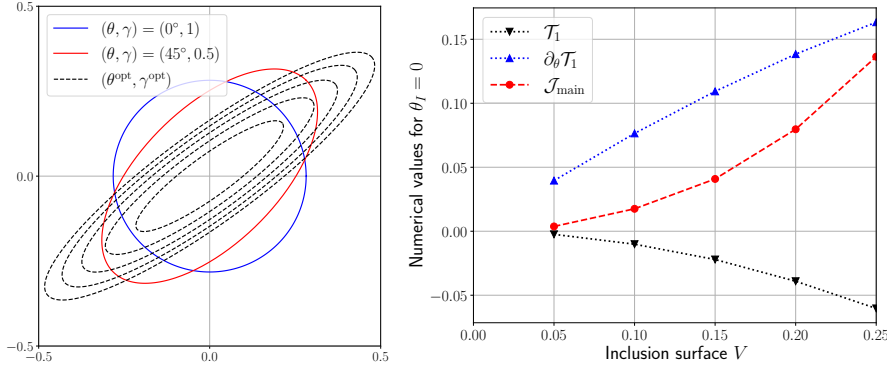


Fig. 8: Left: Investigated ellipses. Test cases with surface  $|\Omega_i| = 0.25$  and “optimal” ellipses for normal incidence  $\theta_I = 0$  with increasing surfaces  $|\Omega_i| \in \{0.05, 0.25\}$ . Right: Values of  $\mathcal{T}_1$ ,  $\partial_\theta \mathcal{T}_1$  and  $\mathcal{J}_{\text{main}}$ , computed numerically for these “optimal” ellipses.

Ellipse	$\mathcal{T}_1$	$\partial_\theta \mathcal{T}_1$	$\mathcal{J}_{\text{main}} = (\mathcal{T}_1 / \partial_\theta \mathcal{T}_1)^2$
$(\theta, \gamma) = (0^\circ, 1)$ (disk)	-0.11	0	$\emptyset$
$(\theta, \gamma) = (45^\circ, 0.5)$	-0.10	$8.6 \times 10^{-2}$	1.4
$(\theta^{\text{opt}}, \gamma^{\text{opt}}) \approx (36^\circ, 0.23)$	-0.06	0.16	0.14

Table 2: Case  $\theta_I = 0$  (normal incidence). Values of functions  $\mathcal{T}_1$ ,  $\partial_\theta \mathcal{T}_1$  and  $\mathcal{J}_{\text{main}}$  for several ellipses with the same surface  $|\Omega_i| = 0.25$ , see Figure 8. For the disk, one has  $\mathcal{B}_2 = 0$  and therefore  $\partial_\theta \mathcal{T}_1 = 0$ , so that  $\mathcal{J}_{\text{main}}$  is not defined.

536 As illustrated in Figures 9 and 10 for  $\theta_I = 30^\circ$  and  $\theta_I = 45^\circ$ , respectively, the  
 537 curves  $(\theta, \gamma)$  that achieve  $\mathcal{T}_1 = o(\varepsilon^2)$  are numerically extracted, the leading-order ap-  
 538 proximation of  $\partial_\theta \mathcal{T}_1(\theta_I)$  is computed along them, and an optimal couple is determined,  
 539 similarly to the case  $\theta_I = 0$ .

540 For an ellipse with these characteristics and surface  $|\Omega_i| = 0.25$ , the values of  
 541  $\mathcal{T}_1$ ,  $\partial_\theta \mathcal{T}_1$  and  $\mathcal{J}_{\text{main}}$  are then computed by numerically solving the cell problems, and  
 542 compared the two other ellipses represented in Figure 8. Tables 3 and 4 summarize  
 543 the results. In these two cases, the “asymptotically optimal” ellipse gives much better  
 544 results than the two other test-cases.

Ellipse	$\mathcal{T}_1$	$\partial_\theta \mathcal{T}_1$	$\mathcal{J}_{\text{main}} = (\mathcal{T}_1 / \partial_\theta \mathcal{T}_1)^2$
$(\theta, \gamma) = (0^\circ, 1)$ (disk)	-0.11	0.05	4.8
$(\theta, \gamma) = (45^\circ, 0.5)$	-0.054	0.12	0.20
$(\theta^{\text{opt}}, \gamma^{\text{opt}}) \approx (52^\circ, 0.34)$	-0.019	0.17	0.012

Table 3: Case  $\theta_I = 30^\circ$ . Values of functions  $\mathcal{T}_1$ ,  $\partial_\theta \mathcal{T}_1$  and  $\mathcal{J}_{\text{main}}$  for several ellipses with the same surface  $|\Omega_i| = 0.25$ .

545 **5. Topological optimization of microstructured interfaces.** While in the  
 546 previous section, we used the analytical information given by the topological deriva-  
 547 tive to analyse the case of a unique elliptic inclusion, the aim in this section is to use

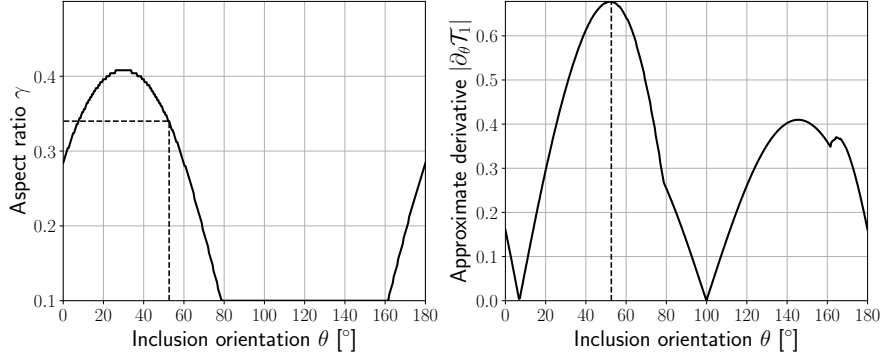


Fig. 9: Case  $\theta_1 = 30^\circ$ . Couples  $(\theta, \gamma)$  that achieve  $\mathcal{T}_1 = o(\varepsilon^2)$  (left), corresponding leading-order approximation of  $\partial_\theta \mathcal{T}_1$  (right), and numerical extraction of the optimal parameters  $(\theta^{\text{opt}}, \gamma^{\text{opt}}) \approx (53^\circ, 0.34)$  (dashed lines).

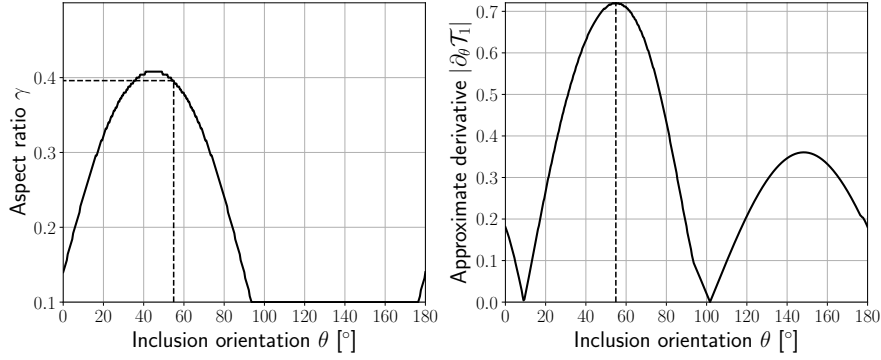


Fig. 10: Case  $\theta_1 = 45^\circ$ . Couples  $(\theta, \gamma)$  that achieve  $\mathcal{T}_1 = o(\varepsilon^2)$  (left), corresponding leading-order approximation of  $\partial_\theta \mathcal{T}_1$  (right), and numerical extraction of the optimal parameters  $(\theta^{\text{opt}}, \gamma^{\text{opt}}) \approx (55^\circ, 0.40)$  (dashed lines).

Ellipse	$\mathcal{T}_1$	$\partial_\theta \mathcal{T}_1$	$\mathcal{J}_{\text{main}} = (\mathcal{T}_1 / \partial_\theta \mathcal{T}_1)^2$
$(\theta, \gamma) = (0^\circ, 1)$ (disk)	-0.10	0.078	1.8
$(\theta, \gamma) = (45^\circ, 0.5)$	-0.032	0.13	0.058
$(\theta^{\text{opt}}, \gamma^{\text{opt}}) \approx (54^\circ, 0.4)$	-0.011	0.16	0.0047

Table 4: Case  $\theta_1 = 45^\circ$ . Values of functions  $\mathcal{T}_1$ ,  $\partial_\theta \mathcal{T}_1$  and  $\mathcal{J}_{\text{main}}$  for several ellipses with the same surface  $|\Omega_i| = 0.25$ .

548 the topological derivative in an optimization algorithm to minimize a functional with  
 549 no *a priori* on the geometry of the inclusion. The efficiency of both methodologies  
 550 will be investigated through numerical examples in Section 5.3.

551 One aims at generating a microstructure minimizing an objective cost functional  
 552  $\mathcal{J}(\mathbf{m}_{\text{eff}})$ . An optimal microstructure is defined by the phase distribution  $\mathbf{m}_{\text{opt}}$  in the  
 553 bounded cell  $\Omega^a$ . The cost functional depends on the macroscopic behaviour which

554 is described by the effective parameters  $\mathbf{m}_{\text{eff}}$  (2.14) that themselves depend on  $\mathbf{m}$   
 555 based on the homogenized model. We therefore consider the following optimization  
 556 problem:

$$557 \quad (5.1) \quad \text{Find} \quad \mathbf{m}_{\text{opt}} = \arg \min_{\mathbf{m}} \tilde{\mathcal{J}}(\mathbf{m}) \quad \text{with} \quad \tilde{\mathcal{J}}(\mathbf{m}) = \mathcal{J}(\mathbf{m}_{\text{eff}}).$$

558 In this context, and given the optimization problem (5.1), one looks for the topological  
 559 derivative  $\mathcal{D}\tilde{\mathcal{J}}$ . If  $\mathcal{J}$  is differentiable with respect to the effective parameters,  $\mathcal{D}\tilde{\mathcal{J}}$   
 560 is computed thanks to the chain rule:

$$561 \quad (5.2) \quad \mathcal{D}\tilde{\mathcal{J}} = \frac{\partial \mathcal{J}}{\partial \mathcal{B}} \mathcal{D}\mathcal{B} + \frac{\partial \mathcal{J}}{\partial \mathcal{B}_2} \mathcal{D}\mathcal{B}_2 + \frac{\partial \mathcal{J}}{\partial \mathcal{S}} \mathcal{D}\mathcal{S} + \frac{\partial \mathcal{J}}{\partial \mathcal{C}_1} \mathcal{D}\mathcal{C}_1 + \frac{\partial \mathcal{J}}{\partial \mathcal{C}} \mathcal{D}\mathcal{C}.$$

562 The final objective is to have at hand an optimization algorithm in order to compute  
 563 the optimal material distribution in the sense of (5.1).

### 564 5.1. Optimization scheme.

565 **5.1.1. FFT-based computation of the cell problems.** In order to perform  
 566 topological optimization, multiple computations of the band problem (2.9) are re-  
 567 quired. Accurately solving this band problem with a numerical efficiency is therefore  
 568 crucial. The main difficulty compared to classical cell problems with periodicity condi-  
 569 tions on all boundaries that are involved in volume homogenization consists in dealing  
 570 with the unboundedness in the  $y_1$ -direction. This problem has been tackled in [16].  
 571 This relies on the reformulation of the problem in a bounded cell, which is recalled in  
 572 Appendix A. Then the solution of this equivalent bounded problem is decomposed as  
 573 follows

$$574 \quad (5.3) \quad \Phi = \Phi_{\text{per}} + \Phi_{\text{bound}}.$$

575 The two terms of this decomposition are

- 576 • The bi-periodic function  $\Phi_{\text{per}}$  that satisfies:

$$577 \quad (5.4) \quad \nabla \cdot (\mu(\mathbf{y}) (\mathbf{I}_2 + \nabla \Phi_{\text{bound}} + \nabla \Phi_{\text{per}})) = \mathbf{0} \text{ in } \Omega^a,$$

578 together with  $\int_{\Omega^a} \Phi_{\text{per}} = 1$  for uniqueness. This is an usual cell problem,  
 579 which appears in homogenization of bi-periodic media, with a source term  
 580 that is given by  $\mathbf{I}_2 + \nabla \Phi_{\text{bound}}$ . For a given function  $\Phi_{\text{bound}}$ , this problem is  
 581 solved using a FFT-accelerated algorithm [28].

- 582 • The boundary corrector  $\Phi_{\text{bound}}$  that ensures that the boundary conditions  
 583 associated to the DtN conditions in (2.9) are satisfied:

$$584 \quad (5.5) \quad (\partial_{\mathbf{n}} - \Lambda) \Phi_{\text{bound}} \left( \pm \frac{a}{2h}, \cdot \right) = -(\partial_{\mathbf{n}} - \Lambda) \Phi_{\text{per}} \left( \pm \frac{a}{2h}, \cdot \right).$$

585 Using Fourier series expansion, an explicit expression of the boundary cor-  
 586 rector has been proposed in [16].

587 The problem is then solved using a fixed-point algorithm iterating on  $\Phi^n$  whose  
 588 behaviour has not been investigated theoretically but which has been observed to  
 589 converge in practice. The various fields are discretized on a regular  $N_1 \times N_2$  grid  
 590 mapping the inner cell  $\Omega^a$  and the stopping criterion is the following

$$591 \quad (5.6) \quad \frac{\|\Phi^{n+1} - \Phi^n\|_{L^2(\Omega^a)}}{\|\Phi^n\|_{L^2(\Omega^a)}} < \delta_{\text{FFT}},$$

592 where  $\delta_{\text{FFT}}$  is a user-chosen parameter.

593 **5.1.2. Material updating.** In the configuration mentioned in Introduction,  
 594 there are only two phases:  $\Omega_m$  which is the homogeneous matrix outside the mi-  
 595 crostructured array, and  $\Omega_i \subset \Omega^a$  which is the inclusion phase. Consequently the only  
 596 material modification allowed in the optimization process is a phase conversion from  
 597  $(\rho_i, \mu_i)$  to  $(\rho_m, \mu_m)$  or conversely. Accordingly, the material perturbation  $\Delta \mathbf{m}$  in the  
 598 topological derivatives of Proposition 3.23 is chosen as:

$$599 \quad (5.7) \quad \Delta \mathbf{m} = (\rho_i - \rho_m, \mu_i - \mu_m) \text{ in } \Omega_m \quad \text{and} \quad \Delta \mathbf{m} = (\rho_m - \rho_i, \mu_m - \mu_i) \text{ in } \Omega_i.$$

Moreover, the shape of the perturbation  $\mathcal{P}$  is a disk so that the expression of the polarization tensor is given by (3.27) with  $\gamma = 1$ . The use of the boundary corrector approach described above requires that the phase at the boundaries  $y_1 = \pm \frac{a}{2h}$  is  $\Omega_m$ . Consequently, one defines an optimization domain

$$\Omega^{\text{design}} = [-b; b] \times [-1/2; 1/2] \quad \text{with} \quad b < \frac{a}{2h}$$

600 in which material updates are allowed. Since the material is made of two phases, a  
 601 common way to characterize it is to use a *level-set* function  $\Psi$  that satisfies:

$$602 \quad (5.8) \quad \begin{cases} \Psi(\mathbf{z}) > 0 \text{ in } \Omega^{\text{design}} \cap \Omega_m \\ \Psi(\mathbf{z}) < 0 \text{ in } \Omega^{\text{design}} \cap \Omega_i \end{cases} \quad \text{and} \quad \|\Psi\|_{L^2(\Omega^{\text{design}})} = 1.$$

603 A projection algorithm introduced in [6] for topological optimization can then be used  
 604 [4, 7, 33, 20]. The main steps are recalled in this subsection.

605 First, one defines a signed normalized topological derivative  $\overline{\mathcal{D}\mathcal{J}}^{(n)}$  at iteration  $n$  as:

$$606 \quad (5.9) \quad \overline{\mathcal{D}\mathcal{J}}^{(n)}(\mathbf{z}) = \begin{cases} \mathcal{D}\mathcal{J}^{(n)}(\mathbf{z}) / \|\mathcal{D}\mathcal{J}^{(n)}\|_{L^2(\Omega^{\text{design}})} & \text{in } \Omega^{\text{design}} \cap \Omega_m \\ -\mathcal{D}\mathcal{J}^{(n)}(\mathbf{z}) / \|\mathcal{D}\mathcal{J}^{(n)}\|_{L^2(\Omega^{\text{design}})} & \text{in } \Omega^{\text{design}} \cap \Omega_i. \end{cases}$$

607 When  $\overline{\mathcal{D}\mathcal{J}}^{(n)}$  satisfies the sign condition (5.8), then  $\mathcal{D}\mathcal{J}^{(n)}(\mathbf{z}) > 0$  is satisfied in  
 608 the whole optimization domain  $\Omega^{\text{design}}$ . Consequently, in this case, the leading-order  
 609 approximation of the cost functional  $\mathcal{J}$  cannot be decreased anymore by a phase  
 610 change in  $\Omega^{\text{design}}$ . Therefore,  $\overline{\mathcal{D}\mathcal{J}}^{(n)}$  satisfying (5.8), is a sufficient optimal condition  
 611 that ensures that the material configuration corresponds to a local minimum of  $\mathcal{J}$ .  
 612 The iterative updating strategy of [6] for  $\Psi$  aims at fulfilling this condition. At each  
 613 iteration, the new level-set function  $\Psi^{(n+1)}$  is computed as:

$$614 \quad (5.10) \quad \Psi^{(n+1)}(\mathbf{z}) = \frac{1}{\sin(\Theta^{(n)})} \left[ \sin((1 - \kappa^{(n)})\Theta^{(n)})\Psi^{(n)}(\mathbf{z}) + \sin(\kappa^{(n)}\Theta^{(n)})\overline{\mathcal{D}\mathcal{J}}^{(n)}(\mathbf{z}) \right],$$

615 with the angle  $\Theta^{(n)}$  being defined by the projection

$$616 \quad (5.11) \quad \Theta^{(n)} = \cos^{-1} \left( \overline{\mathcal{D}\mathcal{J}}^{(n)}, \Psi^{(n)} \right)_{L^2(\Omega^{\text{design}})}.$$

617 The parameter  $\kappa^{(n)}$  in (5.10) is chosen so that the cost functional decreases at each  
 618 iteration. In practice, it is initialized to  $\kappa^{(0)} = 1$  and then at each iteration it is  
 619 determined down to a minimal value  $\kappa_{\min}$  within an inner optimization loop that  
 620 writes as:

$$621 \quad 1. \text{ Initialization to } \kappa^{(n)} = \min(2, \kappa^{(n-1)})$$

622 2. While the cost functional does not decrease  
 623 • set  $\kappa^{(n)} = \kappa^{(n)}/2$   
 624 • if  $\kappa < \kappa_{\min}$ , the level-set algorithm is stopped: the cost functional cannot  
 625 be decreased by the level-set projection  
 626 The stopping criterion of the level-set method associated with the updating (5.10) is  
 627 set as:

$$628 \quad (5.12) \quad |\Theta^{(n)}| < \delta_{\Theta}$$

629 with  $\delta_{\Theta}$  a user-chosen tolerance parameter.

630 *Remark 5.1.* Different initializations are possible for the level-set function  $\Psi^{(0)}$ ,  
 631 here we chose to compute it as  $f/||f||_{L^2(\Omega^{\text{design}})}$  with  $f$  being defined by:

$$632 \quad (5.13) \quad f(\mathbf{z}) = \begin{cases} \bar{\mu} - \mu(\mathbf{z}) & \text{if } \mu_{\text{m}} < \mu_{\text{i}}, \\ \mu(\mathbf{z}) - \bar{\mu} & \text{if } \mu_{\text{m}} > \mu_{\text{i}}, \end{cases}$$

633 where  $\bar{\mu} = (\mu_{\text{m}} + \mu_{\text{i}})/2$ .

634 **5.2. Perimeter and surface constraints.** One may want to reach a given  
 635 phase ratio in the microstructure. Consequently, we denote by  $\mathcal{A}$  the target surface  
 636 of phase  $\Omega_{\text{i}}$  in the unit cell, and we now consider the following cost functional:

$$637 \quad (5.14) \quad \mathcal{J}_{\text{main}} + \lambda \left( \frac{|\Omega_{\text{i}}|}{\mathcal{A}} - 1 \right)^2$$

638 where we added a penalization term to tend to satisfy the surface condition. The  
 639 parameter  $\lambda$  is a user-chosen parameter which is chosen so that the final configuration  
 640 is made of a surface  $|\Omega_{\text{i}}| \in [\mathcal{A} - \mathcal{A}_{\text{err}}; \mathcal{A} + \mathcal{A}_{\text{err}}]$  with  $\mathcal{A}_{\text{err}}$  also chosen by the user. An  
 641 augmented Lagrangian strategy [29] could be carried out rather than this quadratic  
 642 term with a “user-controlled” parameter  $\lambda$ , but this is beyond the scope of this paper.

643 Furthermore, for manufacturing purposes, one aims at getting smooth final con-  
 644 figurations that are not necessary obtained if we only minimize the cost functional  
 645 (5.14). Consequently one wants to minimize the following cost functional

$$646 \quad (5.15) \quad \mathcal{J}(\mathbf{m}_{\text{eff}}) = \mathcal{J}_{\text{main}} + \lambda \left( \frac{|\Omega_{\text{i}}|}{\mathcal{A}} - 1 \right)^2 + \alpha_{\text{per}} \text{Per}(\Omega_{\text{i}})$$

647 with  $\text{Per}(\Omega_{\text{i}}) = \int_{\partial\Omega_{\text{i}}} d\sigma$  the perimeter of the inclusions phase in a unit cell. In [5],  
 648 a regularized perimeter functional  $\text{Per}_{\epsilon}$  has been introduced to take into account  
 649 perimeter minimization in topology optimization. This functional has been proved  
 650 to converge to the exact perimeter as the regularization parameter  $\epsilon$  tends to 0. In  
 651 practice, the main idea is to solve sequentially the approximate problems for  $n =$   
 652  $1, \dots, N_{\text{per}}$ :

$$653 \quad (5.16) \quad \min \mathcal{J}_{\epsilon_n} := \mathcal{J}_{\text{main}} + \lambda \left( \frac{|\Omega_{\text{i}}|}{\mathcal{A}} - 1 \right)^2 + \alpha_{\text{per}} \text{Per}_{\epsilon_n}(\Omega_{\text{i}})$$

654 with  $\epsilon_{n+1} = \epsilon_n/2$ , while  $\epsilon_0$  and  $N_{\text{per}}$  are user-chosen parameters.



655 **5.3. Numerical examples.** In this section, the desired macroscopic effect is to  
 656 minimize the fields along a given direction  $\theta_{\min}$  with  $(r, \theta)$  the polar coordinates centered at  $\mathbf{X}_{\mathcal{S}} = (-35, 0)$ , where the source (2.17) is located. Following the discussion  
 657 of Section 2.2, we then want to have a change of sign for  $\mathcal{T}_1$  at  $\theta_{\min}$ . We consequently  
 658 minimize the regularized cost functional (5.16). The physical parameters are still  
 659 the one typical of steel in concrete given by Table 1, while the numerical parameters  
 660 are given in Table 5. In a first example, we chose  $\theta_I = 0$  with a surface  $\mathcal{A} = 0.2$ .

Table 5: Numerical parameters.

$\kappa_{\min}$	$\delta_{\Theta}$	$N_1$	$N_2$	$\delta_{\text{FFT}}$	$\epsilon^0$	$N_{\text{per}}$
$10^{-3}$	$10^{-1}$	101	101	$10^{-3}$	1	10

661 In the cost functional (5.16) the coefficients for the surface penalization  $\lambda$  and the  
 662 perimeter penalization  $\alpha_{\text{per}}$  are chosen so that  $\mathcal{A}_{\text{err}} = 0.06$ . Their values for each  
 663 test case is given in Table 6. Four different initializations are chosen: an ellipse of  
 664 semi-axes lengths (0.15, 0.3) and tilted of  $-\pi/4$ , the same ellipse but tilted of  $\pi/4$ ,  
 665 a random initialization with the same ratio of both materials, and the “asymptotically optimal ellipse” computed in Section 4. The initial configurations, the final configurations obtained after the optimization process, and the maps of the cumulative energy associated with the effective final configurations are plotted for these four cases in Figure 11. The initial and final values of the cost functional are also given in Tables 6 and 7, respectively. We recover the symmetry of the configuration between the first two cases. We observe that the cost functional is well decreased in every example, so we reach a better configuration by topological optimization than with the optimal ellipse. In addition, it seems that the number of iterations and the value of the cost functional are smaller when we initialize by this asymptotically optimal ellipse, so this can be considered as a valuable initialization to improve the results of the topological optimization process. A second example, for  $\theta_I = \pi/4$ ,  $\mathcal{A} = 0.3$  and  $\mathcal{A}_{\text{err}} = 0.06$  is described by Table 8, Table 9 and Figure 12. It confirms that the topological optimization algorithm decreases the cost functional. However, for the first two initializations the target angle of  $\pi/4$  does not seem to be reached so accurately, as it can be noticed in Figures 12c and 12f. In this case, initializing by the optimal ellipse seems even more relevant since the result obtained in Figure 12i is more satisfying, with a cost functional and a number of iterations which are lower than for the other initializations.

Table 6: Initial values for the different configurations with objective  $\theta_I = 0$ : surface and perimeter parameters, and values of functionals before optimization.

	$\lambda$	$\alpha_{\text{per}}$	$\mathcal{J}$ init.	$\mathcal{J}_{\text{main}}$ init.
ellipse (0.15, 0.3, $-\pi/4$ )	0.5	0.2	1.21	$9.72 \cdot 10^{-1}$
ellipse (0.15, 0.3, $\pi/4$ )	0.5	0.2	1.21	$9.72 \cdot 10^{-1}$
random	0.5	0.2	$5.23 \cdot 10^3$	$5.23 \cdot 10^3$
optimal ellipse	0.15	$5 \cdot 10^{-2}$	$1.02 \cdot 10^{-1}$	$3.61 \cdot 10^{-1}$

685 **6. Conclusion.** In this work, formulas were derived for the sensitivities of the  
 686 homogenized model that describes the propagation of low-frequency scalar waves

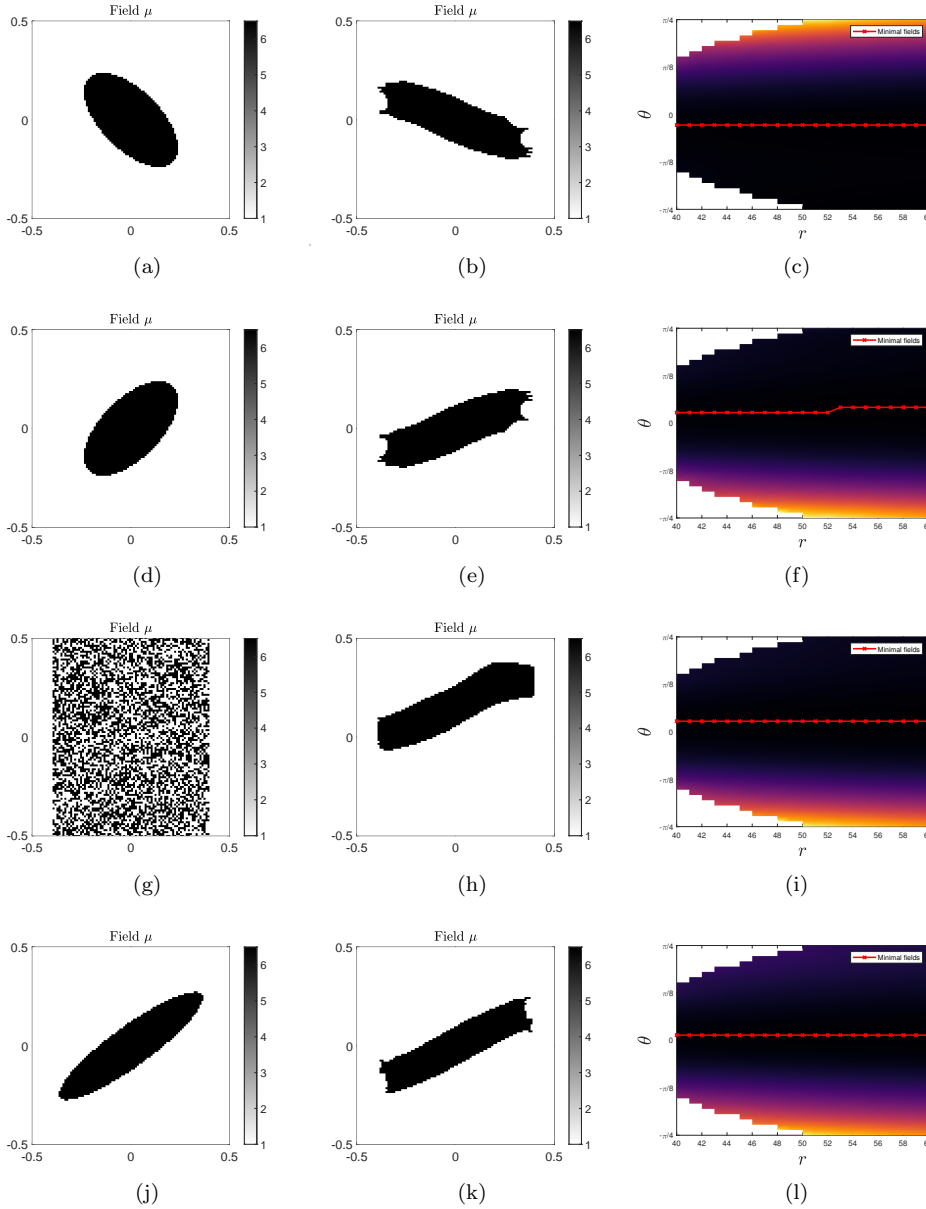


Fig. 11: Test cases for  $\theta_1 = 0$  and  $\mathcal{A} = 0.2$ . From left to right: initial configuration, final configuration, and cumulative energy in the effective medium associated to the final configuration where the position of the minimal value for a given  $r$  is denoted by the red crosses.

687 through a row of inclusions embedded in a homogeneous matrix. To do so, we con-  
 688 sidered asymptotic expansions for a unit cell where a perturbation is introduced. The  
 689 expression of the sought topological derivatives of the effective parameters involve the  
 690 solution of band cell problems in an unperturbed unit cell, and the usual polarization

Table 7: Final values for the different configurations with objective  $\theta_I = 0$ : number of iterations, final surface, and values of functionals after optimization.

	$N_{\text{iter}}$	$ \Omega_i  \text{ end}$	$\mathcal{J} \text{ end}$	$\mathcal{J}_{\text{main}} \text{ end}$
ellipse $(0.15, 0.3, -\pi/4)$	103	0.15	$2.24 \cdot 10^{-1}$	$1.4 \cdot 10^{-2}$
ellipse $(0.15, 0.3, \pi/4)$	103	0.15	$2.24 \cdot 10^{-1}$	$1.4 \cdot 10^{-2}$
random	82	0.16	$1.93 \cdot 10^{-1}$	$7.2 \cdot 10^{-3}$
optimal ellipse	60	0.14	$6.76 \cdot 10^{-2}$	$2.1 \cdot 10^{-3}$

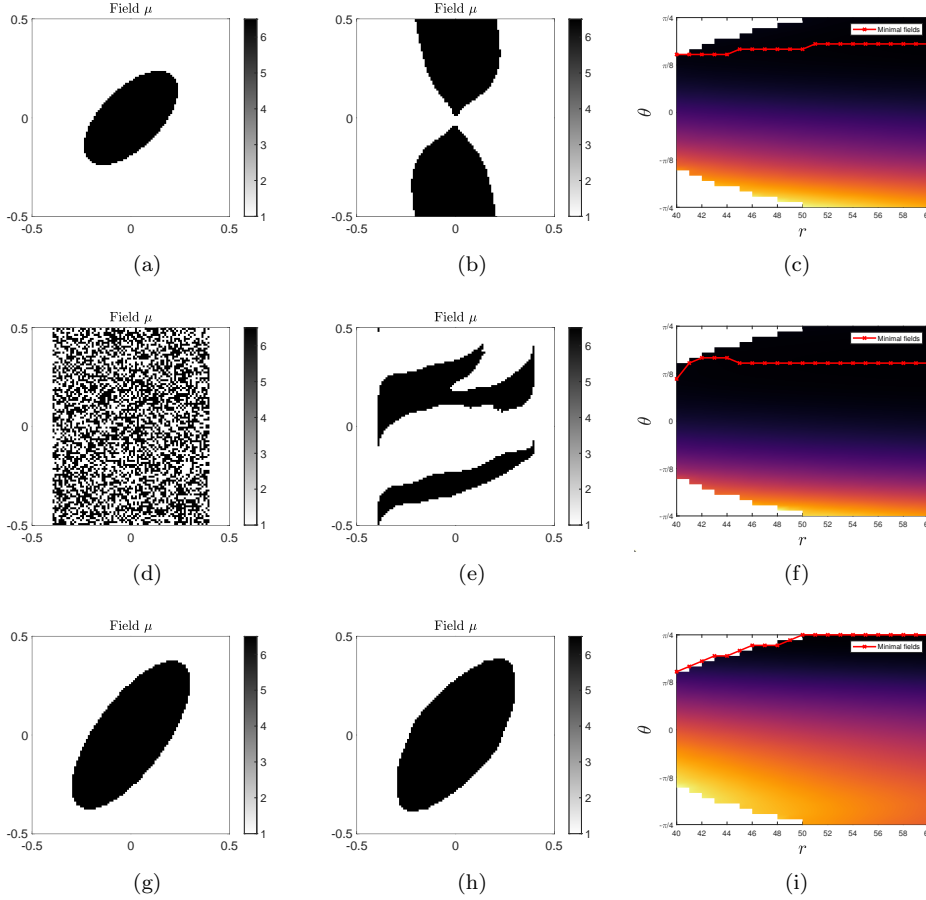


Fig. 12: Test cases for  $\theta_I = \pi/4$  and  $\mathcal{A} = 0.3$ . From left to right: initial configuration, final configuration, and cumulative energy in the effective medium associated to the final configuration where the position of the minimal value for a given  $r$  is denoted by the red crosses.

691 tensor. The numerical computation of these band cell problems had been tackled in  
 692 a previous work, while the polarization tensor is known analytically for elliptic per-  
 693 turbations, for example. The expression of the topological derivatives were validated

Table 8: Initial values for the different configurations with objective  $\theta_I = \pi/4$ : surface and perimeter parameters, and values of functionals before optimization.

	$\lambda$	$\alpha_{\text{per}}$	$\mathcal{J}$ init.	$\mathcal{J}_{\text{main}}$ init.
ellipse (0.15, 0.3, $\pi/4$ )	0.3	$7 \cdot 10^{-2}$	1.51	1.40
random	1	$1 \cdot 10^{-1}$	$2.03 \cdot 10^{-1}$	$2.11 \cdot 10^{-4}$
optimal ellipse	0.3	$7 \cdot 10^{-2}$	$6.27 \cdot 10^{-2}$	$3.30 \cdot 10^{-3}$

Table 9: Final values for the different configurations with objective  $\theta_I = \pi/4$ : number of iterations, final surface, and values of functionals after optimization.

	$N_{\text{iter}}$	$ \Omega_i $ end	$\mathcal{J}$ end	$\mathcal{J}_{\text{main}}$ end
ellipse (0.15, 0.3, $\pi/4$ )	49	0.30	$2.84 \cdot 10^{-2}$	$9.72 \cdot 10^{-5}$
random	52	0.24	$1.35 \cdot 10^{-1}$	$7.99 \cdot 10^{-4}$
optimal ellipse	28	0.28	$2.96 \cdot 10^{-2}$	$8.76 \cdot 10^{-5}$

694 numerically, and used to perform an analytical analysis of the sensitivity of the model  
 695 when considering elliptic inclusions. Then a topological optimization process was  
 696 developed to minimize a proposed cost functional, which objective was to minimize  
 697 the transmitted fields along a given direction. The material distribution is updated  
 698 at each iteration thanks to a level-set method and using the topological derivatives  
 699 obtained in the first part. Surface and perimeter constraints were also added to the  
 700 cost functional in order to reach local minima which are smoother and avoid trivial  
 701 solutions.

702 This study sets a framework for optimization of microstructured interfaces based  
 703 on their homogenized properties. This work could be extended to other configurations,  
 704 for instance:

- 705 • resonant interfaces, obtained e.g. for highly contrasted inclusions [39, 38].  
 706 In this case, frequency-dependent coefficients have been derived, and while  
 707 homogenization-based optimization procedures exist for fully periodic reso-  
 708 nant media e.g. [40], they are quite scarce for such interfaces, at the best of  
 709 our knowledge.
- 710 • high-frequency behavior. Again, the specific homogenization procedure for  
 711 higher frequencies or shorter wavelengths is well-known for fully periodic  
 712 media, and has been used for optimization [32], but could be extended to  
 713 interfaces.
- 714 • *graded* metasurfaces. By relaxing the periodicity assumption and allowing  
 715 for slow variations of the periodicity cell size along the interface, one may  
 716 obtain graded interfaces (sometimes called *quasi-periodic* [35]) able to pro-  
 717 duce stronger macroscopic effects than their strictly periodic counterparts.  
 718 Optimization procedures also exist for such configuration [30].

## 719 Appendix A. Dirichlet-to-Neumann operator.

720 In this section, the steps used in [16] to obtain the cell problem (2.9) with DtN  
 721 boundary conditions are briefly recalled. The problem initially derived in [25], posed

722 in the infinite strip  $\Omega$ , reads :

$$723 \quad (\text{A.1}) \quad \begin{cases} \nabla \cdot (\mu(\mathbf{y}) (\nabla_{\mathbf{y}} \Phi(\mathbf{y}) + \mathbf{I}_2)) = \mathbf{0} \text{ in } \Omega, \\ \mu(\mathbf{y}) [\nabla_{\mathbf{y}} \Phi(\mathbf{y}) + \mathbf{I}_2] \cdot \mathbf{n} \text{ and } \Phi \text{ are continuous on } \partial\Omega_i, \\ \Phi \text{ is } y_2\text{-periodic,} \\ \lim_{y_1 \rightarrow \pm\infty} \nabla_{\mathbf{y}} \Phi(y_1, y_2) = \mathbf{0}. \end{cases}$$

724 The variations of the physical parameters are restricted to  $\Omega^a$  due to its definition  
725 in (2.7). Introducing the half-strips  $\Omega_a^+ = [\frac{a}{2h}, +\infty[ \times I$  and  $\Omega_a^- = ] -\infty, -\frac{a}{2h}] \times I$ ,  
726 see Figure 2, the restrictions  $\Phi^\pm := \Phi|_{\Omega_a^\pm}$  satisfy  $\Delta \Phi^\pm = \mathbf{0}$  in  $\Omega_a^\pm$ , along with  
727 the periodicity and decaying conditions. The modal decomposition of these fields,  
728 classically found in the literature on waveguides [22, 13] and also used in [25] to find  
729 approximate solutions, then reads:

$$730 \quad (\text{A.2}) \quad \Phi^\pm(y_1, y_2) = \sum_{n \in \mathbb{Z}} \varphi_n^\pm e^{\mp |\xi_n| (y_1 \mp \frac{a}{2h})} \Psi_n(y_2), \text{ with } \Psi_n(y_2) = e^{i\xi_n y_2}, \xi_n = 2n\pi.$$

731 The modes  $\{\Psi_n\}$  are orthonormal for the  $L^2$  scalar product  $(\cdot, \cdot)_I$  on any vertical  
732 section  $I$ , i.e. they satisfy:

$$733 \quad (\text{A.3}) \quad (\Psi_p, \Psi_q)_I = \delta_{pq}, \text{ with } (f, g)_I := \int_I f(y_2) \overline{g(y_2)} dy_2.$$

734 Consequently, choosing the particular section  $I^+ = \{(y_1, y_2) \in \Omega_a^+, y_1 = \frac{a}{2h}\}$ , see  
735 Figure 2, yields the expression of the modal coefficients in the right half-strip:

$$736 \quad (\text{A.4}) \quad \varphi_n^+ = \left( \Phi^+ \left( \frac{a}{2h}, \cdot \right), \Psi_n \right)_I = \int_I \Phi^+ \left( \frac{a}{2h}, y_2 \right) \overline{\Psi_n(y_2)} dy_2.$$

737 One differentiates the decomposition (A.2) with respect to  $y_1$  and uses the expression  
738 of the coefficients (A.4) to get the following *Dirichlet-to-Neumann* (DtN) operator  
739 linking the traces of  $\Phi$  and of its normal derivative on the section  $I^+$  where  $\Phi = \Phi^+$ :

$$740 \quad (\text{A.5}) \quad \partial_{y_1} \Phi \left( \frac{a}{2h}, \cdot \right) = \Lambda \left[ \Phi \left( \frac{a}{2h}, \cdot \right) \right], \text{ with } \Lambda[f](y_2) = - \sum_{n \in \mathbb{Z}} (f, \Psi_n)_I |\xi_n| \Psi_n(y_2).$$

741 Similarly, focusing on the particular section  $I^- = \{(y_1, y_2) \in \Omega_a^-, y_1 = -\frac{a}{2h}\}$ , see  
742 Figure 2, provides the expression of the “left” modal coefficients of  $\Phi^-$ . The DtN  
743 relation is finally found to be the same for both interfaces  $I^\pm$ , up to the direction of  
744 the outer normal derivative:

$$745 \quad (\text{A.6}) \quad \partial_{\mathbf{n}} \Phi \left( \pm \frac{a}{2h}, \cdot \right) = \Lambda \left[ \Phi \left( \pm \frac{a}{2h}, \cdot \right) \right], \text{ where } \partial_{\mathbf{n}} = \pm \partial y_1.$$

746 The problem posed in the infinite band (A.1) can thus be rewritten as the problem  
747 (2.9) with DtN boundary conditions on the bounded cell (2.7).

748 **Appendix B. Properties of Green’s functions.** The definition of the full-  
749 space fundamental solution  $G_\infty$  in (3.9) implies:

$$750 \quad (\text{B.1}) \quad -\mu_\star \Delta_{\mathbf{r}} G_\infty(\mathbf{r}; \mu_\star) = \delta(\mathbf{r}) \quad \text{and} \quad \nabla_{\mathbf{r}} G_\infty(\mathbf{r}; \mu_\star) = -\frac{\mathbf{r}}{2\pi\mu_\star \|\mathbf{r}\|^2}.$$

751 From the problem (3.8), the decomposition of the fundamental solution  $G$  given in  
 752 (3.9) and the equalities above, the complementary part  $G_c$  is defined as the solution  
 753 of the PDE:

$$\begin{aligned}
 (B.2) \quad -\nabla_{\mathbf{y}} \cdot \left( \frac{\mu(\mathbf{y})}{\mu_m} \nabla_{\mathbf{y}} G_c(\mathbf{y}, \mathbf{x}) \right) &= \nabla_{\mathbf{y}} \cdot \left( \frac{\mu(\mathbf{y}) - \mu(\mathbf{x})}{\mu_m} \nabla_{\mathbf{y}} G_{\infty} \left( \mathbf{y} - \mathbf{x}; \frac{\mu(\mathbf{x})}{\mu_m} \right) \right) \\
 &= -\nabla_{\mathbf{y}} \cdot \left( \frac{[\mu(\mathbf{y}) - \mu(\mathbf{x})] (\mathbf{y} - \mathbf{x})}{2\pi\mu(\mathbf{x})\|\mathbf{y} - \mathbf{x}\|^2} \right)
 \end{aligned}$$

755 along with the boundary conditions:

$$(B.3) \quad \begin{cases} G_c(\cdot, \mathbf{x}) + G_{\infty} \left( \cdot - \mathbf{x}; \frac{\mu(\mathbf{x})}{\mu_m} \right) & \text{is } y_2\text{-periodic,} \\ -(\partial_{\mathbf{n}} + \Lambda) [G(\mathbf{y}, \mathbf{x})] \Big|_{y_1 = \pm \frac{a}{2h}} & = (\partial_{\mathbf{n}} + \Lambda) \left[ G_{\infty} \left( \mathbf{y} - \mathbf{x}; \frac{\mu(\mathbf{x})}{\mu_m} \right) \right] \Big|_{y_1 = \pm \frac{a}{2h}} \quad \forall \mathbf{y} \in I^{\pm}. \end{cases}$$

757 The right-hand side of the PDE (B.2) is seen to be regular as  $\mathbf{y} \rightarrow \mathbf{x}$  as soon as  
 758 the material coefficient  $\mu$  is  $C^1$  in a neighborhood of  $\mathbf{x}$ . Therefore,  $G_c(\cdot, \mathbf{x})$  and its  
 759 gradient are ensured to be regular functions when  $\mathbf{x}$  is itself in the neighborhood of  
 760 the perturbation point  $\mathbf{z}$ , which is not located on a material interface. Using the  
 761 rescaled coordinates  $(\mathbf{y}, \mathbf{x}) = (\mathbf{z} + \varepsilon\bar{\mathbf{y}}, \mathbf{z} + \varepsilon\bar{\mathbf{x}})$ , one obtains the asymptotic behavior:

$$(B.4) \quad \nabla_{\mathbf{y}} G_c(\mathbf{y}, \mathbf{x}) = \nabla_{\mathbf{y}} G_c(\mathbf{z}, \mathbf{z}) + o(1) = O(1) \quad \text{as } \varepsilon \rightarrow 0.$$

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