A stable numerical algorithm for the design of anti-reflection coating for solar cells

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Abstract: We present an efficient numerical algorithm for the design of anti-reflection coating (ARC). In contrast to the widely used direct design where the behaviour of the field is investigated, we consider the inverse problem. Our purpose is to determine the best material for the ARC which matches with some sought values of the field at the surface. Mathematically, we solve an inverse scattering problem to identify the refractive index of the ARC. For modelling, the light propagation throughout a stratified ARC the time-harmonic Maxwell equations are reduced into one dimensional Helmholtz equation with prescribed boundary conditions. From this BVP, we derive an equivalent formulation as a Fredholm integral equation. The problem is nonlinear and ill-posed. We apply Born approximation for linearisation. To obtain stable solutions, we present numerical results using the method of approximate inverse (AI). We also carry out numerical tests to compare AI to Tikhonov-Phillips method.

Keywords: anti-reflection coatings; ARCs; inverse problems.

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1 Introduction

Anti-reflection coatings (ARCs) are thin films which are deposited on optical materials to enhance their reflection and/or transmission properties. They are widely used in many application areas such as displays, ophthalmics, camera lenses to mention just few. In particular, ARCs increase significantly the performance of solar cells, see Chen (2001, 2001). These thin films with specified refractive index are deposited onto the solar cells to capture the sun light and compel the propagation of the electromagnetic waves across a boundary between two media with two different refractive indices, see, e.g., Abazid et al. (2013), Mahdjoub and Zighed (2005) and Nubile (1999).

The design of ARC is usually performed in a direct way where a prototype with specified optical properties of the coating is considered and the generated electromagnetic field is investigated. The constitutive properties are calibrated until the desired effect is realised. Our approach is based here on the optimal contrast ansatz. The objective is to determine the refractive index for the ARC from given values of the electromagnetic field at the surface. Thus, we solve an inverse electromagnetic scattering problem to identify the space dependent refractive index of the optical coating from specified reflection coefficients at the surface for multiple frequencies. For the physical modelling, we consider a stratified medium with space-dependent refractive index. From the Maxwell equations an inverse scattering problem for the Helmholtz equation in one dimension is derived. The methods for solving such an inverse problem can be classified according to two main approaches: applying nonlinear techniques, e.g., iterative algorithms or solving a linearised inverse problem. The nonlinear methods recover the unknowns of the problem iteratively from an *a priori* guess by solving a sequence of forward problems via, e.g., finite difference schemes (Lesnic, 2010). For further methods, we refer to Chen and Rokhlin (1992) based on trace formula and to Dunn and Hariharan (1984) using Spline approximation projection. For linearised inversion schemes, we may cite, e.g., Hagin (1981) based on approximations of Born or Rytov type which are valid for media with low contrasts.

For solving our inverse scattering problem, we have to overcome two difficulties: on the one hand the nonlinearity due to the dependence of field on the object's contrast function, on the other hand the ill-posedness of the problem as large errors on the solution are induced by errors on the data even for a small noise.

We linearise the mathematical model using the Born approximation, see Kak, A.C. and Slaney (1988) and Natterer (2004). In this framework, we assume the scattered field to be small enough and neglected in comparison with the incident field so that we get a linear Fredholm integral equation of the first kind. For practical use, we remain in the scope of the Born approximation which requires some limitations on the contrast function and on the relevant range of the wave numbers.

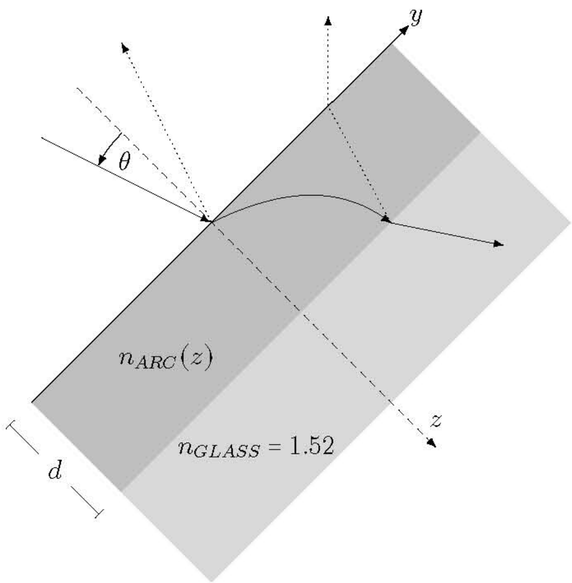
The ill-posedness of the inverse problem is caused by the non-uniqueness of the solution and the ill-conditioning of the integral operator. We apply a regularisation method to stabilise the solution (Lakhal and Louis, 2008; Lakhal, 2010, 2013). For the analytical and numerical study of regularisation methods for ill-posed problems we refer to Louis (1989, 1999). We apply here the method of the approximate inverse which is a stable and flexible regularisation scheme. It is efficient and robust for solving linear problems (Louis, 1999) and nonlinear problems (Louis, 1996, 1998). It is also powerful for image reconstruction (Louis, 2008), for feature reconstruction (Louis, 2011), and for solving inverse problems on Banach-spaces (Schuster and Schöpfer, 2010; Kohr, 2013).

We outline the content of this paper as follows: in Section 2, we present the physical background and derive the boundary value problem (BVP) from the Maxwell equations. In Section 3, we transform the model into an equivalent integral equation of Lippmann-Schwinger type. In Section 4, we deal with linearisation of problem using Born approximation. The application of the method of the approximate inverse to solve the linearised problem is treated in the same section. In the last section, we present some numerical results.

2 Physical background

For the sake of completeness we recall in this section some classical results about the physics of electromagnetic waves, see Born and Wolf (1999). Based on the Maxwell's equations in stratified media we use the mathematical modelling as a BVP for the Helmholtz equation in one dimension. We deal with the case of a normal incidence, namely the incident angle $\theta = 0$, see Figure 1.

Figure 1 ARC in contact with a glass substrate



We consider a plane time-harmonic wave propagating through a stratified non-magnetic medium with a constant magnetic permeability μ_0 and a dielectric permittivity $\varepsilon = \varepsilon(z)$ where z is the direction of stratification and of incidence. We suppose the electric wave to be linearly polarised in the direction perpendicular to the plane of incidence, i.e., a transverse electric (denoted by TE) wave. An electromagnetic wave is said to be transverse magnetic (denoted by TM) when it is linearly polarised with its magnetic wave orthogonal to the plane of incidence. We lose no generality here by considering only a TE wave since any plane wave with an arbitrary polarisation may be decomposed into two waves, one is TE and the other is a TM wave. Then, we may use the duality between the electric and the magnetic fields in the Maxwell's equations to deduce results on TM from corresponding results on TE. For a TE wave, the polarisation is along the x-direction, this means $E_y = E_z = 0$. The Maxwell's equations read

$$\nabla \times \mathbf{E} - i\omega\mu_0\mathbf{H} = 0, \tag{1}$$

$$\nabla \times \mathbf{H} + i\omega\varepsilon(z)\mathbf{E} = 0. \tag{2}$$

The coating space-dependent permittivity is given by

$$\varepsilon(z) = \varepsilon_0 n^2(z) = \varepsilon_0\left(1 + f(z)\right), \tag{3}$$

with $n(z)$ and $f(z)$ the refractive index and the contrast function of the coating respectively. We have the free space wave number $\kappa = \omega\sqrt{\mu_0\varepsilon_0}$. We further set the magnetic permeability $\mu_0 = 1$ since we have a non-magnetic medium. Inserting the TE-wave in the Maxwell equations, we get

$$\frac{\partial^2 E_x}{\partial y^2} + \frac{\partial^2 E_x}{\partial x^2} + \kappa^2 n^2(z)E_x = 0. \tag{4}$$

Using a separation ansatz $E_x = v(y)u(z)$, we get the differential system provided that the complex valued functions u and v do not vanish:

$$-\frac{v''(y)}{v(y)} = \frac{u''(z)}{u(z)} + \kappa^2\varepsilon(z), \tag{5}$$

where the left hand side depends on y and the right hand side depends on z. It yields that there exists a positive constant for physically relevant solutions

$$\frac{v''(y)}{v(y)} = -a^2, \tag{6}$$

and

$$u''(z) + \kappa^2 n^2(z)u(z) = a^2 u(z). \tag{7}$$

Let α be such that $\alpha^2 = \frac{\alpha^2}{\kappa^2}$, then

$$u''(z) + \kappa^2\left(n^2(z) - \alpha^2\right)u(z) = 0. \tag{8}$$

It follows that

$$v(y) = v(0)\left(c_1 e^{i\kappa\alpha y} + c_2 e^{-i\kappa\alpha y}\right), \tag{9}$$

with the constants c_1, c_2. Consequently

$$E_x = u(z)\left(c_1 e^{i\kappa\alpha y} + c_2 e^{-i\kappa\alpha y}\right), \tag{10}$$

where the complex-valued function u, depending on z, satisfies the differential equation (8). In the framework of ARC, we consider an incident wave $u_{inc}(z) = e^{i\kappa n_0 z}$, where n_0 is the refractive index of the air environment ($n_0 = 1$). The ARC has a given thickness d and a refractive index $n_{ARC}(z) = n(z)$, in contact with a glass substrate of uniform refractive index $n_{Glass} = n_s = 1.52$. Let the interval $\Omega = (0, d) \in \mathbb{R}$ be the bounded domain of the relevant coating with the points $z = 0$ and $z = d$ as the ARC boundaries. We consider only wave propagation in the z-direction, i.e., we set $\alpha = 0$ in (8), where u'' is the second derivative of u with respect to the model variable z. Denoting the magnitude of E_x with u, we get the scalar Helmholtz equation

$$u''(z) + \kappa^2 n^2(z)u(z) = 0, \quad z \in (0,d), \tag{11}$$

where u'' is the second derivative of u with respect to the model variable z. Equation (11) represents our model in the coating's interval (0, d). For the sake of scaling into the interval [0, 1], we replace x with x / d to obtain

$$u''(z) + \kappa^2 d^2 n^2(z)u(z) = 0, \quad z \in (0,1). \tag{12}$$

If we denote with $\beta = \kappa d$ the non-dimensionalised wave number, we get

$$u''(z) + \beta^2 n^2(z)u(z) = 0, \quad z \in (0,1). \tag{13}$$

Equation (13) is the second order differential Helmholtz equation with variable coefficient. It represents our model problem with the related boundary conditions. These are generated by the continuity of the tangential components of electric and magnetic fields across the boundaries $z = 0$ and $z = 1$. The continuity at the upper interface of the slab ($z < 0$) implies that each tangential component of the electromagnetic fields is expressed as sum of the incident and reflected (scattered) fields. Since the magnetic field H is indicated by the gradient of the electric field E, the continuity condition is thus reduced into the magnitudes of the electromagnetic field $u(0)$ together with its first derivative $u'(0)$. The solution $u(z)$ of equation (13) at $z < 0$ is a linear combination between the incident and reflected fields

$$u(z) = e^{in_0\beta z} + \mathcal{R}(\beta)e^{-in_0\beta z}, \quad z < 0. \tag{14}$$

The first derivative of $u(z)$ is given by

$$u'(z) = in_0\beta e^{in_0\beta z} - in_0\beta\mathcal{R}(\beta)e^{-in_0\beta z}, \quad z < 0, \tag{15}$$

where $\mathcal{R}(\beta)$ is called the *reflection coefficient*. Practically, the reflection coefficient can be measured for any value of β which is ranging in the interval $[\beta_{\min}, \beta_{\max}]$. In the case of the inverse problem of our model, the varying of the wave number β is motivated by the need of identifiablity of the solution of the inverse problem.

By taking the values of $u(z)$, $u'(z)$ at $z = 0$ we obtain the boundary condition

$$u'(0) + in_0\beta\, u(0) = 2in_0\beta. \tag{16}$$

The continuity at the lower interface of the slab ($z > 1$) considers only the transmitted wave. The second boundary condition is hence similarly produced by taking the values of $u(1)$ and $u'(1)$. The solution $u(z)$ of equation (13) at $z > 1$ is given by

$$u(z) = \mathcal{T}(\beta)e^{-in_s\beta z}, \quad z > 1, \tag{17}$$

where $\mathcal{T}(\beta)$ is the transmission coefficient. The first derivative $u'(z)$ is given by

$$u'(z) = +in_s\beta\mathcal{T}(\beta)e^{in_s\beta z}. \tag{18}$$

We take the values of $u(z)$, $u'(z)$ at $z = 1$ to obtain the second boundary condition

$$u'(1) - in_s\beta\, u(1) = 0. \tag{19}$$

Considering the equation (13) in addition to the slab boundary conditions (16), (19) produces mainly our model as a BVP:

$$(BVP)\begin{cases} u''(z) + \beta^2 u(z) = -\beta^2 f(z)u(z), z \in (0,1), \\ u'(0) + in_0\beta\, u(0) = 2in_0\beta, \\ u'(1) - in_s\beta u(1) = 0. \end{cases} \tag{20}$$

In the direct problem, we are concerned with the determination of the scattered electromagnetic field for a given incident field impinging upon our medium with given electromagnetic properties, namely the given space-dependent refractive index of the coating. However, in the inverse problem, we have to determine the refractive index of the coating depending on the given incident and scattered fields which are represented by the reflection coefficients.

3 Integral equation formulation

In this section, we formulate the BVP (20) as Fredholm integral equation of the first kind.

We have

$$u''(x) + \beta^2 u(x) = -\beta^2 f(x)u(x). \tag{21}$$

It is well known from the theory of differential equation that the total solution of equation (21) is the sum of solutions of its homogeneous and inhomogeneous form

$$u(x) = u_{\text{hom}}(x) + u_{\text{inhom}}(x). \tag{22}$$

The fundamental solution of the homogeneous Helmholtz equation with respect to the boundary conditions is given as

$$u_{\text{hom}}(x) = e^{i\beta x} + \eta e^{-i\beta(x-2)} =: u^0(x). \tag{23}$$

where $\eta := \frac{1-n_s}{1+n_s}$. We write the solution of the inhomogeneous Helmholtz equation using the integral operator

$$u_{\text{inhom}}(x) = -\beta^2 \int_0^1 K_\beta(x,y)u(y)f(y)dy \tag{24}$$

for a given contrast function f of the coating. We get a Fredholm equation of the second kind with respect to the field u

$$u(x) + \int_0^1 \underbrace{\beta^2 K_\beta(x,y)f(y)}_{=:\widehat{K}_\beta(x,y)} u(y)dy = u^0(x), \quad x \in (0,1). \tag{25}$$

Equation (25) is known in the scattering theory as Lippmann-Schwinger integral equation. Formulating (25) using operator notation produces:

$$(\mathcal{I} + K)u = u^0 \tag{26}$$

with the identity operator $\mathcal{I}$ and the integral operator K given by:

$$Ku(x) = \int_0^1 \widehat{K}_\beta(x,y)u(y)dy. \tag{27}$$

The integral kernel $K_\beta(x, y)$ corresponding to our model is given as:

$$K_\beta(x,y) = \begin{cases} \frac{1}{2i\beta} e^{-i\beta(x-y)} + \frac{\eta}{2i\beta} e^{-i\beta(x+y-2)} & \text{for } x \le y \\ \frac{1}{2i\beta} e^{+i\beta(x-y)} + \frac{\eta}{2i\beta} e^{-i\beta(x+y-2)} & \text{for } x > y \end{cases} \tag{28}$$

The inverse problem is concerned with the determination of refractive indices of the optical coating based on measurements of the electric field at the surface of the coating for different values of the wave numbers.

The integral formulation of the BVP is

$$u(x,\beta) = u^0(x,\beta) - \beta^2 \int_0^1 K_\beta(x,y) u(y,\beta) f(y) dy \tag{29}$$

for $x \in (0, 1)$. The electric field is measured at $x = 0$, then

$$\int_0^1 \underbrace{\beta^2 K_\beta(0,y) u(y,\beta)}_{=:\hat{K}(y,\beta)} f(y) dy = \underbrace{u^0(0,\beta) - (0,\beta)}_{=:g(\beta)} \tag{30}$$

where

$$K_\beta(0,y) = \frac{1}{2i\beta}\left(e^{i\beta y} + \eta e^{-i\beta y} e^{2i\beta}\right). \tag{31}$$

For a given field u we have to find the contrast function f. This inverse problem faces two difficulties. First of all, it is nonlinear because the dependence of the field u on the contrast function f is nonlinear. Secondly, the problem is ill-posed as the underlying operator is a compact operator between two Hilbert spaces. Hence, we need to apply regularisation methods. We refer to Louis (1989) for general analytical study of regularisation methods of ill-posed problems. We will apply the method of approximate inverse as a regularisation method in the next section.

4 Method of solution

4.1 The linearised problem via Born approximation

We linearise the problem using the Born approximation method where we suppose that u_{inhom} is very small compared to u^0 so that it can be neglected in (30) to get:

$$u(y,\beta) \approx u^0(y,\beta) \tag{32}$$

Then

$$\int_0^1 \underbrace{\beta^2 K_\beta(0,y) u^0(y,\beta)}_{=:\tilde{K}(y,\beta)} f(y) dy = \underbrace{u^0(0,\beta) - u(0,\beta)}_{=:(\beta)}. \tag{33}$$

In operator notation equation (33) reads as

$$A : X = L_2([0,1]) \to L_2([\beta_{\min}, \beta_{\max}]) = Y \tag{34}$$

$$Af(\beta) = \int_0^1 \tilde{K}(y,\beta) f(y) dy = g(\beta), \tag{35}$$

where

$$\tilde{K}(y,\beta) = \frac{\beta}{2i} e^{2i\beta y} + \frac{\beta\eta^2}{2i} e^{-2i\beta(y-2)} + \frac{\beta\eta}{i} e^{2i\beta}. \tag{36}$$

The linearised problem seeks *f* as a solution of the equation:

$$Af(\beta_j) = g(\beta_j) \qquad j = 1,\ldots,M \tag{37}$$

where β_j are samplings of the wave numbers. The Born approximation is a practical and feasible linearising method. The condition for the validity of the Born approximation is that the contrast function f is compactly supported and satisfies the inequality

$$\kappa d \sup_{x\in(0,d)} |f(x)| < 4\pi c \tag{38}$$

where *c* is a small constant, say $c = 0.16$, see, e.g., Natterer (2004). The left hand side of this inequality is a rough estimate for the phase shift between the incident field and the wave propagation throughout the object. The range of the wave numbers $[\beta_{\min}, \beta_{\max}]$ taken in the numerical test examples must satisfy the condition above in order to get a good reconstruction.

4.2 The approximate inverse

We use the method of the approximate inverse (AI), see Louis (1996). AI is a stable regularisation method since the reconstruction kernel ψ_x^γ is precomputed independently from the data *g*. Some other advantage of this method is the flexibility in the choice of the mollifier δ_x^γ appropriately to the problem. For the linear compact operator *A* in (34), this method solves the equation (37) by computing an approximation

$$f_\gamma(x) = \langle f, \delta_x^\gamma \rangle_X \quad \text{with} \quad \delta_x^\gamma \approx \delta_x. \tag{39}$$

The suitable mollifier δ_x^γ converges (as γ tends to zero) to the Delta distribution δ_x for the reconstruction point *x*. To relate the data *g* to the solution we have to determine a reconstruction kernel ψ_x^γ by solving the following auxiliary problem:

$$A^*\psi_x^\gamma = \delta_x^\gamma. \tag{40}$$

It holds:

$$f_\gamma(x) = \langle f, \delta_x^\gamma \rangle_X \tag{41}$$

$$= \langle f, A^*\psi_x^\gamma \rangle_X \tag{42}$$

$$= \langle Af, \psi_x^\gamma \rangle_Y \tag{43}$$

$$= \langle g, \psi_x^\gamma \rangle_Y =: S_\gamma g(x) \tag{44}$$

The adjoint operator of *A* is:

$$A^* : L_2([\beta_{\min}, \beta_{\max}]) \to L_2([0,1]) \tag{45}$$

$$\left(A^*, g\right)(y) = \int_{\beta_{\min}}^{\beta_{\max}} \tilde{K}^*(y,\beta) g(\beta) d\beta, \qquad y \in [0, 1]. \tag{46}$$

Applying the adjoint operator on the reconstruction kernel we get

$$\left(A^* \psi_x^\gamma\right)(y) = \int_{\beta_{\min}}^{\beta_{\max}} \tilde{K}^*(y,\beta) \psi_x^\gamma(\beta) d\beta = \delta_x^\gamma(y), \qquad y \in [0, 1] \tag{47}$$

with

$$\tilde{K}^*(y,\beta) = \overline{\tilde{K}(y,\beta)} = \frac{-\beta}{2i} e^{-2i\beta y} - \frac{\beta\eta^2}{2i} e^{+2i\beta(y-2)} - \frac{\beta\eta}{i} e^{-2i\beta}. \tag{48}$$

The reconstruction kernel can then be computed numerically.

5 Numerical results

For testing the proposed reconstruction method, we consider the contrast function

$$f(x) = \begin{cases} x & \text{for } 0 \le x \le \frac{1}{2} \\ -x+1 & \text{for } \frac{1}{2} < x \le 1 \end{cases} \tag{49}$$

The ARC is laid above the glass film which covers the solar cell. The refractive index $n(x)$ of our inhomogeneous layer must fall gradually from that of air environment to the glass substrate. Therefore, it ranges between the values 1 and 1.52 which are the refractive indices of the air and the glass respectively. Since $n^2 = 1 + f$, then the contrast function varies between the values 0 and 1.25 which are realistic boundaries for the contrast function. In our numerical reconstructions, we chose low contrasts ($f = 0$ till $f = 0.5$) to coincide with the Born approximation which is valid for low contrasts.

To generate the data, we solve the forward problem using a quadrature method (trapezoidal rule) to obtain a solution of the Fredholm integral equation of the second kind (25), avoiding the inverse crime. A comparison between exact and numerical solution of the electric field for a constant contrast function is given in Figure 2. The reconstruction kernel ψ_x^γ is calculated numerically as a solution of equation (40) independently of the data. For the reconstruction of the constant contrast function $f(x) = 0.1$ in the interval [40,900], see Figure 3. We test the validity of the Born approximation by considering the same function in the interval [15,900] where the condition of this approximation is not satisfied, see Figure 4. For reconstruction of the space-dependent contrast function $f = \frac{1}{4} y$, see Figure 5. The data are generated using the direct solver. In the case of example (49), we also validate the linearisation with the Born approximation. Therefore, we compare the numerical solution of equation (25) with the linearised integral equation (33), see Figure 6. For the inversion, we compare the calculated results using AI with the classical method of Tikhonov-Phillips which uses the minimiser $\|Af - g\|^2 + \gamma^2 \|f\|^2$, see Figure 7. A reconstruction with perturbed data for the same example is represented in Figure 8.

Figure 2 Direct simulation L_2 – Relative error = 0.0023 for λ = 80 nm(see online version for colours)

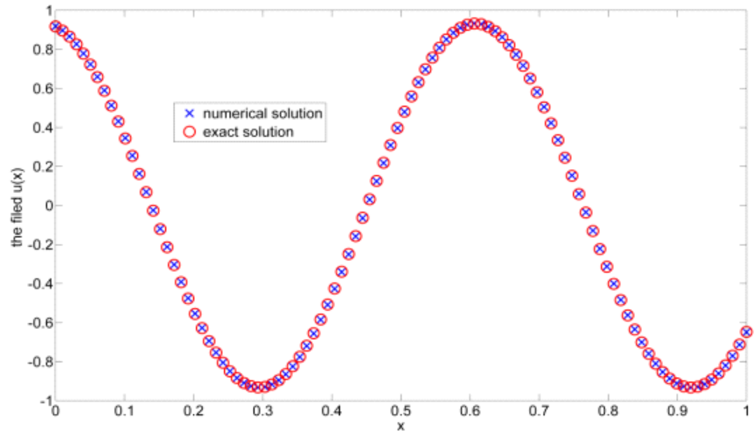


Figure 3 The inverse problem: reconstruction of $f(x)$ = 0.1 in the interval [40, 900] L_2 – Relative error = 0.1350 for the method of AI (see online version for colours)

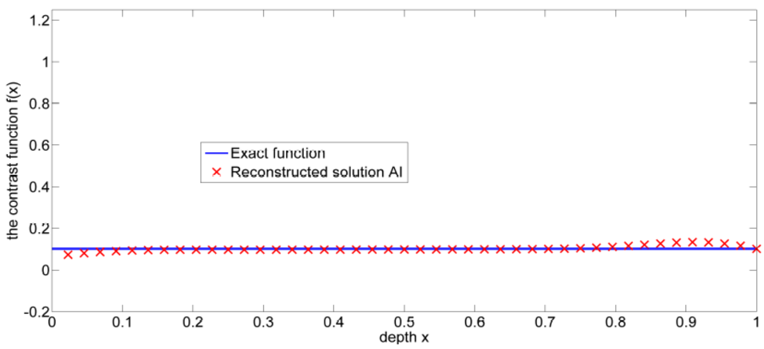
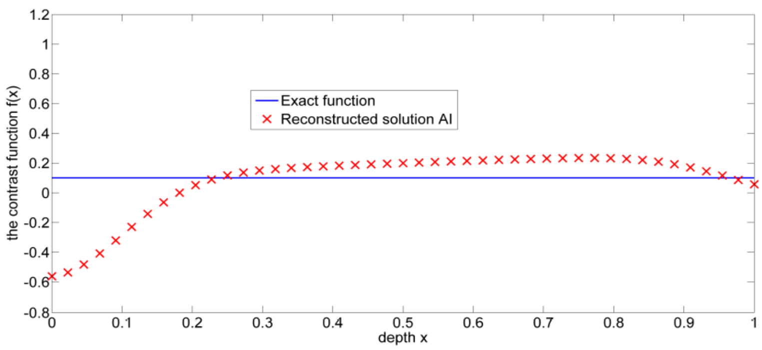
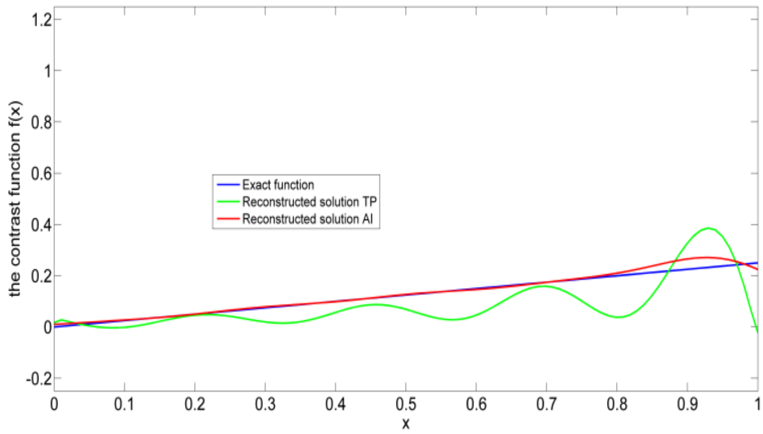


Figure 4 The inverse problem: bad reconstruction of $f(x)$ = 0.1 in the interval [15, 900] (see online version for colours)



Notes: Since this interval dose not satisfy the validity of Born approximation (38), L_2 – Relative error = 2.0911 for the method of AI.

Figure 5 The inverse problem: reconstruction of the function $f(x) = \frac{1}{4}x$ for exact solution (in blue) and reconstructed solution for the AI (in red) and TP (in green) as methods of regularisation (see online version for colours)



Notes: The relative errors are 0.0905 and 0.5355, respectively, with simulated data considered for a wave number ranging between 60 and 1,300 nm.

Figure 6 Linearisation validity: L_2 – Relative error = 0.1178 for simulated data (in blue) and one-time linearised data (in red) using the first Born approximation (see online version for colours)

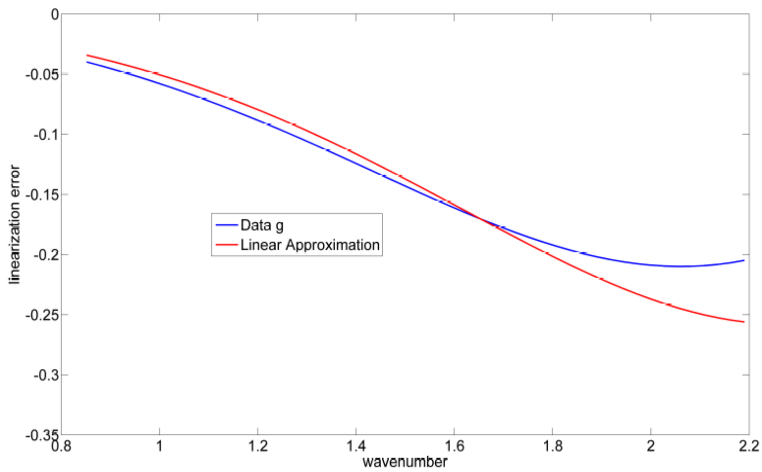
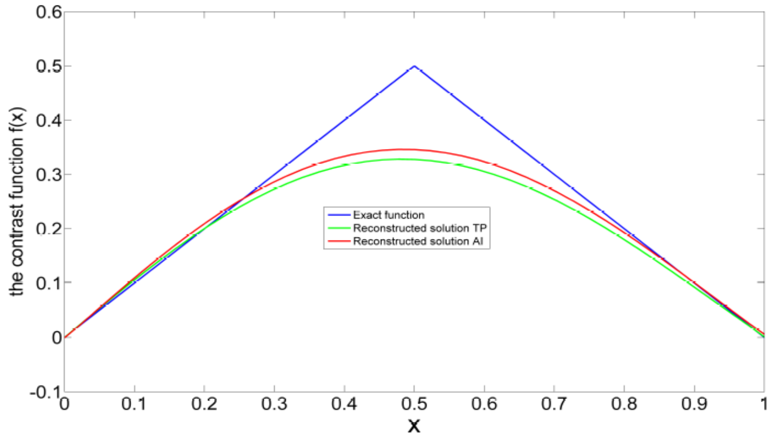
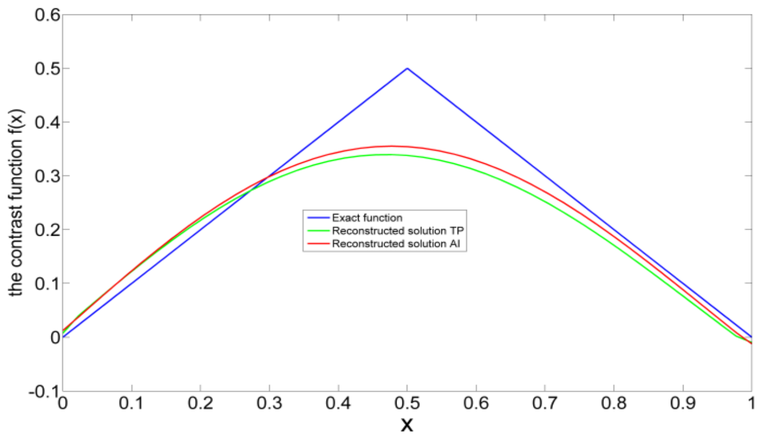


Figure 7 The inverse problem: exact solution (in blue) and reconstructed solution for the approximate inverse (in red) and Thikhonov-Phillips (in green) as methods of regularisation (see online version for colours)



Notes: The relative errors are 0.2282 and 0.1911; respectively, with simulated data considered for a wave number ranging between 350 and 900 nm.

Figure 8 The inverse problem: reconstruction of example (49) with perturbed data of level 0.2% with relative errors 0.1996 and 0.2336 for AI and TP respectively (see online version for colours)



6 Conclusions

For the design of ARCs we solved an inverse scattering problem. This approach enables us to apply a stable numerical algorithm for determining the optimal refractive index of the coating from the desired reflection coefficients at the surface. Choosing the best material for the ARC depends on appropriate given reflection coefficients (data). If the data are given in the sense of energy-control, then the best material will be determined via our algorithm. We tested our approach using simulated data generated by a direct solver. We also checked the validity of the Born approximation for the linearisation of the inverse problem. We tested the stability of the method of the approximate inverse and compare it to the widely used Tikhonov-Phillips regularisation. The extension of this contribution using nonlinear approximation of higher order and its validation with experimentally generated data will be subject to a future work.

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