

Mykhaylo ANDRIYCHUK¹, Uliana MARIKUTSA²

8. MODELING MATERIALS WITH DESIRED REFRACTIVE INDEX

The explicit solution to the diffraction problem on a set of small particles, supplemented into homogeneous material, is used for modeling the materials with the desired refractive index. The consideration concerns to the case of acoustic scalar scattering and the solution to initial scattering problem is built using an asymptotic approach. The closed form solution is reduced for the scattering problem. This lets an explicit formula for the refractive index of the resulting inhomogeneous material to be obtained. The numerical calculations show the possibility of getting the specific values of refractive index including its negative values.

8.1. INTRODUCTION

The materials with the specific physical properties, in particular with negative refractive index play an important role in the process of improving the radiation performances of the different IC and radioelectronic devices. Such materials are used widely for improving the radiation performances of microstrip antennas of different types, microwave filters and field transformers. There are different approaches to forming specific properties of the medium (material) by embedding into it a series of inclusions. This leads to the formation of the physical properties of resulting material that are different to those that are inherent to the properties of initial material. The theoretical prediction of the existence of such materials was made in the pioneer work [1] and thereon, such materials were designed by the variety recipes. As early as the eighties of the last century, these materials received the name *chiral* and began to be used in various areas of antenna technology [2], manufacturing of electronic devices [3], [4], and telecommunications equipment [5]. The goal of this paper is to propose the numerical approach (based on [6] and [7]) for modeling the material with the specific refractive index, including its negative values. The approach foresees reducing

¹ Ivan Franko National University of Lviv, Ukraine

² Lviv Polytechnic National University, Ukraine

an explicit solution to the respective acoustic scattering problem, and the explicit formula for the resulting refractive index based on the asymptotic solution to acoustic wave scattering problem on a set of big number of embedded particles of small size. The chapter is organized as follows: Section 8.2 is devoted to statement of diffraction problem and outline of application limits of geometrical and physical parameters of the material under consideration. The analytical form of solution will be derived in Section 8.3, and the numerical aspects of solving the respective system of linear algebraic equations (SLAE) will be presented here. The explicit formula for the refractive index of resulting inhomogeneous material will be derived in Section 8.4. The numerical results, related to exactness of asymptotic solution to the initial diffraction problem and properties of material with obtained refractive index will be presented in Section 8.5. A short conclusion finalizes the discussed topic under consideration.

8.2. STATEMENT OF SCATTERING PROBLEM

A combination of both the asymptotic method and numerical simulation is used to solve the problem of creating a material with specified scattering characteristics, particularly, with a given refractive index. The initial diffraction problem is solved by assumption: $ka \ll 1$, and $d \gg a$, a is the characteristic size of the particle, d is the distance between adjacent particles, $k = 2\pi/\lambda$ is the wave number.

An asymptotic solution to the scattering problem on many particles by assumptions: $d = O(\sqrt[3]{a})$, and $M = O(a^{-1})$ was obtained in [6], M is the total number of particles contained in a given domain $D \subset R^3$.

The impedance boundary conditions

$$\zeta_m = q(x_m)/a^\kappa \quad (8.1)$$

are prescribed on the boundary S_m of m -th particle, where ζ_m is boundary impedance, $x_m \in D_m$, $q_m = q(x_m)$; $q(x)$ is arbitrary function, continuous in \bar{D} ; $Im q \leq 0$, and $d = O(a^{(2-\kappa)/3})$, where $M = O(1/a^{2-\kappa})$, and $\kappa \in (0,1)$.

The incident field satisfies Helmholtz equation in the whole R^3 , by this, the scattered field satisfies the radiation conditions. We assume that a small particle is a sphere of radius a with center in point x_m , $1 \leq m \leq M$.

The full field u_M satisfies equation

$$[\nabla^2 + k^2 n_0^2(x)]u_M = 0 \text{ in the domain } R^3 \setminus \bigcup_{m=1}^M D_m, \quad (8.2)$$

and boundary conditions

$$\partial u_M / \partial N = \zeta_m u_M \text{ in } S_m, \text{ where } 1 \leq m \leq M, \quad (8.3)$$

and

$$u_M = u_0 + v_M, \quad (8.4)$$

u_0 is the solution of problem (8.2) – (8.4) at $M=0$ (namely, when D does not contain the particles), $u_0 = e^{ik\alpha \cdot x}$ is the incident field, and field v_M satisfies the radiation conditions.

Let $q(x)$ belong to $C(D)$, $\Delta_p \subset D$ is arbitrary subdomain of D , and $K(\Delta_p)$ is the total number of particles in Δ_p determined by

$$K(\Delta_p) = 1/a^{2-\kappa} \int_{\Delta_p} N(x)dx \cdot [1 + o(1)] \quad \text{at } a \rightarrow 0, \quad (8.5)$$

where function $N(x) \geq 0$ is given and continuous in domain D .

It was substantiated in [6] that there exists some specific field $u_e(x)$ (limiting field), which satisfies the next condition

$$\lim_{a \rightarrow 0} \|u_e(x) - u(x)\| = 0, \quad (8.6)$$

and solution to the initial diffraction problem (8.2) – (8.4) can be sought from the equation

$$u(x) = u_0(x) - 4\pi \int_D G(x, y)q(y)N(y)u(y)dy, \quad (8.7)$$

where $G(x, y)$ is the Green function for Helmholtz equation (8.2) for the case of absence of the particles. This fact allows us to use the approximate solution $u_e(x)$ instead of exact solution $u(x)$ and to obtain an explicit formula for refractive index of constructed inhomogeneous material.

8.3. THE SEMIANALYTICAL FORM OF SOLUTION TO SCATTERING PROBLEM

In order to derive the explicit formula for approximate field, we introduce the concept of limiting (effective) field $u_e(x)$. In paper [6], it was substantiated that the exact solution to problem (8.2) – (8.4) can be presented in the form

$$u_M(x) = u_0(x) + \sum_{m=1}^M \int_{S_m} G(x, y) v_m(y) dy. \quad (8.8)$$

Despite the fact that this last equation contains an unknown function $v_m(y)$ in the integrand, in contrast to formula (8.7), where all functions in the integrands are known, it is used to obtain an approximate solution to the original diffraction problem. For this goal, we define the effective field $u_e(x, a) = u_e^{(m)}(x)$, which acts on the m -th particle as

$$u_e(x) = u_M(x) - \int_{S_m} G(x, y)v_m(y)dy, \quad x \in R^3, \quad (8.9)$$

and the next relation for the neighboring points is valid $|x - x_m| \sim a$. We present the exact formula (8) in form

$$u_M(x) = u_0(x) + \sum_{m=1}^M G(x, x_m) R_m + \sum_{m=1}^M \int_{S_m} [G(x, y) - G(x, x_m)] v_m(y) dy, \quad (8.10)$$

where the values R_m are

$$R_m = \int_{S_m} v_m(y) dy. \quad (8.11)$$

Using the known relation for function $G(x, y)$ from [8], and the asymptotic formula for values R_m [6], we obtain the next formula for $u_M(x)$

$$u_M(x) = u_0(x) + \sum_{m=1}^M G(x, x_m) R_m + o(1) \text{ at } a \rightarrow 0 \text{ for } |x - x_m| \geq a. \quad (8.12)$$

The values R_m are defined by the asymptotic formula

$$R_m = -4\pi q(x_m) u_e(x_m) a^{2-\kappa} [1 + o(1)], \text{ if } a \rightarrow 0, \quad (8.13)$$

and asymptotic formula for function v_m is

$$v_m = -q(x_m) u_e(x_m) \cdot \frac{1}{a^\kappa} \cdot [1 + o(1)], \text{ if } a \rightarrow 0. \quad (8.14)$$

Using last two formulas, we obtain the asymptotic representation of the effective field in the vicinity of particles

$$u_e^{(j)}(x) = u_0(x) - 4\pi \sum_{m=1, m \neq j}^M G(x, x_m) q(x_m) u_e(x_m) a^{2-\kappa} [1 + o(1)], \quad (8.15)$$

which is valid in the domains $|x - x_j| \leq a$, where $1 \leq j \leq M$.

In order to calculate the values of the effective field everywhere using formula (8.15), we should know the values $u_e(x_m)$. They can be easily obtained as solutions to the following SLAE

$$u_j = u_{0j} - 4\pi \sum_{m=1, m \neq j}^M G(x_j, x_m) q(x_m) u_m a^{2-\kappa} \text{ for } j = 1, \dots, M, \quad (8.16)$$

where $u_j = u(x_j)$ and $j = 1, 2, \dots, M$. The matrix of SLAE (8.16) is diagonally dominant, therefore it is convenient for solving numerically. It was proven in [9] that this SLAE has a unique solution for sufficiently small a .

In order to justify the exactness of solution to SLAE (8.16), which is used for determination of the effective field, we derive different SLAE, corresponding to the

limiting equation (8.7). Let us divide the domain D , where the small particles are located, into an union of the small non-intersecting cubes Δ_p with centers at points y_p , the side of such cubes can be chosen as $O(d^{1/2})$. Because the limited quantity of cubes cannot give whole D , we consider their smallest partition that contains D , and define values $n_0^2 = 1$ in the cubes, which do not belong to domain D .

In order to find the solution to equation (8.7), we apply the collocation method proposed in [9]. In accordance with this method, we obtain such SLAE

$$u_j = u_{0j} - 4\pi \sum_{p=1, p \neq j}^P G(x_j, x_p) q(y_p) N(y_p) u_p |\Delta_p|, \quad j = 1, \dots, P \quad (8.17)$$

where P is the number of cubes that form a partition of D , y_p is a center of p -th cube, $|\Delta_p|$ is its volume. Since the value of d is small, diameter Δ_p can be of an order larger than distance d between particles. Since $P \ll M$, then solving SLAE (8.17) is much easier than solving SLAE (8.16) in terms of the number of calculations.

As a result, we have two different SLAE (8.16) and (8.17). Solving both the SLAE, we can compare their solutions and evaluate the area of accuracy of asymptotic solution (8.15). This evaluation has also a practical importance as allows the determination of the optimal parameters of the domain D , which provide the possibility to create the refractive index that is the closest to the desired one.

8.4. REFRACTIVE INDEX OF THE OBTAINED MATERIAL

The explicit formula (8.7) for the effective field opens the way to determining the refractive index of the obtained material. It is important from the practical point of view, how the calculated refractive index $n_M^2(x)$ differs from those obtained from the theoretical assumptions. We confine here by the real refractive index and formulate the constructive algorithm to obtain the desired one. It consists of three steps.

- Step 1: using known $n_0^2(x)$ and unknown $n^2(x)$, we calculate function $p(x) = k^2 [n_0^2(x) - n^2(x)] = p_1(x)$.
- Step 2: using the relation $p(x) = 4\pi q(x)N(x)$ we determine

$$N(x)q(x) = \frac{p_1(x)}{4\pi}. \quad (8.18)$$

Equation (8.18) for two unknown functions $q(x)$ and $N(x)$ has infinite number of solutions $\{q(x), N(x)\}$, for which the conditions $N(x) \geq 0$ are fulfilled. In this connection, the solution to (8.18) we determine as

$$q(x) = \frac{p_1(x)}{4\pi N}. \quad (8.19)$$

Calculation of $N(x)$ and $q(x)$ by (8.19) finalized Step 2 of our procedure.

- Step 3: is completely constructive and its goals are the following:
 - to create on the small particle of radius a the necessary impedance $q(x_m)/a^\kappa$;

- to embed the particles that satisfies the properties (8.19) into domain with the initial properties.

The application of the above algorithm was considered in [10] for the case of complex function $q(x)$, the above algorithm can be applied if material is lossless.

8.5. NUMERICAL MODELING

8.5.1. Checking the applicability of asymptotic solution

Exactness of solution of the limiting equation (8.7)

The computational check for the determination of the exactness of solution to (8.7) foresees carrying out the calculations with a set of different problem's parameters. We calculate the absolute and relative errors in the process of growth of the number of collocation points. The dependence of error of the parameter $p = \sqrt[3]{P}$, where P is the total number of the small domains (cubes) in D for $k = 1.0$, $l_D = 0.5$, and $a = 0.01$ for the different values of function $q(x)$ are shown in Fig. 8.1 and Fig. 8.2 (dimension of k is cm^{-1} , and linear sizes of D are prescribed in cm) respectively. The solution, which corresponds to $p = 20$ ($P = 20^3$), is considered as a benchmark.

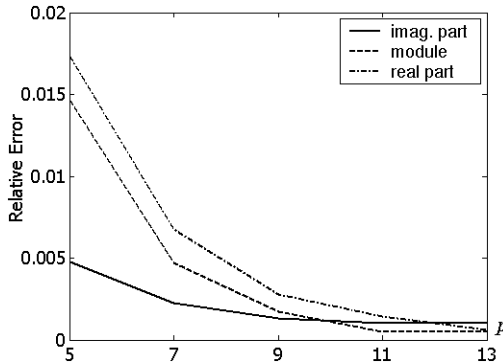


Fig. 8.1. The relative error versus parameter p , $q(x) = k^2(0.008 - 0.0011i)$

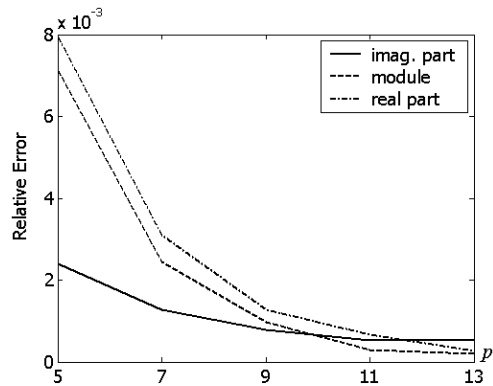


Fig. 8.2. The relative error versus parameter p , $q(x) = k^2(0.008 - 0.0027i)$

The relative error of solution to (8.7) is equal to 1.05% and 0.023% for the real and imaginary parts if $p = 5$ (5^3 collocation points), it diminishes to 0.72% and 0.053% respectively at $p = 6$ (6^3 collocation points), and to values 0.287% and 0.018% at $p = 8$ (8^3 collocation points), (see Fig. 8.1). This error is less than 0.009% for the real part of solution if $p = 12$, it tends to zero if value p grows. The error depends of the values of function $q(x)$ too, it diminishes if the imaginary part of $q(x)$ decreases (see Fig. 8.2). The error of real part of solution if $p = 19$ is equal to 0.009%, and error of imaginary part is thousandths of a percent. The obtained results confirm that calculation of the values of

approximate field can be carried out with the high enough accuracy, and this accuracy is attained in a wide range of the geometrical and physical parameters of the material under investigation.

The results of computations show that the relative error depends of the parameter k to a large extent. In Fig. 8.3 and Fig. 8.4, the error is shown at $k = 2.5$ and $k = 0.75$ respectively, $q(x) = k^2(0.008 - 0.0011i)$. One can see that the error is of one order larger at $k = 2.5$. The maximal error (if $p = 5$) at $k = 0.75$ is less on 27% than those for $k = 1.0$.

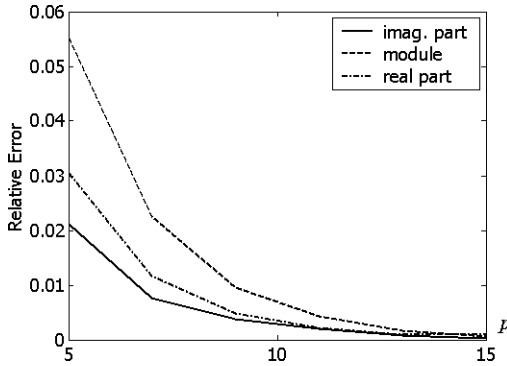


Fig. 8.3. The relative error versus parameter p , $k = 2.5$

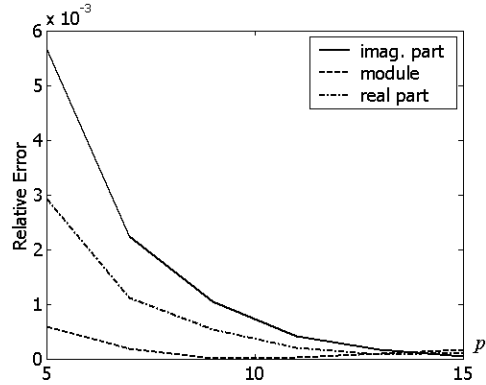


Fig.8.4. The relative error versus parameter p , $k = 0.75$

Comparison of solutions to limiting equation (8.7) and asymptotic SLAE (8.16)

In the previous subsection, we consider the solution to SLAE (8.17) with $p = 20$ as benchmark solution to equation (8.7). The maximal value of relative error for this p does not exceed 0.009% for wide range of the problem's parameters. The numerical calculations are presented for the different sizes of D and different functions $N(x)$. The obtained results for small values m are shown in Table 8.1 for $l_D = 1.0$, $k = 1.0$, and $N(x) = 40$. The values of a_{est} , which are received by formula (8.20), when the expected number $K(\Delta_p)$ of particles is changed by M . For this case, the radius of particle is determined as

$$a_{est} = \left(M / \int_{\Delta_p} N(x) dx \right)^{1/(2-\kappa)}. \quad (8.20)$$

Table 8.1. The optimal parameters of domain D at small m , $N(x) = 40$

m	8	10	12	14	16
a_{est}	0.1397	0.0682	0.0378	0.0247	0.0152
a_{opt}	0.1054	0.0603	0.0369	0.0252	0.0169
d	0.1329	0.1099	0.0917	0.0787	0.0679
Relative error	2.47%	0.42%	0.41%	1.09%	0.77%

The values of a_{opt} in the third row correspond to the optimal values of radius a , which guarantees the minimal error for module of solution to equation (8.7) and system (8.16).

In the fourth row, the values of distance d between particles are shown. The maximal value of error is attained at $m = 8$, the error diminishes if m grows. The numerical results for large m with the same initial data are shown in Table 8.2. The minimal error of solution is attained at $m = 65$ (total number of particles $M=27.46 \cdot 10^4$), and it is equal to 0.20%.

Table 8.2. The optimal parameters of domain D at large m , $N(x) = 40$

m	25	35	45	55	65
a_{est}	0.0079	0.0024	0.00121	$6.45 \cdot 10^{-4}$	$3.96 \cdot 10^{-4}$
a_{opt}	0.0076	0.0022	0.0010	$6.31 \cdot 10^{-4}$	$3.89 \cdot 10^{-4}$
d	0.0514	0.0329	0.0241	0.0198	0.0171
Relative error	0.53%	0.31%	0.34%	0.23%	0.20%

Table 8.3 contains the comparable results for $N(x) = 4$ with the same set of initial data. One can see that the relative error diminishes if the number M of particles increases (one should note that the relative error depends on parameters a and l_D too). This error tends to relative error of solution to equation (8.7) if the value of m becomes larger than 80 ($M = 5.12 \cdot 10^5$).

Table 8.3. The optimal parameters of domain D at large m , $N(x) = 4$

m	25	35	45	55	65
a_{est}	$9.98 \cdot 10^{-4}$	$3.30 \cdot 10^{-4}$	$1.51 \cdot 10^{-4}$	$8.19 \cdot 10^{-5}$	$4.99 \cdot 10^{-5}$
a_{opt}	$1.02 \cdot 10^{-3}$	$3.32 \cdot 10^{-4}$	$1.51 \cdot 10^{-4}$	$8.20 \cdot 10^{-5}$	$4.99 \cdot 10^{-5}$
d	0.0526	0.0345	0.0256	0.0204	0.0169
Relative error	0.19%	0.09%	0.1108%	0.06%	0.02%

Investigation of difference between solutions to SLAE (8.16) and (8.17)

The comparison of solutions to SLAE (8.16) and (8.17) was carried out for the different values of a at different p and m . The relative error of SLAE (8.16) diminishes if p increases while m remains constant. As an example, if p increases to 50%, then the relative error diminishes to 11.7% (if $p = 8$ and $p = 12$, $m = 15$).

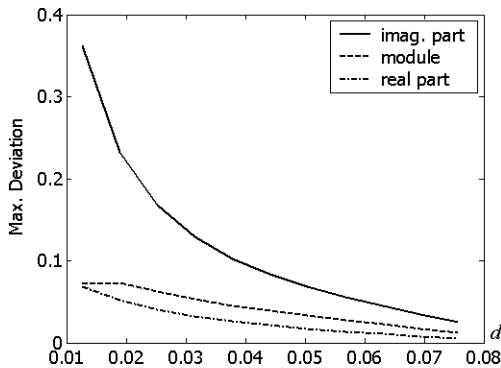


Fig. 8.5. Dependence of deviation of the solution's components of distance d between particles, $N(x) = 10$

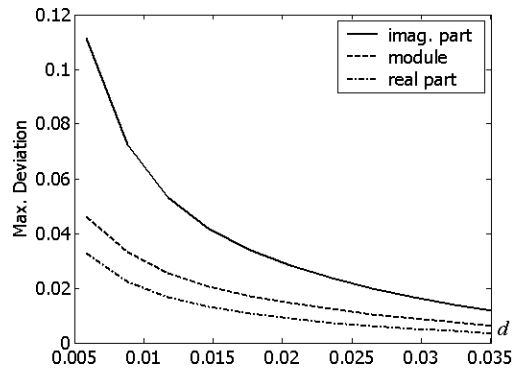


Fig 8.6. Dependence of deviation of the solution's components of distance d between particles, $N(x) = 30$

The differences in solutions to SLAE (8.16) and (8.17) in the real part, imaginary part, and module are shown in Figs. 8.5 and 8.6 if $p = 7$ and $m = 15$. By this, the difference of real parts do not exceed 3.9% at $a = 0.01$, it is less than 3.3% at $a = 0.007$, and it is less than 1.85% if $a = 0.004$, $d = 9a$, and $N(x) = 20$. Respectively, this difference is less than 0.075% if $p = 11$, $a = 0.001$, and $N(x) = 30$, $d = 15a$ (m is the same). The numerical results, obtained for a wide range of d , show that its optimal value exists, and starting from this value, the deviations of solutions begin to increase again. Such optimal values of d are presented in Table 8.4 for the different constant $N(x)$. The results obtained testify that the optimal distance between particles increases if the number of particles grow. For the small number of particles, the optimal distance is of the same order that a , for the set number of particles ($M = 15^3$, namely $m = 15$). This distance is of an order larger. The values of the minimal and maximal errors, which are attained for the optimal d , are shown in Table 8.5.

Table 8.4. Optimal values of d for the different constant $N(x)$

	Value of $N(x)$				
	10	20	30	40	50
$a = 0.004$	0.0711	0.0468	0.0468	0.0469	0.0381
$a = 0.01$	0.0864	0.0559	0.0595	0.0594	0.0496

Table 8.5. The relative error of solution to SLAE (8.16) in % (min/max) for the optimal d

	Value of $N(x)$				
	10	20	30	40	50
$a = 0.004$	0.69/0.09	5.17/0.48	0.48/0.109	0.95/0.121	0.28/0.06
$a = 0.01$	2.39/0.19	1.67/0.29	0.51/0.09	2.4/0.41	1.47/0.17

The obtained results allow us to conclude that the optimal value of d diminishes slower, when function $N(x)$ grows, additionally this trend is more significant for the smaller a .

5.2. Modeling the material with the desired refractive index

Numerical calculations are carried out for the case $N(x) = \text{const}$. For simplicity, we consider the case when a given domain D consists of the same subdomains Δ_p . This limit is not essential for the numerical modeling.

Numerical calculations were performed for the case when $D = \bigcup_{p=1}^P \Delta_p$, and $P = 20^3$, D is some cube with side $l_D = 0.5$ and particles are placed uniformly in domain D (the relative error of the solution to system (8.16) does not exceed 0.01% for this P). Let the initial domain D be the material with the initial refractive index $n_0^2(x) = 1$. Then the values $N(\Delta_p)$ can be calculated using the formula (8.5). On the other hand, we can choose the number m such that $M = m^3$ is closest to number $N(\Delta_p)$. It is easy to see that the corresponding $n^2(x)$ for such M is calculated by such formula

$$\tilde{n}^2(x) = -\frac{4\pi M q(x)}{k^2} + n_0^2 \quad (8.21)$$

that is, the obtained value of the refractive index differs on $n^2(x)$. To obtain the minimum difference, we choose numbers m_1 and m_2 that satisfy the inequality $M_1 < N(\Delta_p) < M_2$ where $M_1 = m_1^3$ and $M_2 = m_2^3$. Therefore, if we have the value $N(\Delta_p)$ for the fixed a , we can obtain the numbers M_1 and M_2 , and to calculate also the nearest to the $n^2(x)$ values by the formula (8.21).

The dependence of the maximal relative error for the calculated values of $\tilde{n}^2(x)$ on radius a of a particle is shown in Fig. 8.7 for $N(x)=50$ for complex function $q(x)$ (in Figs. 8.7 – 8.9, the solid and dashed lines correspond to the real part and imaginary part).

The obtained results testify that the relative error considerably depends on the parameters M_1, M_2 , and $K(\Delta_p)$. This error is smallest if the value of numbers M_1 or M_2 are much closer to value $K(\Delta_p)$. The error has periodic character that is defined by the properties of functions $K(\Delta_p)$ and by the values of parameters M_1 and M_2 . The mean of error in the period grows if a increases. The comparable results are shown in Fig. 8.8 and Fig. 8.9 at $N = 20$ and $N = 50$ respectively.

The minimal value of error 0.49% is attained for $a = 0.015$ and it is equal to 0.51% if $a = 0.008$, and 0.26% if $a = 0.006$ for $N(x) = 5, 20, 50$ respectively.

The uniform placement of particles in domain D is the simplest from the practical point of view. Using the data, given in Figs. 8.7 – 8.9, we can evaluate the number M of particles, which is necessary to obtain the refractive index more closer to the desired one (at given parameter l_D of domain D). The respective results are shown for $l_D = 0.5$ in Fig. 8.10. The values $m = \sqrt[3]{M}$ are shown on the y axis. The solid, dashed and dot-dashed lines correspond to values $N(x) = 5, 20, 50$ respectively. The knowledge about the optimal number of particles in the domain D is the subsequent step to creating a material with the given refractive index.

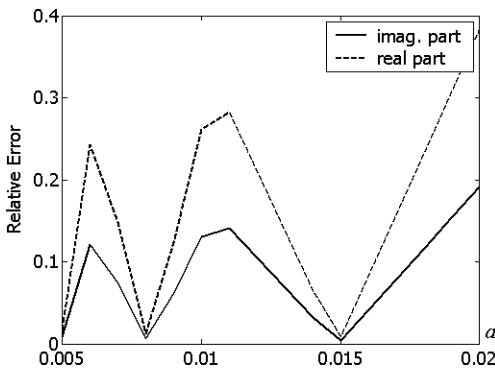


Fig. 8.7. The maximal relative error of the modeled refractive index $\tilde{n}^2(x)$, $N = 5$

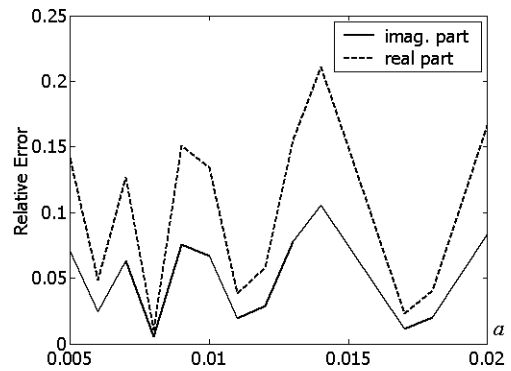


Fig. 8.8. The maximal relative error of the modeled refractive index $\tilde{n}^2(x)$, $N = 20$

The data shown in Fig. 8.10 testify that the optimal number of particles diminishes if their radius a grows. The estimation $\sqrt[3]{a^{(2-\kappa)}}$ determines the distance d between particles. This distance differs from that is determined by uniform placement of particles in D . As an example, for $N = 5, a = 0.0107$ it is equal to 0.1361, and the calculated d is equal to 0.119 and 0.159 for $m = 5$ and $m = 4$ respectively. The computations show that the relative difference between these two values of d is quite proportional to the relative error of the refractive index.

Since this value d does not depend on the diameter of D in accordance to estimation $d = \sqrt[3]{a^{(2-\kappa)}}$, it can be applied as an additional parameter for optimization while choosing the alternative values of m . On the other hand, we can evaluate the number of particles in D by the known formula [10]. With $K(\Delta_p)$, we can calculate the quantity M of particles if they are distributed uniformly in D . The distance between particles is calculated easy too if l_D is prescribed.

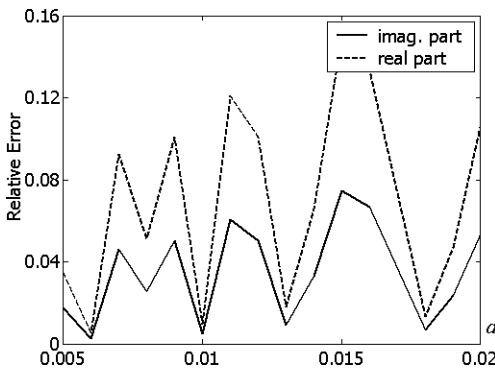


Fig. 8.9. The maximal relative error of the calculated refractive index $\hat{n}^2(x)$, $N = 50$

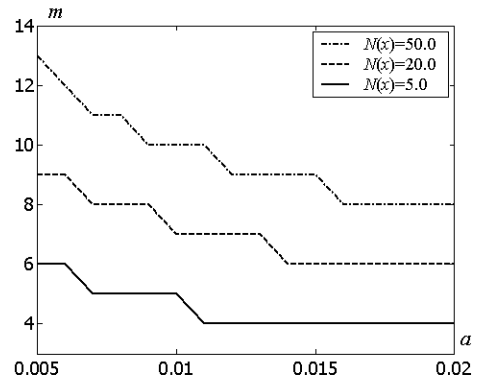


Fig. 8.10. The optimal value of m versus radius a of particles for different $N(x)$

8.6. CONCLUSIONS

The asymptotic approach has been developed to solve the problem of acoustic scattering on a set of small size particles (bodies) placed in a homogeneous material. The scattering problem is reduced to solving a corresponding SLAE whose dimension is equal to the number of particles. The solutions of this system are used in the formula of explicit representation of the components of the scattered field. Numerical calculations are performed that determine the accuracy of the obtained solution depending on the physical parameters of the problem.

The obtained numerical results demonstrate the possibility of applying the proposed technique to create materials with specified acoustic properties, in particular the refractive index. A constructive algorithm for modeling the material with the desired refractive index is proposed.

The results of numerical modeling open up the possibility of engineering solutions for practical applications. As an example, uniform placement of particles is the easiest way to

engineering design, and the answer to how many particles should be placed in a given domain is given by the numerical simulation results.

The engineering problems regarding the placement of a large number of small particles in a given domain D and creating on their surface the necessary impedance $\zeta = q(x)/a^\kappa$ require the separate technological solutions.

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