

Improvement of Mishchenko's T -matrix code for absorbing particles

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The use of Gaussian elimination with backsubstitution for matrix inversion in scattering theories is discussed. Within the framework of the T -matrix method (the state-of-the-art code by Mishchenko is freely available at <http://www.giss.nasa.gov/~crmim>), it is shown that the domain of applicability of Mishchenko's FORTRAN 77 (F77) code can be substantially expanded in the direction of strongly absorbing particles where the current code fails to converge. Such an extension is especially important if the code is to be used in nanoplasmonic or nanophotonic applications involving metallic particles. At the same time, convergence can also be achieved for large nonabsorbing particles, in which case the non-Numerical Algorithms Group option of Mishchenko's code diverges. Computer F77 implementation of Mishchenko's code supplemented with Gaussian elimination with backsubstitution is freely available at <http://www.wave-scattering.com>. © 2005 Optical Society of America
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1. Introduction

Matrix inversion is, unfortunately, an unavoidable step in many single-scattering^{1–6} and multiple-scattering^{7–10} theories. For instance, the method of choice in acoustic and electromagnetic wave scattering off a general scatterer of finite size is the so-called Waterman extended boundary condition method (EBCM), also known as the T -matrix method.^{1,2} EBCM yields the single-scatterer T matrix as the product

$$T = -\text{Rg}(Q)Q^{-1}, \quad (1)$$

where $\text{Rg}(Q)$ and Q are known matrices given in terms of surface integrals.^{1–5} In the case of a multiple-scattering off a finite stack of arbitrarily stacked parallel planes of periodically arranged scatterers, the method of choice is the so-called LEED or LKKR method.^{7–10} (Here the respective acronyms LEED and LKKR specify the application of the same *ab initio* multiple-scattering theory to different waves rather than the use of two different methods: LEED stands for the low-energy electron diffraction,^{7,8} whereas one uses the notion of LKKR, which

stands for the layer Korringa–Kohn–Rostocker method,^{9,10} when dealing with multiple scattering of classical waves.) Each plane of periodically arranged scatterers is characterized by a pair of transmission matrices, Q^I and Q^{IV} , and by a pair of reflection matrices, Q^{II} and Q^{III} , which are the respective members of a pair that characterizes transmission and reflection properties with regard to waves incident to the two opposite sides of the plane. Given the reflection and transmission matrices Q_1 and Q_2 of two layers of periodically arranged scatterers, the reflection and transmission matrices of a stack formed by the two layers are then calculated according to^{7,9,10}

$$\begin{aligned} Q^I &= Q_2^I [1 - Q_1^{III} Q_2^{III}]^{-1} Q_1^I, \\ Q^{II} &= Q_2^{II} + Q_2^I Q_1^{II} [1 - Q_2^{III} Q_1^{III}]^{-1} Q_2^{IV}, \\ Q^{III} &= Q_1^{III} + Q_1^{IV} Q_2^{III} [1 - Q_1^{III} Q_2^{III}]^{-1} Q_1^I, \\ Q^{IV} &= Q_1^{IV} [1 - Q_2^{III} Q_1^{III}]^{-1} Q_2^{IV}. \end{aligned} \quad (2)$$

(The same “fusion” rules also yield the reflection and transmission matrices of any finite stack, provided that the reflection and transmission matrices of any two stack-forming substacks have been determined.^{7,9}) Matrix inversion in Eqs. (1) and (2) then renders the above methods inherently fragile in the following sense. Ideally, as the angular-momentum cutoff value l_{\max} , which determines the size of the matrix to be inverted, increases a numerical implementation should converge to a certain numerical

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value with ever-increasing accuracy. When we start from a small value of l_{\max} , this is indeed the case. However, when l_{\max} increases beyond a certain value, l_c , the numerical implementations of the above methods collapse and cease to provide a reasonable answer. (This is not the case with the so-called bulk KKR method, which involves only the calculation of a determinant.¹¹) The reason behind this is that the calculation of the matrix inverse becomes an ill-conditioned process strongly influenced by round-off errors: Even small numerical errors in the computed elements of Q result in large errors in the elements of Q^{-1} . Fortunately, in many important cases, the critical value of l_c is larger than the value of the angular-momentum cutoff l_{\max} , which guarantees a reasonable convergence, thereby allowing the application of the above scattering theories to a limited range of parameters.

This paper discusses the use of Gaussian elimination with backsubstitution (see Section 2.2 of Ref. 12) for performing matrix inversion. My focus is on the T -matrix method¹⁻⁵ and its state-of-the-art implementation by use of Mishchenko's code (freely available at <http://www.giss/nasa.gov/~crmin>).

In the T -matrix method¹⁻⁵ Eq. (1) is first rewritten as

$$TQ = -\text{Rg}(Q), \quad (3)$$

where T , Q , and $\text{Rg}(Q)$ are considered to be square matrices. Therefore the matrix inversion becomes equivalent to solving matrix equation $X \cdot A = B$, where A , X , and B denote $N \times N$ square matrices. The state-of-the-art Mishchenko's T -matrix-method F77 code comes with two options to perform matrix inversion, namely Numerical Algorithms Group (NAG) and non-NAG options. These options can be activated by setting the value of the integer variable ICHOICE to 1 and 2. The NAG option uses a decomposition of an $N \times N$ matrix A into a product $A = PLU$ (the so-called LU factorization), where P is a permutation matrix, L is a lower triangular matrix, and U is an upper triangular matrix, which is performed by NAG routine F07ARF. Matrix P enters here because the routine uses partial pivoting with row interchanges. After the initial LU -factorization step, the actual inverse of the complex square matrix A is computed by NAG routine F07ARF, which first forms U^{-1} and then solves the equation $XPL = U^{-1}$ for X . The second, non-NAG option is a Gaussian elimination (also known as the Gauss-Jordan elimination; see Section 2.1 of Ref. 12) performed by the set of routines INV1 \supset INVERT \supset (DECOMP, SOLVE) in conjunction with routine PROD, where the notion ROUT1 \supset ROUT2 indicates that ROUT1 calls routine ROUT2.

Compared with the NAG-option, the non-NAG option fails when the equal-volume-sphere radius of a nonabsorbing homogeneous dielectric particle exceeds a certain threshold value. On the other hand, in

the case of nonspherical particles, both options fail when absorption [imaginary part of the refractive index (MRI)] exceeds a certain threshold value (see Table 2 below). It will be shown that the use of Gaussian elimination with backsubstitution (see Sec. 2.2 of Ref. 12) can substantially expand the domain of applicability of Mishchenko's F77 code in the direction of strongly absorbing particles, where the current code fails to converge. Such an extension is especially important if the code is to be used in nanoplasmonic or nanophotonic applications involving small metallic particles.^{11,13,14} At the same time, convergence can also be maintained for large nonabsorbing particles, in which case the non-NAG option of Mishchenko's code fails.

2. Gaussian Elimination with Backsubstitution

Let us consider a $N \times N$ square matrix A . Gaussian elimination with backsubstitution, as described, for instance, in Sections 2.1-2 of Ref. 12, is used to solve matrix equation $\mathbf{x} \cdot A = \mathbf{b}$, for an unknown row vector \mathbf{x} , and a given row vector \mathbf{b} . A 4×4 example then looks as follows:

$$[x_1, x_2, x_3, x_4] \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} = [b_1, b_2, b_3, b_4]. \quad (4)$$

An application of Gaussian elimination with backsubstitution to Eq. (3) then amounts to repeatedly solving equations $\mathbf{x} \cdot Q = \mathbf{b}$, with the right-hand side \mathbf{b} being each time a different row of the $-\text{Rg}(Q)$ matrix. After the row vector \mathbf{x} is determined, it becomes a corresponding row of the T matrix.

The Gaussian elimination step is performed by the ZGER routine, whereas the step of backsubstitution is performed by the ZSUR routine. The Gaussian elimination routine ZGER has 23 execution lines, which first perform a partial pivoting. The partial pivoting comprises the step of finding an element with the largest magnitude in the n th row to the right of and including the a_{nn} matrix diagonal element. (Note in passing that Gaussian elimination with no pivoting is numerically unstable in the presence of any round-off error, even when a zero pivot is not encountered.) If the element with the largest magnitude is found in the j th column, where $j > n$, the n th and j th columns are interchanged, with the subsequent adjusting of labeling of matrix elements. However, in contrast to full Gaussian elimination, in the present case only the elements of the n th and j th columns below and including the respective n th elements are affected by partial pivoting, i.e., column permutations. Afterward, for j from $n + 1$ to N , the a_{nj}/a_{nn} multiple of the n th column is subtracted from the j th column as if it were the conventional Gaussian elimination of matrix elements in the n th row to the right of the diagonal a_{nn} element (see, e.g., Sections 2.1-2 of Ref. 12), but with the following differences:

1. Only the elements below the n th element of the j th column are affected by the subtraction.

2. The subtraction is performed if and only if both a_{nn} and a_{nj} are larger than a certain small numerical value EMACH.

Hence, after Gaussian elimination is performed by ZGER, our model 4×4 Eq. (4) would look as follows:

$$[x_1, x_2, x_3, x_4] \begin{bmatrix} a'_{11} & a_{12} & a_{13} & a_{14} \\ a'_{21} & a'_{22} & a_{23} & a_{24} \\ a'_{31} & a'_{32} & a'_{33} & a_{34} \\ a'_{41} & a'_{42} & a'_{43} & a'_{44} \end{bmatrix} = [b'_1, b'_2, b'_3, b'_4], \quad (5)$$

where the prime symbol indicates modified elements. The first difference, together with the partially pivoting step of the elements of the n th and j th columns, $j > n$, only below and including the respective column n th elements, is a cosmetic change aimed at saving computer time. If the conventional full Gaussian elimination were performed, all the elements above the diagonal would be rendered identically zero. However, in what follows, nothing changes [see Eq. (6) below] if one instead simply assumes that the upper diagonal elements are zero, without actually performing the additional elimination.

using the pivoting information supplied by ZGER. Before backsubstitution is performed (see, e.g., Section 2.2 of Ref. 12),

$$x_j = \frac{1}{a_{jj}} \left[b'_j - \sum_{k=j+1}^N x_k a'_{kj} \right], \quad (6)$$

ZSUR tests if the diagonal matrix element a'_{jj} is less than EMACH. If yes, then the value of a'_{jj} is reset to be equal to $(1 + i) \cdot \text{EMACH}$, where $i = \sqrt{-1}$. This is the provision that may protect the modified backsubstitution from an overflow. EMACH is usually set to be equal to the machine precision ϵ and hence depends on the available computer precision. Roughly speaking, the machine precision ϵ is the smallest floating point number such that $\epsilon + 1 > 1$; i.e., for all floating point numbers $u < \epsilon$, the result of the operation $u + 1$ on your computer will be 1.

In summary, to implement modified Gaussian elimination with backsubstitution in Mishchenko's T -matrix code, one must perform the following changes:

1. The Gaussian elimination routine ZGER and the backsubstitution routine ZSUR replace the earlier set of routines $\text{INV1} \supset \text{INVERT} \supset (\text{DECOMP}, \text{SOLVE})$ and PROD . This change amounts to replacing the entire part between labels 5 and 70 in the subroutine TT with the following shortened block:

```

5  CALL ZGER (ZQ, IPIV, NNMAX, NPN2, EMACH)           ! Gaussian elimination of ZQ to
                                                         ! a lower diagonal matrix

DO 6 I=1, NNMAX
    DO K=1, NNMAX                                     ! Initialization of the right-hand side
                                                         ! of the matrix equation ZX*ZQ=ZB

        ZX (K)=DCMPLX (RGQR (I, K), RGQI (I, K))
    ENDDO

    CALL ZSUR (ZQ, IPIV, ZX, NNMAX, NPN2, EMACH)      ! Solving ZX*ZQ=ZB by
                                                         ! backsubstitution
                                                         ! (ZX overwritten on exit)

        DO K=1, NNMAX

*
*  Assign T-matrix elements=-RG(Q)*[Q**(-1)]
*

            TR1 (I, K)=-DBLE(ZX (K))
            TI1 (I, K)=-DIMAG(ZX (K))
        ENDDO
6  CONTINUE
70 RETURN

```

The backsubstitution routine ZSUR has 21 execution lines. It first rearranges the right-hand side by

2. Additionally, the real*8 arrays $F, B, \text{WORK}, A, C, D, E$ in the subroutine TT are substituted by a

Table 1. Comparison of the Total Extinction Efficiency as Calculated by Mishchenko's Code with Three Different Inversion Techniques for the Case of a Sphere in Vacuum^a

r	MRR	MRI	LU	Gauss–Jordan	G.w.b. ^b
30	1.45	0	2.15780	2.15781	2.15781
30	1.45	0.01	2.22722	2.22723	2.22723
30	1.45	0.1	2.73525	2.73526	2.73526
30	1.45	1	4.87930	4.87931	4.87931
30	0.419	8.42	4.64827	4.64729	4.64729
500	1.45	0	1085.04	$1.75 \times 10^{-42\dagger, n.c.}$	1085.05
500	1.45	0.01	1084.16	1087.58	1087.58
500	1.45	0.1	1081.52	1081.52	1081.52
500	1.45	1	1089.37	1089.37	1089.37
500	0.419	8.42	1082.60	1082.60	1082.60

^aCalculations are shown as a function of radius AXI and refractive index MRR + i *MRI for a fixed incidence wavelength of LAM = 100.

^bG.w.b., Gaussian elimination with backsubstitution.

[†]Indicates that nearly singular matrices were encountered during the calculation. *n.c.*, the calculation did not converge.

single complex*16 array ZX(NPN2).

3. A new real variable EMACH is introduced in the subroutine TT.

3. Numerical Results

Gaussian elimination with backsubstitution was implemented as an additional alternative to Mishchenko's T -matrix code, which can be activated by the option ICHOICE = 3. In what follows, the convergence of Mishchenko's T -matrix code with the respective LU -factorization (ICHOICE = 1), Gauss–Jordan elimination (ICHOICE = 2), and Gaussian elimination with backsubstitution (ICHOICE = 3) options was investigated as a function of the equal-volume-sphere radius, AXI, and the relative refractive index, MRR + i *MRI. Particles were considered to be in vacuum and light incidence at vacuum wavelength of LAM = 100 was fixed at angles THET0 = 30°, THET = PHI0 = PHI = 0. Following recommendations, we kept the value of a precision variable DDELTA at 0.001. The array dimensions were kept the same as in the on-line version. Hence the maximum cut-off value of l_{\max} , as determined by the parameter NPN1, was 100. Here AXI, LAM, MRR, MRI, THET0, THET, PHI0, and PHI have the same meaning as in Mishchenko's original code.

The ICHOICE = 2 option numerical values in Tables 1 and 2, which are labeled with a superscript †, indicate that nearly singular matrices were encountered during the calculation. This label is particular to the ICHOICE = 2 option: Only in this case does the program calculate the so-called condition number of a matrix to be inverted. The values with superscript *n.c.* represent the cases in which the program was heading in the wrong direction and could not converge, owing most likely to the inherent fragility of the T -matrix method. In what follows, * denotes the values for which the resulting albedo was found to be larger than 1.

The spherical particle case is summarized in Table 1. (Following the recommendations for the NP = -1 option, we represented the sphere as an almost

spherical spheroid, with the rotational axis 0.0001 larger than the minor horizontal axis.) For absorbing particles, the performance of all three options is essentially equivalent in the range considered. The only difference appears to be in the convergence for large nonabsorbing particles, in which case the ICHOICE = 2 option begins to fail. For instance, for fixed LAM = 100, MRR = 1.45, and MRI = 0, the ICHOICE = 2 option does not converge for AXI \geq 500.

A comparison for the case of a prolate spheroid with an aspect ratio of 2 is summarized in Table 2. Here, for fixed LAM = 100, MRR = 1.45, and MRI = 0, the ICHOICE = 2 option does not converge, beginning with AXI = 115. Nevertheless, by choosing the imaginary part MRI as small as 10^{-6} , the convergence can be recovered again, with the result being substantially the same as for MRI = 0. More serious convergence problems were encountered for absorbing particles. By fixing MRR at 1.45, the values of MRI were stepped up by 0.1. The largest value of MRI at a given AXI then corresponds to the last value before all three options failed. For small spheroids (the equal-volume-sphere radius AXI is smaller than the vacuum wavelength LAM), it was found that the code with Gaussian elimination with backsubstitution can produce converged results with MRI that are more than 60% larger than those of either of the two remaining options. Results can also be obtained for the refractive index of 0.419 + i *8.42, which corresponds to that of gold at a wavelength of 1319 nm (see the AXI = 60 case in Table 2). With increasing AXI, the relative improvement of the MRI convergence range by the ICHOICE = 3 option relative to the other two options steadily decreases and is as low as 48% for AXI = 115 and 20% for AXI = 200. Eventually, for AXI = 300, the advantage of the ICHOICE = 3 option was marginal.

In the present case it has been checked that the outputs listed in Tables 1 and 2 are independent of the values of EMACH taken between 0 and 10^{-12} .

Table 2. Comparison of the Total Extinction Efficiency as Calculated by Mishchenko's Code with Three Different Inversion Techniques for the Case of a Prolate Spheroid with an Aspect Ratio 2 in Vacuum^a

AXI	MRR	MRI	<i>LU</i>	Gauss–Jordan	G.w.b. ^b
60	1.45	0	26.0297	26.0297	26.0297
60	1.45	1	20.0207	20.0207	20.0207
60	1.45	5.2	20.0089	19.1891 [†]	19.1891
60	1.45	5.3	19.1649*	19.1495 [†]	19.14954
60	1.45	5.4	19.1486*	20.1056 [†]	20.0440
60	1.45	5.5	18.8501*	20.2431 ^{†,*}	20.0207
60	1.45	8.6	<i>n.c.</i>	[†] , <i>n.c.</i>	18.4337
60	0.419	8.42	60.3485 ^{n.c.}	49.1987 ^{†,n.c.}	18.3566
115	1.45	0	82.1884	2.606×10^{-140} ^{†,n.c.}	82.1884
115	1.45	0.000001	82.1883	82.1883	82.1883
115	1.45	2.4	75.2908	75.1667 [†]	75.2750
115	1.45	2.5	75.4117	78.3078 ^{†,*}	75.3604
115	1.45	2.6	74.5664	74.7042 [†]	75.4077
115	1.45	2.7	77.7777*	74.9373 [†]	75.4134
115	1.45	2.8	85.6298*	77.7298 ^{†,*}	75.3814
115	1.45	3	165.776*	68.8598	75.2149
115	1.45	4	0.4444 ^{n.c.}	[†] , <i>n.c.</i>	73.1770
200	1.45	0	209.298	7.58×10^{-95} [†]	209.298
200	1.45	0.000001	209.298	209.298 [†]	209.298
200	1.45	1	199.838	199.838 [†]	199.838
200	1.45	1.3	203.474	204.1621 [†]	203.426
200	1.45	1.4	204.471	215.393 ^{†,*}	204.606
200	1.45	1.5	206.321	808.928 ^{†,n.c.}	205.758
200	1.45	1.6	213.231*	808.928 ^{†,n.c.}	206.869
200	1.45	1.8	-108.293*	808.928 ^{†,n.c.}	208.929
300	1.45	0	401.726	7.58×10^{-64} [†]	401.726
300	1.45	0.000001	401.727	401.694 [†]	401.727
300	1.45	0.4	427.810	427.810	427.810
300	1.45	0.8	431.935	431.910 [†]	431.913
300	1.45	0.9	433.643	436.991 ^{*,†}	433.693

^aCalculations are shown as a function of the equal-volume-sphere radius AXI and refractive index $MRR + i \cdot MRI$. Light incidence at the vacuum wavelength of $\lambda = 100$ was fixed at the angle $\theta = 30^\circ$.

^bG.w.b., Gaussian elimination with backsubstitution.

*Albedo returned larger than 1.

[†]Indicates that nearly singular matrices were encountered during the calculation.

n.c., the calculation did not converge.

4. Discussion and Conclusions

The results presented in Section 3 have demonstrated that Mishchenko's code, when equipped with the new ICHOICE = 3 option in which matrix inversion is performed by Gaussian elimination with backsubstitution, is superior to both *LU*-factorization (ICHOICE = 1) and Gauss–Jordan elimination (ICHOICE = 2). This finding is consistent with earlier experience with Gaussian elimination with backsubstitution when I built a two-dimensional photonic LKKR method,¹⁰ or when I tried to improve the three-dimensional photonic LKKR program¹¹ of Stefanou *et al.*⁹ [In the latter case, the method goes as far back as the LEED F77 program by Pendry⁷ (see routines ZGE and ZSE therein).] In the LKKR methods, the problem was to find the solution of an equation $A \cdot \mathbf{x} = \mathbf{b}$; i.e., the multiplication by matrix *A* was from the left. It turned out to be extremely difficult to improve the performance of Gaussian elimination with backsubstitution. Even the singular-value decomposition performed by the F02XEF NAG routine, when the

decomposition was equipped with the trick of an explicit zeroing of the small elements of the diagonal matrix in the singular-value decomposition (see Section 2.6, pp. 55–56 of Ref. 12), did not result in an improvement. Although the NAG routines may have wider range of applicability, it appears that, for generic scattering applications, the modified Gaussian elimination with backsubstitution may provide some advantage, especially for absorbing particles. The use of Gaussian elimination with backsubstitution is particularly advantageous when scattering properties are to be determined over many wavelengths; for instance when Mishchenko's *T*-matrix code is implemented within the *ab initio* multiple-scattering LKKR theory,¹³ or when various optimization tasks are performed. Indeed, when the NAG option reports an error, the whole program stops and an error message is issued. On the other hand, the modified Gaussian elimination with backsubstitution enables one to perform an uninterrupted execution (it can easily be supplemented with matrix singularity

checks to provide a warning if necessary). Moreover, the option is very simple and compact, requiring a mere 44 execution lines.

To conclude, Gaussian elimination with backsubstitution has substantially expanded the domain of applicability of Mishchenko's F77 code in the direction of strongly absorbing particles, where the original current code failed to converge. Such an extension is especially important if the code is to be used in nanoplasmonic or nanophotonic applications involving small metallic particles, such as, for instance, surface-enhanced Raman scattering, metalodielectric photonic crystals involving complex nonspherical particles,^{11,13} and design of near-field optical probes with optimal field enhancement.¹⁴ At the same time, convergence must also be maintained for large non-absorbing particles, in which case the non-NAG option of Mishchenko's code was diverging. The application of Gaussian elimination with backsubstitution to matrix inversion may also prove to be useful in other scattering methods, such as the separation of variable method⁶ and the method of auxiliary sources. The computer F77 implementation of Mishchenko's code supplemented with Gaussian elimination with backsubstitution is freely available at <http://www.wave-scattering.com>.

References

1. P. C. Waterman, "New formulation of acoustic scattering," *J. Acoust. Soc. Am.* **45**, 1417–1429 (1969).
2. P. C. Waterman, "Symmetry, unitarity, and geometry in electromagnetic scattering," *Phys. Rev. D* **3**, 825–839 (1971).
3. L. Tsang, J. A. Kong, and R. T. Shin, *Theory of Microwave Remote Sensing* (Wiley, New York, 1985).
4. M. I. Mishchenko, L. D. Travis, and D. W. Mackowski, "T-matrix computation of light scattering by nonspherical particles: a review," *J. Quant. Spectrosc. Radiat. Transfer* **55**, 535–575 (1996).
5. M. I. Mishchenko, L. D. Travis, and A. A. Lacis, *Scattering, Absorption, and Emission of Light by Small Particles* (Cambridge U. Press, Cambridge, UK, 2002).
6. V. G. Farafonov, N. V. Voshchinnikov, and V. V. Somsikov, "Light-scattering by a core-mantle spheroidal particle," *Appl. Opt.* **35**, 5412–5425 (1996).
7. J. B. Pendry, *Low Energy Electron Diffraction* (Academic, London, 1974).
8. J. M. McLaren, S. Crampin, D. D. Vvedensky, R. C. Albers, and J. B. Pendry, "Layer KKR electronic structure code for bulk and interface geometries," *Comput. Phys. Commun.* **60**, 365–389 (1990).
9. N. Stefanou, V. Yannopoulos, and A. Modinos, "Heterostructures of photonic crystals: frequency bands and transmission coefficients," *Comput. Phys. Commun.* **113**, 49–77 (1998).
10. V. Poborchii, T. Tada, T. Kanayama, and A. Moroz, "Silver-coated silicon-pillar photonic crystals: enhancement of a photonic band gap," *Appl. Phys. Lett.* **82**, 508–510 (2003).
11. A. Moroz, "Metallo-dielectric diamond and zinc-blende photonic crystals," *Phys. Rev. B* **66**, 115109 (2002).
12. W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in 77* (Cambridge U. Press, Cambridge, UK, 2001); see also <http://www.nr.com>.
13. I. Ederra, R. Gonzalo, C. Mann, A. Moroz, and P. de Maagt, "(Sub)mm-wave components and subsystems based on EBG technology," in *Proceedings of International Conference on Electromagnetics in Advanced Applications (ICEAA 2003)*, (n.p., 2003), pp. 643–646.
14. J. T. Krug, II, E. J. Sánchez, and X. S. Xie, "Design of near-field optical probes with optimal field enhancement by finite difference time domain electromagnetic simulation," *J. Chem. Phys.* **116**, 10895–10901 (2002).