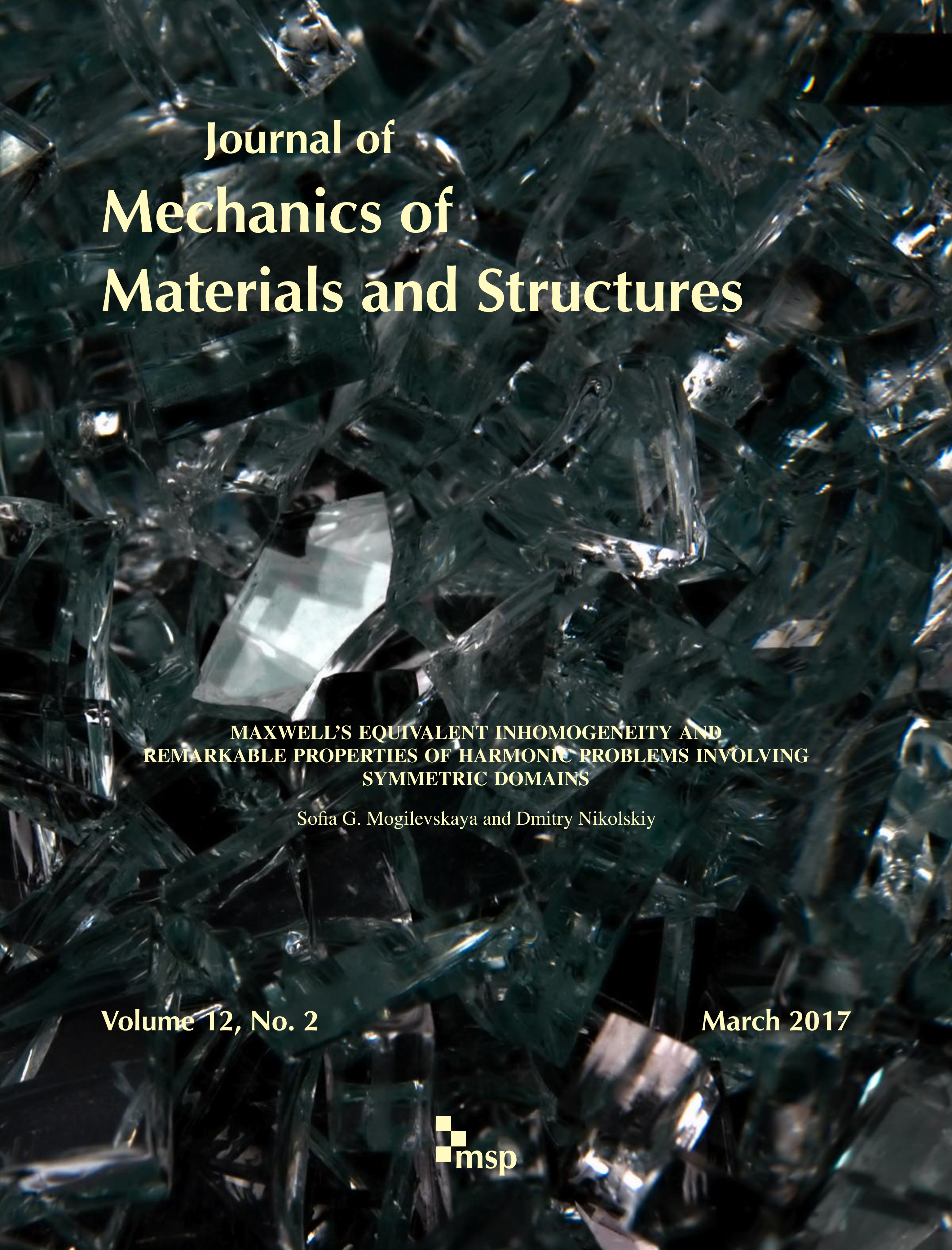

Journal of
Mechanics of Materials and Structures

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Volume 12, No. 2 March 2017

msp

JOURNAL OF MECHANICS OF MATERIALS AND STRUCTURES
Vol. 12, No. 2, 2017
dx.doi.org/10.2140/jomms.2017.12.179

MAXWELL'S EQUIVALENT INHOMOGENEITY AND REMARKABLE PROPERTIES OF HARMONIC PROBLEMS INVOLVING SYMMETRIC DOMAINS

SOFIA G. MOGILEVSKAYA AND DMITRY NIKOLSKIY

This paper revisits the Maxwell concept of equivalent inhomogeneity in the context of two-dimensional harmonic problems involving composite or porous materials of periodic structure. As previously done for elasticity problems, here the scheme is modified to accommodate for the shape of the equivalent inhomogeneity and for the interactions between the constituents of the cluster. New numerical results for periodic materials with hexagonal arrangements of fibers (holes) demonstrate that, with these modifications, the scheme allows for accurate estimates of the effective material properties. It is also shown that, as for elasticity problems, some harmonic symmetric inhomogeneities possess remarkable properties. Under the action of uniform far-fields, the averages of the fields within these inhomogeneities preserve the structure of the applied far-fields.

1. Introduction

This paper presents further studies of the Maxwell [1892] homogenization scheme that is based on the concept of an equivalent inhomogeneity. The concept suggests that a cluster that represents the material in question affects the fields at large distances away from it in the same manner as an equivalent inhomogeneity whose properties are equal to the effective ones.

The idea has a long history (see, e.g., [Milton 2002; Torquato 2002], and the references therein) and has been reinvented in a few later publications, e.g., [Kuster and Toksöz 1974; Hasselman and Johnson 1987; Lu and Song 1996; Lu 1998; Shen and Yi 2000; 2001; 2004]. In recent years, the concept has attracted even more attention, (e.g., [McCartney and Kelly 2008; McCartney 2010; Koroteeva et al. 2010; Mogilevskaya et al. 2010; 2012a; 2012b; 2013; Weng 2010; Pyatigorets and Mogilevskaya 2011; Levin et al. 2012; Mogilevskaya and Crouch 2013; Kushch 2013; Kushch et al. 2014; Kushch and Knyazeva 2016; Kushch and Sevostianov 2016]) and, in some of these publications, was generalized to include information on the geometrical arrangement of the constituents of the cluster and their interactions.

The original Maxwell scheme and its later modifications in application to the material with overall isotropy adopted either a spherical (three-dimensions) or a circular (two-dimensions) shape of the equivalent inhomogeneity. However, the papers [Jasiuk et al. 1992; 1994; Sevostianov and Kachanov 2011; Kushch and Sevostianov 2015] (see also the references therein) have demonstrated that the shape has an influence on the far-field asymptotic behavior. Some of these publications, although not directly related to Maxwell's concept, are relevant because the analysis of the far-fields is a cornerstone of the original Maxwell concept.

Keywords: Maxwell equivalent inhomogeneity, harmonic problems, composite and porous materials, effective properties.

In the context of Maxwell's scheme, the issue of shape was investigated in [Sevostianov and Giraud 2013; Sevostianov 2014; Kushch et al. 2014; Kushch and Sevostianov 2016; Kushch and Knyazeva 2016]. These authors studied more general cases that involved materials with overall anisotropic behavior and suggested using a more general shape of the equivalent inhomogeneity (elliptical for two-dimensional and ellipsoidal for three-dimensional problems). Their major arguments were based on the availability of closed form analytical solutions for the fields due to these inhomogeneities, see [Eshelby 1957; 1959; 1961]. In [Mogilevskaya and Nikolskiy 2015], it was demonstrated numerically that, for two-dimensional *elastic* materials with hexagonal symmetry, the estimates for the effective bulk and shear moduli based on a hexagonal shape of the equivalent inhomogeneity are more accurate than those based on circular shape. In addition, while circular-based estimates for some materials diverge with the size of the cluster, their hexagonal counterparts converge. Also in that paper, it was numerically discovered that two-dimensional regular polygonal and other symmetric inhomogeneities possess some remarkable properties. Under the action of uniform far-fields, the averages of the fields within these inhomogeneities have the same structure as that of the applied far-fields. In [Mogilevskaya and Stolarski 2015], these properties have been rigorously proved for a wider class of two- and three-dimensional elastic problems, which included anisotropic and nonuniform materials subjected to either far-field loads or constant transformational strains within the inhomogeneity.

In this paper, we use the approach in [Mogilevskaya and Nikolskiy 2015] to study the issue of the shape of Maxwell's inhomogeneity in the context of problems governed by the Laplace equation (harmonic problems). New developments presented here include new numerical results on the effective properties (e.g., conductivities) of two-dimensional materials with hexagonal symmetry, including the convergence studies. As previously done for elasticity problems in the above cited paper, some remarkable properties of symmetric inhomogeneities are numerically discovered here for harmonic problems.

The paper is structured as follows. In Section 2, the classical concept of Maxwell's equivalent inhomogeneity for harmonic problems is described and the generalized Maxwell approach is briefly reviewed. In Section 3, we consider the problem of finding the property of an arbitrarily shaped inhomogeneity whose asymptotic far-fields' expansions contain the same leading terms as those for the circular inhomogeneity of the same area. In Section 4, we analyze the obtained interrelations between the properties of the arbitrarily shaped and circular inhomogeneities. This analysis leads to the discovery of some remarkable properties of regular polygonal and other symmetric inhomogeneities. In Section 5, using the results on the effective properties obtained with the use of circular equivalent inhomogeneity (see [Mogilevskaya et al. 2012b]), we recalculate the effective properties for the periodic materials using a hexagonal shape for that inhomogeneity. We demonstrate that these new estimates converge faster with the size of the cluster than the corresponding circular inhomogeneity-based estimates. The discussion of the obtained results and the direction for future work are presented in Section 6.

2. Maxwell's scheme and a review of the generalized Maxwell approach that accounts for interaction

The original Maxwell scheme is based on the idea that a cluster that represents the material in question (Figure 1, left, for the two-dimensional case) affects the fields at large distances away from it in the same manner as an equivalent circle (sphere) (Figure 1, right) whose property (e.g., thermal or electric

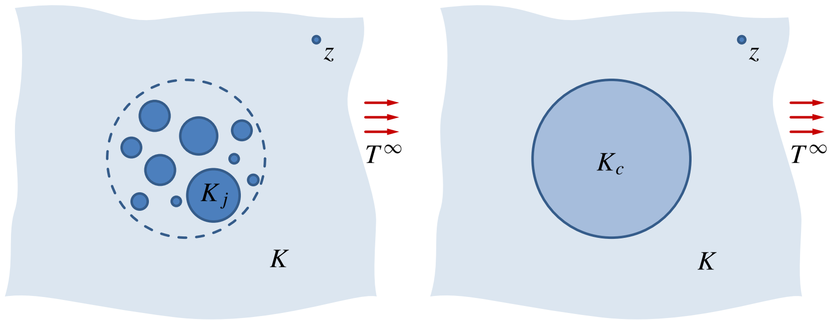

Figure 1. Cluster of circular inhomogeneities (left) and equivalent inhomogeneity (right).

conductivity) is equal to the effective one. The radius R of the equivalent circle/sphere is chosen such that the ratio of the total area (volume) occupied by the constituents of the cluster to that of the equivalent circle (sphere) reflects the volume fraction of the material.

Below we review the basics of the scheme and its generalization in the context of the steady-state heat conduction problem. However, the scheme can be easily reformulated in terms of any harmonic problem (e.g., antiplane elasticity in two dimensions). We assume that the cluster consists of N nonoverlapping fibers/particles that are perfectly bonded to the material matrix. In the original Maxwell's scheme the fibers/particles are of circular/spherical shapes. In that scheme, the geometrical arrangement of the fibers/particles is neglected (from large distances away, they are perceived as to be located at the same point), and the interactions between them are not accounted for (the contribution of every fiber/particle to the far-fields is evaluated under the assumption that this fiber/particle is the only one in the matrix). Maxwell [1892], who considered the three-dimensional case, assumed that all particles had the same conductivities k_p that are different from the conductivity k of the matrix. The latter restriction is easy to lift as it was done in [McCartney and Kelly 2008; Mogilevskaya et al. 2012a] for the three-dimensional case and in [Mogilevskaya et al. 2012b] for the two-dimensional case (the latter paper considered the scheme in the context of antiplane problem).

With the above assumptions, Maxwell's scheme yields the following result for the effective conductivity k_{ef} of the material (both for two- and three-dimensional problems):

$$\frac{k_{\text{ef}}}{k} = \frac{1-(d-1)B^0}{1+B^0}, \qquad B^0 = \sum_{j=1}^{N} c_j \left(1 - \frac{k_j}{k}\right) \frac{1}{(d-1)+k_j/k}, \tag{1}$$

in which k_j is the conductivity of the j-th circular fiber (spherical particle) of radius a_j, the variable d is the dimension of the problem ($d = 2$ in two-dimensions, $d = 3$ in three-dimensions), and c_j is the so-called volume fraction of j-th particle/fiber ($j = 1, \ldots, N$) that is defined as

$$c_j = \left(\frac{a_j}{R}\right)^d. \tag{2}$$

The papers [Mogilevskaya et al. 2012a; 2012b; 2013; Kushch et al. 2013; 2014; Kushch and Knyazeva 2016; Kushch and Sevostianov 2016] generalized the Maxwell scheme by precisely evaluating the far-fields due to the cluster using semianalytical methods. These methods explicitly account for the geometrical arrangements of the particles/fibers in the cluster and their interactions. The effective constants were obtained by comparing the dipole coefficients in the multipole expansions of far-fields with the dipole coefficients for the equivalent inhomogeneities. The effective conductivity (that was assumed to be the same as that of the equivalent inhomogeneity) was expressed by equations similar to that of (1)–(2) but with different parameters, B^0 (see e.g., [Mogilevskaya et al. 2012a, Equations (16)–(18)] with $B^0 = A^*_{10}$ for spherical particles). In the generalized approach in [Koroteeva et al. 2010; Mogilevskaya et al. 2012a; 2012b], the shape of the equivalent inhomogeneity was assumed to be the same (circular or spherical) as that in the original Maxwell's approach while [Kushch et al. 2014; Kushch and Knyazeva 2016; Kushch and Sevostianov 2016] suggested the use of an elliptical (ellipsoidal) shape when the overall behavior of the materials is anisotropic.

We now consider the two-dimensional case, assuming that shape of the equivalent inhomogeneity may be arbitrary, and formulate the following auxiliary problem: determine the property of a noncircular inhomogeneity such that the asymptotic expansions of the far-fields induced by it have the same leading terms as that induced by the circular inhomogeneity.

3. The expressions for the far-fields induced by the inhomogeneity

We assume that the circular inhomogeneity of radius R and conductivity k_c has its center at the origin of the Cartesian coordinate system x_1Ox_2 (Figure 2, left). The counterpart problem of the inhomogeneity D of arbitrary shape and conductivity k_I is shown on Figure 2, right, where L is the boundary of that inhomogeneity. For both problems, it is assumed that the temperature gradient $T^\infty = \alpha x_1$ is applied at infinity. Both problems are governed by the Laplace equation. The solution for the first problem is well-known (see, e.g., [Honein et al. 1992]). The temperature at the point $z = x_1 + ix_2$ located inside the matrix can be written in the form

$$T(z) = T^\infty(z) + \alpha \frac{1 - k_c/k}{1 + k_c/k} \operatorname{Re} \frac{R^2}{\bar{z}}, \tag{3}$$

in which $\bar{z} = x_1 - ix_2$.

The solution for the second problem is also available in [Linkov 2002; Dobroskok and Linkov 2009] and [Dong and Lo 2013]. The temperature at the same point z is

$$T(z) = T^\infty(z) + (1 - k_I/k) \operatorname{Re} \frac{1}{2\pi i} \int_L \frac{T(\tau)\,\mathrm{d}\tau}{\tau - z}. \tag{4}$$

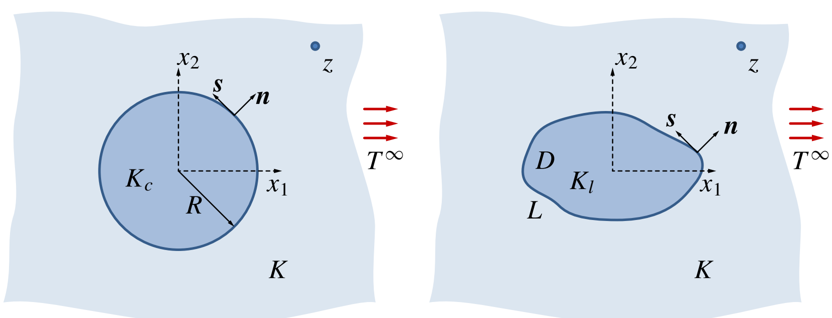

Figure 2. Circular inhomogeneity (left) and arbitrarily shaped inhomogeneity (right)

Assuming that the point z is located far away from the inhomogeneity, one can obtain the following asymptotic expansion for the complementary temperature $T^{\text{com}}(z) = T(z) - T^{\infty}(z)$:

$$T^{\text{com}}(z) = -(1 - k_I/k)\,\text{Im}\,\frac{1}{2\pi}\left\{\frac{1}{z}\int_L T(\tau)\,\mathrm{d}\tau + \frac{1}{z^2}\int_L T(\tau)\tau\,\mathrm{d}\tau + O\left(\frac{1}{z^3}\right)\right\}. \tag{5}$$

The comparison of (3) with the leading terms of (5) yields the following set of equations:

$$\text{Re}\int_L T(\tau)\,\mathrm{d}\tau = 0, \tag{6}$$

$$\text{Im}\int_L T(\tau)\,\mathrm{d}\tau = -2\pi R^2 \frac{\alpha}{1 - k_I/k}\,\frac{1 - k_c/k}{1 + k_c/k}. \tag{7}$$

It can be shown that

$$\text{Re}\int_L T(\tau)\,\mathrm{d}\tau = -\int_D \frac{\partial T(\tau)}{\partial x_2}\,\mathrm{d}D, \tag{8}$$

$$\text{Im}\int_L T(\tau)\,\mathrm{d}\tau = \int_D \frac{\partial T(\tau)}{\partial x_1}\,\mathrm{d}D, \tag{9}$$

which indicates that these integrals are proportional to the corresponding average temperature gradients within the inhomogeneity.

4. Analysis of the equations of Section 3

It follows from (6) and (8) that

$$\int_D \frac{\partial T(\tau)}{\partial x_2}\,\mathrm{d}D = 0, \tag{10}$$

which indicates that the average temperature gradient within the inhomogeneity has only the x_1 component, as is the case for the applied temperature field. Certainly, it could only be valid for the problems with particular types of symmetry. Using virtually the same arguments as those presented in [Mogilevskaya and Stolarski 2015], it could be proved that (10) is valid for the inhomogeneities whose shapes possess certain types of rotational symmetry. For such problems, the interrelation between the property of the inhomogeneity associated with the problem and that of the circular inhomogeneity can be obtained from (7) and (9) as follows:

$$\frac{k_I}{k} = 1 - 2\frac{1 - k_c/k}{1 + k_c/k}\,\frac{\alpha}{\Xi}, \tag{11}$$

in which

$$\Xi = \frac{1}{\pi R^2}\int_D \frac{\partial T(z)}{\partial x_1}\,\mathrm{d}D. \tag{12}$$

5. Results

5.1. ***Interpretation of the equations of Section 4.*** We now assume that the area of the inhomogeneity is the same as that of the circle, πR^2. It can be seen that the expression in the right-hand side of (12) is the

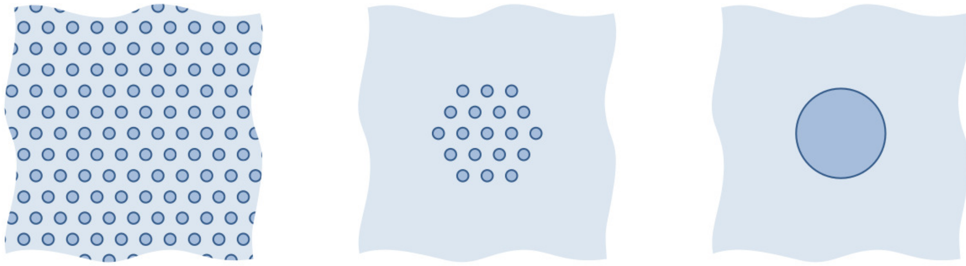

Figure 3. Infinite hexagonal array of inhomogeneities (left), finite cluster of inhomogeneities and equivalent hexagonal inhomogeneity in homogeneous matrix material (middle), finite cluster of inhomogeneities and equivalent circular inhomogeneity (right).

area average of the temperature gradient in the corresponding direction. Therefore, the conductivity of the inhomogeneity D is expressed by (11) via the corresponding property of the circular inhomogeneity of the same area and via the average given by (12). However, this average also depends on the conductivity of the inhomogeneity D, which has yet to be found.

To resolve this issue, we propose the simple iteration procedure in which the boundary value problem of the inhomogeneity of the same geometry as D but with the properties $(k_I)_0$ taken to be the same as for the corresponding circular inhomogeneity, $(k_I)_0 = k_c$, and is solved first by means of a boundary element code. The conductivities k_c were evaluated in [Mogilevskaya et al. 2012b]. The new conductivity $(k_I)_1$ obtained from (12) is then used in the next iteration. The process is terminated when the difference between the values obtained in last two iterations becomes less than the prescribed accuracy level.

Below, the proposed approach is used to evaluate the effective conductivities of a two-phase composite material with a hexagonal arrangement of fibers (Figure 3, left). The unit cell of this material is a hexagon that possesses desirable symmetry with respect to the coordinate axes. The problem of hexagonal inhomogeneity was solved by using an in-house boundary element code that employs quadratic approximations for the unknown temperature on each straight boundary element. Using this code, we demonstrated numerically that the conditions of (10) are satisfied up to 11 significant digits. These conditions, as explained above, imply that the average directional temperature gradients have the same structure as those of the applied far-field temperature field. These "strange" properties of symmetric inhomogeneities can be proved theoretically for more general classes of two- and three-dimensional anisotropic and nonuniform materials using virtually the same arguments as those used in [Mogilevskaya and Stolarski 2015] for elastic problems.

5.2. ***Circular fibers.*** The cluster of $N = N(p) = 1 + 3p(p+1)$, where $p \geq 1$, circular fibers (holes) of radius r_0 that forms a hexagon D is taken from an infinite double-periodic array of fibers (holes) (Figure 3, left) and placed in an infinite matrix material (Figure 3, middle). The area $|D|$ of the hexagon is

$$|D| = \frac{3\sqrt{3}d^2}{2} p^2, \tag{13}$$

in which d is the distance between the centers of the inhomogeneities.

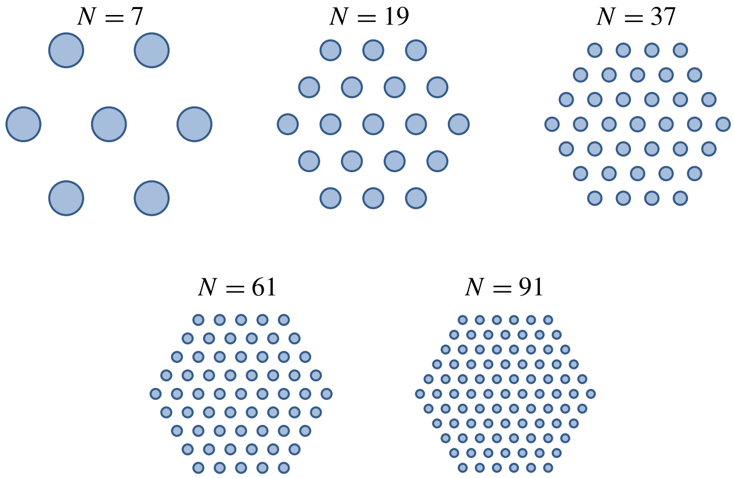

Figure 4. Clusters of N inhomogeneities.

The volume fraction c of the fibers (holes) in the above mentioned double-periodic array is defined as

$$c = \frac{2\pi r_0^2}{\sqrt{3}d^2}. \tag{14}$$

The equivalent circular inhomogeneity (Figure 3, right), considered in [Mogilevskaya et al. 2012b], has the same area as the hexagon. The radius of that inhomogeneity can be found from the equation

$$\pi R^2 = \frac{3\sqrt{3}d^2}{2} p^2. \tag{15}$$

The examples of five clusters of the material with $N = 7$, 19, 37, 61, and 91 fibers are shown in Figure 4. Assume that k_f is the conductivity of the fibers. Consider the cases:

(i) of holes, where $k_f/k = 0$, and

(ii) of high contrast in fibers/matrix conductivities, where $k_f/k = 135$.

The accurate estimates of the normalized effective conductivity (k_{per}/k) were provided to us by Godin [2013] (for both cases) and Kushch [2013] (for the second case). These authors solved the double periodic problem using two different methods. For high-contrast composites, the results obtained by both methods were identical up to the requested five significant digits. The estimates k_c/k are obtained by the method described in [Mogilevskaya et al. 2012b]. Note, these estimates take the full account for the interactions among all fibers of the cluster and its geometry.

The conductivity of the hexagonal inhomogeneity, k_h/k, is calculated from the iteration procedure described in the beginning of this section. The parameter defining the accuracy level was set up as 10^{-5}. The values of the moduli for each iteration were obtained from (11) in which the conductivity needed to evaluate Ξ was taken from the previous iteration. The number of iterations depended on the volume fraction and varied from 1 (for low volume fractions) to 64 (for high volume fractions). The boundary element solution required to evaluate Ξ employed 32 elements on each side of the hexagon.

c	k_c/k					Periodic (k_{per}/k), [Godin 2013]
	$N=7$	$N=19$	$N=37$	$N=61$	$N=91$	
0.1	0.81814	0.81814	0.81814	0.81814	0.81814	0.81818
0.2	0.66635	0.66635	0.66637	0.66638	0.66639	0.66667
0.3	0.53745	0.53748	0.53754	0.53758	0.53761	0.53844
0.4	0.42621	0.42635	0.42650	0.42660	0.42667	0.42845
0.5	0.32868	0.32901	0.32932	0.32953	0.32967	0.33281
0.6	0.24167	0.24224	0.24277	0.24313	0.24337	0.24834
0.7	0.16227	0.16308	0.16387	0.16441	0.16478	0.17208
0.8	0.08705	0.08791	0.08896	0.08970	0.09021	0.10042
0.85	0.04875	0.04940	0.05051	0.05132	0.05189	0.06383

Table 1. Normalized effective conductivity for hexagonal arrays, $k_f/k = 0$. Circular equivalent inhomogeneity.

c	k_h/k					Periodic (k_{per}/k), [Godin 2013]
	$N=7$	$N=19$	$N=37$	$N=61$	$N=91$	
0.1	0.81818	0.81818	0.81818	0.81818	0.81818	0.81818
0.2	0.66661	0.66661	0.66663	0.66664	0.66665	0.66667
0.3	0.53819	0.53822	0.53828	0.53832	0.53835	0.53844
0.4	0.42773	0.42787	0.42802	0.42812	0.42818	0.42845
0.5	0.33129	0.33162	0.33192	0.33213	0.33227	0.33281
0.6	0.24569	0.24625	0.24677	0.24712	0.24736	0.24834
0.7	0.16806	0.16885	0.16962	0.17014	0.17051	0.17208
0.8	0.09506	0.09588	0.09689	0.09761	0.09812	0.10042
0.85	0.05813	0.05876	0.05983	0.06060	0.06116	0.06383

Table 2. Normalized effective conductivity for hexagonal arrays, $k_f/k = 0$. Hexagonal equivalent inhomogeneity.

The results for k_h/k are tabulated in Tables 2 and 4 (the corresponding results for k_c/k are given in Tables 1 and 3). Graphical representation of the results is presented in Figure 5. It could be seen that, while both circular- and hexagon-based estimates seem to converge with the size of the cluster, the latter estimates are more accurate. This is true for both cases of contrast in fiber and matrix conductivities. To better illustrate this fact, the relative errors $\delta = |k_I - k_{\text{per}}|/k_{\text{per}}$ are plotted in Figure 6 for cases (i) and (ii) with volume fractions $c = 0.6$ and 0.85. The results indicate that both estimates converge linearly, i.e.,

$$\lim_{p\to\infty} \frac{|k_I^{(p+1)} - k_{\text{per}}|}{|k_I^{(p)} - k_{\text{per}}|} = \lambda > 0, \tag{16}$$

c	k_c/k					Periodic (k_{per}/k), [Godin 2013; Kushch 2013]
	$N=7$	$N=19$	$N=37$	$N=61$	$N=91$	
0.1	1.2187	1.2187	1.2187	1.2187	1.2187	1.2186
0.2	1.4915	1.4915	1.4915	1.4915	1.4914	1.4908
0.3	1.8426	1.8424	1.8423	1.8421	1.8420	1.8393
0.4	2.3131	2.3124	2.3116	2.3111	2.3107	2.3016
0.5	2.9814	2.9786	2.9760	2.9742	2.9730	2.9464
0.6	4.0179	4.0090	4.0008	3.9954	3.9917	3.9165
0.7	5.8849	5.8582	5.8321	5.8145	5.8026	5.5744
0.8	10.5035	10.4135	10.3056	10.2313	10.1800	9.2521
0.85	17.4471	17.2641	16.9526	16.9526	16.5806	13.9231

Table 3. Normalized effective conductivity for hexagonal arrays, $k_f/k = 135$. Circular equivalent inhomogeneity.

c	k_h/k					Periodic (k_{per}/k), [Godin 2013; Kushch 2013]
	$N=7$	$N=19$	$N=37$	$N=61$	$N=91$	
0.1	1.2186	1.2186	1.2186	1.2186	1.2186	1.2186
0.2	1.4910	1.4910	1.4910	1.4910	1.4909	1.4908
0.3	1.8402	1.8400	1.8399	1.8397	1.8396	1.8393
0.4	2.3053	2.3046	2.3038	2.3033	2.3029	2.3016
0.5	2.9592	2.9564	2.9539	2.9521	2.9510	2.9464
0.6	3.9561	3.9475	3.9397	3.9346	3.9311	3.9165
0.7	5.6970	5.6724	5.6486	5.6325	5.6216	5.5744
0.8	9.7125	9.6377	9.5483	9.4865	9.4438	9.2521
0.85	15.0606	14.9286	14.7037	14.5444	14.4333	13.9231

Table 4. Normalized effective conductivity for hexagonal arrays, $k_f/k = 135$. Hexagonal equivalent inhomogeneity.

where $k_I^{(p)}$ is the conductivity of the equivalent inhomogeneity representing a cluster containing $N = N(p)$ inhomogeneities. The convergence analysis of the tabulated results suggests that the hexagon-based estimates converge with $\lambda \approx 0.8$, which is faster than the circle-based estimates with $\lambda \approx 0.95$.

6. Conclusions

In this paper, we studied the shape of Maxwell's equivalent inhomogeneity for two-dimensional harmonic problems. For problems with hexagonal symmetry, we report new tabulated and graphically illustrated numerical results that are obtained with the use of the modified Maxwell's scheme that accounts for the interactions within the cluster and employs the hexagonal equivalent inhomogeneity. By performing convergence studies, we demonstrated that this scheme provides more accurate estimates for the effective

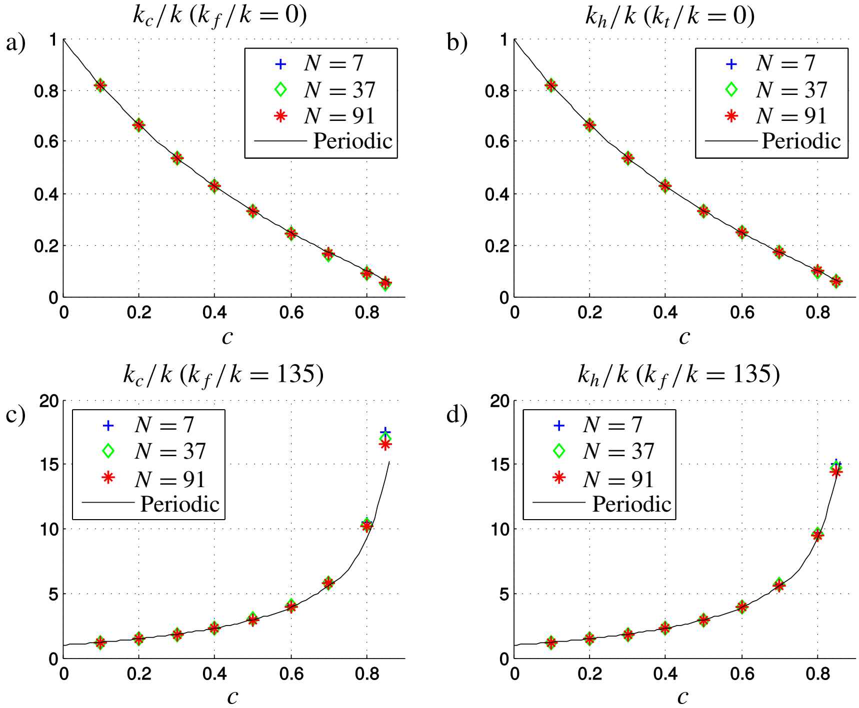

Figure 5. Normalized effective conductivity for hexagonal arrays: a) circular equivalent inhomogeneity, $k_f/k = 0$; b) hexagonal equivalent inhomogeneity, $k_f/k = 0$; c) circular equivalent inhomogeneity, $k_f/k = 135$; d) hexagonal equivalent inhomogeneity, $k_f/k = 135$.

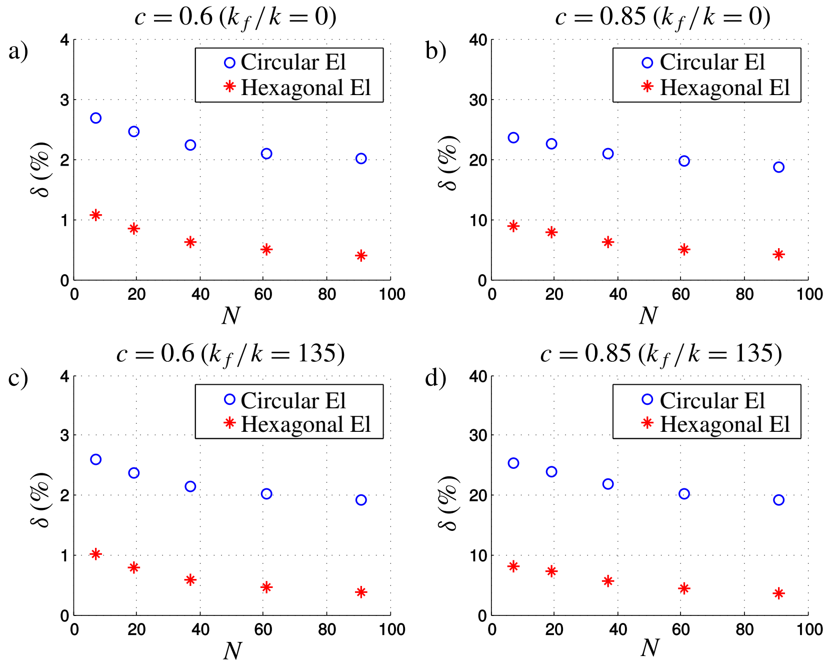

Figure 6. Relative error of normalized effective conductivity $\delta = |k_c - k_{\text{per}}|/k_{\text{per}}$ for circular equivalent inhomogeneity, $\delta = |k_h - k_{\text{per}}|/k_{\text{per}}$ for hexagonal equivalent inhomogeneity.

properties of the materials than that employing circular shape. In addition, we demonstrated numerically that hexagonal inhomogeneities possess remarkable properties. Under the action of a uniform temperature gradient, the averages of the temperature within the inhomogeneity preserves the structure of the applied far-fields. These "strange" properties of symmetric inhomogeneities can be proved theoretically for more general classes of two- and three- dimensional anisotropic and nonuniform harmonic materials using virtually the same arguments as those used in [Mogilevskaya and Stolarski 2015] for elastic problems.

Acknowledgments

The first author gratefully acknowledges the support from the Theodore W. Bennett Chair, University of Minnesota. Special thanks to Volodymyr I. Kushch and Yuri A. Godin for providing benchmark results for hexagonal arrays.

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Received 4 Apr 2016. Revised 6 Oct 2016. Accepted 12 Oct 2016.

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