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Green's function modeling of response of two-dimensional materials to point probes for scanning probe microscopy[★]

V.K. Tewary^{*}, Rebecca C. Quardokus, and Frank W. DelRio

Applied Chemicals and Materials Division, NIST, Boulder, CO 80305, USA

Abstract

A Green's function (GF) method is developed for interpreting scanning probe microscopy (SPM) measurements on new two-dimensional (2D) materials. GFs for the Laplace/Poisson equations are calculated by using a virtual source method for two separate cases of a finite material containing a rectangular defect and a hexagonal defect. The prescribed boundary values are reproduced almost exactly by the calculated GFs. It is suggested that the GF is not just a mathematical artefact but a basic physical characteristic of material systems, which can be measured directly by SPM for 2D solids. This should make SPM an even more powerful technique for characterization of 2D materials.

Keywords

Antidots; Graphene; Green's function; Materials characterization; Scanning probe microscopy; Two-dimensional materials

1. Introduction

Since the advent of graphene [1], many new [2] two-dimensional (2D) materials have been synthesized and tested. These include silicene [3–6], germanene [3], stanene [7], phosphorene [8], geometrically-modified graphene [9,10], hexagonal boron nitride [11], and single-layer transition-metal dichalcogenides (i.e., MoS₂ [12], MoSe₂ [13], WS₂ [14], WSe₂ [15], and PtSe₂ [16]), which have received much attention in recent years. These new materials have the potential to revolutionize the materials industry due to their size and unique electronic, mechanical, thermal, and photonic properties [12,14,15,17,18] (for reviews and other references, see [19,20]). Because of their low dimensionality, small structural changes can significantly affect the transport and other physical properties of 2D materials [9,10]. It is therefore important to develop accurate and fast characterization techniques for these materials, supported by robust and computationally efficient mathematical models. Such techniques are needed to accelerate the industrial application of these materials.

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^{*}Corresponding author. vinod.tewary@nist.gov (V.K. Tewary), rebecca.quardokus@nist.gov (R.C. Quardokus), frank.delrio@nist.gov (F.W. DelRio).

Scanning tunneling microscopy (STM) is a scanning probe microscopy (SPM) technique that uses raster scanning and tunneling electrons to map out the nanoscale topography and electronic properties of conductive surfaces [21]. In addition to the conventional atomic force microscopy (AFM), SPM includes new powerful techniques such as scanning electrostatic microscopy (SESM) and scanning thermal microscopy (SThM). In a typical SPM experiment, one measures the response of the sample to a point probe or a distribution of point probes. Interestingly, that is exactly the mathematical definition of the Green's function – response to a point probe [22]. A Green's function (GF) based method is, therefore, the natural choice for modeling SPM experiments on 2D materials.

Normally GF is understood to be a mathematical technique that is used for solving operator equations. In fact, GF is more than that. An operator in physics represents a process of measurement. The GF corresponding to an operator is the inverse of that operator and gives the response [23] of the material to the measurement process represented by that operator. The GF is independent of the probe and, operating on the probe, it gives the result of that measurement. If, instead of calculating it through various mathematical steps and physical assumptions, the GF can be directly measured, it should prove to be a valuable tool for physical characterization as well as mathematical modeling of materials.

Here we suggest that the GF is a physical entity that contains all the information about the material as modeled by the corresponding operator equation. At least for a 2D material, the GF can be measured directly by SPM. The measurability of the GF is particularly useful because, in principle, it can be used for modeling other related characteristics of that material. This is an interesting example of an apparently mathematical artefact becoming a tool for experimental characterization of 2D materials.

Of course even for 3D materials, SPM yields response to a point force. However, SPM can directly measure the response only at the same surface at which the probe is applied. For ordinary 3D solids, the physical characteristics of a surface are, in general, different than the bulk of the material. Moreover, many other factors contribute to the surface response such as interlayer interactions, presence of randomly distributed point defects as well as topological and extended defects such as dislocations, stacking faults, etc. All these contributions make it very difficult to deconvolve the measured response to extract useful values of the GF. The availability of single layer 2D solids has now made it possible to actually measure the GF.

In this paper we describe a GF method for solving the Poisson equation, or its homogeneous part the Laplace equation, in 2D materials. The Poisson equation gives the distribution of the electric field or voltage in electrostatic experiments such as in SESM or the temperature field in SThM. The Poisson equation is a highly studied equation because of its wide range of applications. Its analytical solution is possible only for fairly simple geometries and infinite solids [24]. For any realistic geometry or for finite solids, one has to resort to partial or fully numerical techniques.

A major advantage of the GF method is that it is partly analytic. We start with an analytical form of the free-space GF for a perfect infinite solid and then impose suitable boundary and/or continuity conditions to simulate finite boundaries and defects. We use the virtual

source (VS) method for satisfying the prescribed boundary conditions. The VS method is analogous to the virtual force method, which was used previously in elastostatics for planar boundaries [25–27]. In this paper, we have adopted this method to boundaries of arbitrary shapes. The test of the reliability of a solution of any boundary value problem is how well the boundary conditions are satisfied. We find that the calculated GF satisfies the boundary conditions almost exactly.

The material system that we consider in this paper is a perfectly flat 2D finite material containing a single rectangular or hexagonal defect of finite size. The VS method is very general and is applicable to material systems containing any number of defects. Further, the defects can be of arbitrary shapes and sizes. A defect may be an antidot or an inclusion of a different material as used for functionalization. An antidot in a 2D material is a hole, which corresponds to a void in a 3D material. Antidots [9,10,28] in graphene are of strong topical interest because they can be engineered to tune the electric and thermal characteristics of the material. Various designs and arrays of antidots and inclusions have been proposed in the literature for making efficient thermoelectric devices for energy harvesting and energy conversion [29]. For all such applications, we need to solve the Poisson/Laplace equation, which is the objective of the present paper.

2. Mathematical formulation

Perhaps the most common numerical technique used for solving the Poisson/Laplace equation is the finite element method (FEM). The FEM is an extremely versatile and powerful technique but computationally rather expensive. It requires inversion of $N_v \times N_v$ matrices where N_v is the number of all the points in the bulk of the material. It is necessary to solve the equation numerically at all the points in the solid even if the results are needed only in a small region, which is often the case.

An alternative to the FEM for linear problems is the boundary element method (BEM), which involves integrals only near the boundaries or discontinuities in the solid where the boundary conditions are prescribed [26]. The BEM requires inversion of $N_s \times N_s$ matrices where N_s is the number of points at the boundary (or surface in 3D systems). Since N_s is much smaller than N_v , the BEM requires inversion of matrices of much lower dimensions as compared to the FEM. However, it does not necessarily have a major advantage over the FEM in terms of computational efficiency. This is because the matrices to be inverted in the FEM are large but sparse, whereas in the BEM they are smaller but dense. Many other methods [25–27,30,31] for calculating the GF are available in the literature such as those based upon integral transforms, complex variables, Dyson's equation, etc. These methods are useful for specific geometries.

We use the GF method, which is intimately linked with the BEM. The BEM uses free-space GF as the starting solution and the Green's or the Gauss theorem with suitable interpolation functions to satisfy the prescribed boundary conditions. For an excellent discussion of the GF and its mathematical properties along with its applications to various materials systems of interest, see the recent monograph by Pan and Chen [32].

In our GF method, we obtain the final GF directly by using a suitable distribution of VSs. The final GF incorporates all the boundary conditions and gives the total response of the material system. Thus, it includes the effect of any defects such as surfaces, boundaries, and discontinuities associated with various defects in the material. The final GF is also called the defect GF in contrast to the free infinite space GF, which is called the perfect GF. In the interest of brevity in this paper, unless stated otherwise, GF will refer to the final GF.

The VS method is somewhat similar to the method of images [24] in electrostatics. The VSs are applied just outside the boundary of the solution domain. The boundary conditions are specified on a contour just inside the boundary. Thus, the contour at which the boundary conditions are prescribed is just inside the solution domain whereas the contour at which the VSs are applied, are just outside the solution domain. This ensures that the VSs give a solution of the homogeneous equation. Further, the differential separation between the loci of the VS and the boundary values avoids the characteristic singularity in the GF at a point where the source and the field points coincide.

The VS method is rapidly convergent and numerically stable. The main computational cost of our GF method is in the calculation of the VSs. However, the VSs are in modular form and can be stored for later use. This can reduce the subsequent computational cost. One computational advantage of our GF method is that we need to numerically solve the main equation only near the boundaries or the discontinuities. In the bulk of the solution domain, the solution is given in a semi-analytic form in terms of the GF and/or its derivatives and the VSs. The most important advantage of the GF method is, as mentioned before, that it gives the response of the material to a point electrostatic or thermal probe, which is directly measurable by SPM.

Fig. 1 shows the geometry of the 2D material that we model. We neglect the discrete atomistic structure of the material so our calculations are valid at length scales larger than the atomistic dimensions. This is consistent with the continuum approximation inherent in the Laplace/Poisson equation. This allows us to neglect the zig-zag structure of the edges and any ripples or unevenness at the surface. Thus, the treatment given here is applicable to graphene as well as other 2D materials beyond graphene.

We consider two separate types of defects – rectangular (Fig. 1(a)) and hexagonal (Fig. 1(b)). The shape of the host solid in both the cases is assumed to be a square. We choose a 2D Cartesian frame of reference. The coordinate axes are assumed to be parallel to the outer edges of the solid with the origin at the center as shown in Fig. 1. We denote the position vector of a point by $\mathbf{r}$ (written in bold) and its X and Y coordinates by the subscripts 1 and 2. Thus $r_1 = X$ and $r_2 = Y$. The magnitude of a vector $\mathbf{r}$ is denoted by r . Unless stated otherwise, we will follow the Einstein's convention of summation over repeated indices.

The upper case letters A–D denote the external boundary whereas the lower case letters a–d (Fig. 1(a)) and a–f (Fig. 1(b)) represent the internal boundary. We denote the external boundary by E and the internal boundary by I . The material is confined into the region between the external and the internal boundaries, that is between E and I . This is the region of interest and constitutes the solution domain.

To calculate the GF, we apply a point source of unit strength at $\mathbf{r} = \mathbf{R}$ and solve the Poisson equation with all the prescribed boundary conditions. The Poisson equation to be solved for the GF, G , is given below

$$\nabla \cdot (K \nabla G) = \delta(\mathbf{r} - \mathbf{R}), \quad (1)$$

where K is a material parameter, ∇ is the gradient operator, and $\delta(\mathbf{r})$ denotes the well-known Dirac delta function of the vector variable $\mathbf{r}$. The material parameter K can denote, for example, the electrical or thermal conductivity for electrostatic or thermal problems. The delta function of a vector variable is defined in terms of the delta functions of its scalar components as

$$\delta(\mathbf{r}) = \delta(r_1)\delta(r_2). \quad (2)$$

We consider the case in which the material is homogeneous in the solution domain so that K is constant over this domain. We also assume K to be isotropic though the present treatment can be easily generalized to the anisotropic cases by taking the tensorial forms of K and the Laplacian. Further, we assume units such that K is unity. With these assumptions, Eq. (1) reduces to the following

$$\nabla^2 G(\mathbf{r}, \mathbf{R}) = \delta(\mathbf{r} - \mathbf{R}). \quad (3)$$

In Eq. (3) for the GF, we have not included any dissipation term, which is of course needed in any physical system. In the GF method the dissipation term may be included by introducing an imaginary part in the representation of the operator [33]. It has the effect of damping singularity and gives a finite width to the delta function type peak in Eq. (3). In many practical systems 2D solids are deposited on a substrate. In such cases the field in the 2D solid is necessarily coupled with the substrate. The coupling will cause dissipation of the field in the 2D solid through the substrate [34]. The field may be electric potential or temperature. Such systems can be phenomenologically simulated in the GF method by expressing the imaginary part as a parametric function of x and y .

The GF is a function of the field point, $\mathbf{r}$, and the source point, $\mathbf{R}$. Once we obtain the solution of Eq. (3), the solution for any general source function is obtained by a simple integration as given below

$$T(\mathbf{r}) = - \int G(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') d\mathbf{r}', \quad (4)$$

where $T(\mathbf{r})$ is the field, which is the response of the material to the probe represented by the source function $\rho(\mathbf{r})$ and the integration is over the distribution of the sources. It can be shown by direct substitution and by using Eq. (3) and the properties of the delta function that $T(\mathbf{r})$ given by Eq. (4) is a solution of the following Poisson equation

$$\nabla^2 T(\mathbf{r}) = -\rho(\mathbf{r}). \quad (5)$$

If $\rho(\mathbf{r})$ corresponds to an ideal point source in a SPM represented by a delta function as in Eq. (3), then the desired solution is just the GF subject to the boundary conditions. For a more realistic SPM tip, the integral in Eq. (4) has to be carried out over the area of the SPM tip.

Further, we observe from Eq. (4) that $T(\mathbf{r})$ follows the same homogeneous boundary conditions as the GF. Hence, the GF gives the complete solution of Eq. (5). Thus, we need to solve Eq. (3) subject to the prescribed boundary conditions as follows.

For each material system 'a' and 'b' shown in Figs. 1(a) and 1(b), respectively, we specify three different sets of boundary conditions as given below. Each set corresponds to a specific type of defect. For each set, the vectors $\mathbf{r}_s$ and $\mathbf{r}'$ are in the solution domain. The vector $\mathbf{r}_s$ lies on a contour which is just inside the boundaries A–D and a–d in Fig. 1(a) or a–f in Fig. 1(b).

- i. Dirichlet boundary conditions on E (external) as well as I (internal) boundaries.

$$G(\mathbf{r}_s, \mathbf{r}') = 0 \quad \text{for } \mathbf{r}_s \text{ on } E \text{ as well as } I. \quad (6)$$

- ii. Dirichlet boundary condition on E and Neumann on I .

$$G(\mathbf{r}_s, \mathbf{r}') = 0 \quad \text{for } \mathbf{r}_s \text{ on } E \quad (7)$$

and

$$\nabla_n G(\mathbf{r}_s, \mathbf{r}') = 0 \quad \text{for } \mathbf{r}_s \text{ on } I \quad (8)$$

- iii. Neumann boundary condition on E and Dirichlet on I .

$$\nabla_n G(\mathbf{r}_s, \mathbf{r}') = 0 \quad \text{for } \mathbf{r}_s \text{ on } E \quad (9)$$

and

$$G(\mathbf{r}_s, \mathbf{r}') = 0 \quad \text{for } \mathbf{r}_s \text{ on } I \quad (10)$$

where ∇_n denotes the normal component of the gradient vector at $\mathbf{r}_s$. The Dirichlet and the Neumann boundary conditions can be used to model different material systems [32]. As is well known, it is not physically meaningful to specify homogeneous Neumann boundary conditions on all the surfaces of a material system.

The particular solution of Eq. (3) that corresponds to the free space GF is given in terms of a logarithmic function and is well known. It is given by [32,35,36]

$$G_0(\mathbf{r}, \mathbf{R}) = (1/2\pi) \ln(|\mathbf{r} - \mathbf{R}|). \quad (11)$$

The unit of distance in Eq. (11) is defined as appropriate for the logarithmic functions. Consider, for example, a scalar field function $f(x) = \ln x$ where x is a distance variable. Suppose the value of $f(x)$ at $x = x_0$ is f_0 . We ‘measure’ the value of the field function with respect to f_0 . So $F(x) = f(x) - f_0 = \ln(x/x_0)$ and $F(x_0) = 0$. Thus, if x is expressed in units of x_0 , $F(x = 1) = 0$. Accordingly, in our formulation, Eq. (11) defines the unit of distance as the distance at which the field is assumed to be zero. For any physical quantity like the voltage or the temperature, the value of the field at unit distance is taken to be the zero point of the field.

The logarithmic term in Eq. (11) shows a singularity in the GF and introduces a size effect. These contributions in case of graphene have been discussed in [35].

The particular solution given by Eq. (11) satisfies Eq. (3) without any boundary conditions. To obtain the final solution, we have to add a solution of the homogeneous equation to Eq. (11). The homogeneous solution is written in terms of the VS functions, $F(\mathbf{r})$, that are integrable and defined to be zero everywhere except on a contour s' , which is just outside the solution domain and is parallel to its boundaries.

In terms of the VS functions, the solution of the homogeneous equation, $G_H(\mathbf{r})$, can be written as

$$G_H(\mathbf{r}, \mathbf{R}) = \int_{s'} G_0(\mathbf{r}, \mathbf{r}'_{s'}) F(\mathbf{r}'_{s'}, \mathbf{R}) d\mathbf{r}'_{s'}, \quad (12)$$

where the integral is over the $\mathbf{r}'_{s'}$. It can be easily shown, by using the property of the delta function, that the result of ∇^2 operating on the integral in Eq. (12) will be zero for $\mathbf{r}$ in the solution domain. This is because by hypothesis $F(\mathbf{r}'_{s'}, \mathbf{R})$ is zero for all values $\mathbf{r}'_{s'}$ inside the solution domain. Hence, Eq. (12) is a solution of the homogeneous equation.

We account for the singularity in $G_0(\mathbf{r}, \mathbf{r}'_{s'})$ in Eq. (12) by letting $\mathbf{r}$ reach the boundary from inside the solution domain without crossing the boundary. It is important to appreciate that both the contours s and s' are parallel to the boundaries and to each other but s lies just inside the boundary whereas s' lies just outside the boundary. The contour s is in the solution domain whereas s' is just outside this domain. The two contours are separated only differentially but they never touch each other. This avoids the singularity in the integral in Eq. (12) and is equivalent to taking the Cauchy principal value of the integral. It is physically justified because the boundary condition is specified at a physical point in the material which must be a part of the solution domain. The VS, on the other hand, is a mathematical artefact and can be chosen at any convenient points.

The complete solution of Eq. (3) is written as

$$G(\mathbf{r}, \mathbf{R}) = G_0(\mathbf{r}, \mathbf{R}) + G_H(\mathbf{r}, \mathbf{R}) \quad (13)$$

where $G_H(\mathbf{r}, \mathbf{R})$ in Eq. (12), which is needed for Eq. (13), is determined by applying the boundary conditions given in Eqs. (6)–(10) corresponding to the three cases (i)–(iii). First consider case (i).

Using Eqs. (6) and (13), we write the following integral equation for determination of $F(\mathbf{r}_s)$

$$G_H(\mathbf{r}_s, \mathbf{R}) = \int_{s'} G_0(\mathbf{r}_s, \mathbf{r}'_{s'}) F(\mathbf{r}'_{s'}, \mathbf{R}) d\mathbf{r}'_{s'} = -G_0(\mathbf{r}_s, \mathbf{R}) \quad (14)$$

where, as described earlier, $\mathbf{r}_s$ and $\mathbf{r}'_{s'}$ scan parallel contours that are differentially close but never touch each other. Thus Eq. (14) becomes an ordinary non-singular Fredholm integral equation that can be solved using the standard techniques.

We solve Eq. (14) numerically by converting the integral into a sum over a discrete set of N_s points on E and I . Effectively, we represent the entire vector space of the solution domain in terms of discrete vectors $\mathbf{r}$. The points at which F are applied and at which G_0 and G_H in Eq. (14) are calculated correspond to the same points at which the boundary conditions are specified. These points constitute a subspace $E+I$ in which $F(\mathbf{r}'_{s'}, \mathbf{R})$ is to be calculated. Equation (14) then becomes a matrix equation as given below:

$$\mathbf{\Gamma} \boldsymbol{\varphi} = -\boldsymbol{\Phi} \quad (15)$$

where $\mathbf{\Gamma}$ is a $N_s \times N_s$ square matrix and $\boldsymbol{\varphi}$ and $\boldsymbol{\Phi}$ are $N_s \times 1$ column matrices in the subspace of $E+I$. The elements of these matrices are given by

$$\Gamma_{s,s'} = G_0(\mathbf{r}_s, \mathbf{r}'_{s'}), \quad (16)$$

$$\varphi_{s'} = F(\mathbf{r}'_{s'}, \mathbf{R}) \quad (17)$$

and

$$\Phi_s = G_0(\mathbf{r}_s, \mathbf{R}). \quad (18)$$

The virtual sources φ_s are now obtained by matrix inversion for which very efficient software codes are available. The matrix inversion required in our method is, in general, numerically quite stable because the diagonal elements of the matrix dominate due to near

singular nature of $G_0(\mathbf{r}_s, \mathbf{r}'_s)$ at $\mathbf{r}_s$ close to $\mathbf{r}'_s$. The numerical results are presented in the next section.

3. Results and discussion

We apply the theory given in Sec. 2 to the two material systems shown in Figs. 1(a) and 1(b). The origin in both figures is taken to be at the center of the square ABCD and the coordinates of A are $(-5, 5)$. The rectangle and the regular hexagon in Figs. 1(a) and 1(b) are also centered at the origin. In Fig. 1(a) (rectangular defect) the coordinates of the corner d are $(-0.75, \sqrt{3}/2)$ with the lengths $dc = 1.5$ and $da = \sqrt{3}$. In Fig. 1(b) (hexagonal defect), the coordinates of the corner d are $(1, 0)$ and the length of the each side of the hexagon is 1.

Thus the areas of the rectangular and the hexagonal defects are equal to $3\sqrt{3}/2$.

We solve Eq. (15) at a discrete set of 1200 points on E and 600 points on I so that $N_s = 1800$. Thus, Eq. (15) is a 1800×1800 matrix equation. Its solution requires inversion of a 1800×1800 matrix. We show in Fig. 2 the calculated values of the homogeneous solution and the prescribed boundary values $G_0(\mathbf{r}_s, \mathbf{R})$ for a rectangular (Fig. 1(a)) and a hexagonal (Fig. 1(b)) defect. The net prescribed values at the boundaries are given by Eq. (13) and are zero in the present case of homogeneous Dirichlet boundary conditions on both E and I .

As a confirmatory test of the method, we calculate the boundary values of the final GF and compare them with the prescribed boundary values. We obtain an almost perfect agreement between the two that shows that the final GF is fully reliable. The numbers on the X axis denote the serial number of the points on E as well as on I . The count starts on E from A to D and, on I , from a to d for rectangular defect and from a to f for hexagonal defect. The two curves are in almost exact agreement and overlap with each other. Hence, for visual convenience, we show the calculated values only at a sample of 20 points on the external boundary and 20 points on the internal boundary. This shows the exact agreement between the calculated and the prescribed values at the boundary.

In a similar manner, we obtain the solutions for cases (ii) and (iii) with the boundary conditions given by Eqs. (7)–(10). In each case the boundary values are reproduced almost exactly as in Fig. 1 and therefore are not shown here.

Using the calculated values of the VS, the values of the GF as obtained from Eq. (13) are shown in the contour plots in Figs. 3–5. These figures correspond to cases (i)–(iii), respectively, with the boundary conditions given by Eqs. (6)–(10). Each figure gives the results for both rectangular (marked as ‘a’) as well as hexagonal (marked as ‘b’) defect. The external boundary is a square in all cases as shown in Fig. 1. The location of the source point, $\mathbf{R}$, is also shown in the figures which is taken to be quite close to the internal boundary. For brevity, the field values in these figures are shown only in the interior region of ABCD and not in the entire square.

As expected, the GF is large near the source point and the contours get deformed near the boundary of the defect. In fact the GF has a logarithmic singularity at $r = R$ as is evident

from Eq. (11). In a numerical application of the GF for some other calculation, the singularity has to be removed by adding an imaginary part in the GF [33] which amounts to adding dissipation as discussed in the previous section. In the present calculations, there was no need to remove this singularity. For the purpose of presentation, the values of the GF in Figs. 3–5 are calculated close to the singularity but not at the actual point of singularity. The singularity in these figures manifests as the limiting value of the curves. From the measurement point of view also, the more interesting feature is how the curves reach the singular point rather than the values at the singularity itself.

We make the following two additional observations in Figs. 3–5.

- i. The values of the GF at the external boundaries do not seem to be sensitive to the geometry of the defect. This is mathematically interesting because normally a 2D material is expected to show a strong size effect due to the logarithmic dependence of the GF as in Eq. (11). The possible reason for a weak size effect in these calculations is that the sign of the homogeneous solution and the particular integral are opposite of each other. This amounts to dipoles of sources for which the total GF does not have a logarithmic singularity. Further, the variation near the outer boundaries is small because the derivative of the log function $[\ln(x)]$ varies as $1/x$ and for a dipole it varies as $(1/x^2)$, which decreases for large x . Consequently, the function is not sensitive to the shape of the outer boundary if it is far enough from the source point.
- ii. The map of the GF clearly shows that it is sensitive to the shape as well as the physical nature of the defect. As remarked earlier, the defect is characterized by prescribing appropriate boundary conditions at the defect boundary. For example, if the defect is an antidot, the appropriate boundary condition will be Neumann type corresponding to free interface for which $\nabla_n T$ or $\nabla_n G$ is zero. The shapes of the GF contours in this case as shown in Fig. 4 are very different compared to those for Dirichlet boundary conditions at the defect shown in Figs. 3 and 5. The Dirichlet boundary conditions are needed if the value of the field T is prescribed at the defect boundary. For example, T can be the temperature for thermal problems and voltage for electrostatic problems. In case the defect is an inclusion, as in a functionalized 2D material, the boundary conditions will be a combination of Dirichlet and Neumann to ensure continuity of the GF at the interface.

To summarize, our results clearly show that G is quite sensitive to nature and size of defects in a material. As suggested in Sec. 1, the GF for a 2D material can be directly measured by SPM. Hence a measurement of G or T by SPM can be a very useful technique for characterization of these materials. We are presently carrying out experiments in this area. In practice, instead of a single point probe, a multiprobe system is experimentally more advantageous [37–41]. One advantage of the GF method as reported in this paper is that it can be applied to any distribution of sources including that in four probe systems. Finally, though we have considered fairly simple geometries in this paper, our method works very well for inclusions of complex shapes.

Our theoretical and experimental results using a multiprobe system will be reported elsewhere.

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Fig. 1. Geometry of the 2D material system. The host solid is a square containing a defect (a): Rectangular defect (b): Hexagonal defect. The area of the defects is the same in both cases. The shaded region in both (a) and (b) denotes the solution domain.

Fig. 2.

Comparison between calculated and prescribed boundary values on the external and internal boundaries for (a) rectangular defect and (b) hexagonal defect for set (i). Full lines denote prescribed values and points denote calculated values. The calculated and the prescribed values agree almost exactly at all the points. Only a sample of calculated values are shown in the interest of visual clarity. The results for sets (ii) and (iii) are exactly similar and, therefore, not shown.

Fig. 3.
Map of the calculated field in the material system shown in Fig. 1 for the boundary conditions in set (i): Dirichlet on E as well as I .

Fig. 4. Map of the calculated field in the material system shown in Fig. 1 for the boundary conditions in set (ii): Dirichlet on E and Neumann on I .

Fig. 5. Map of the calculated held in the material system shown in Fig. 1 for the boundary conditions in set (iii): Neumann on E and Dirichlet on I .