Transformation optics scheme for two-dimensional materials

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Two-dimensional optical materials, such as graphene, can be characterized by surface conductivity. So far, the transformation optics schemes have focused on three-dimensional properties such as permittivity ϵ and permeability μ. In this Letter, we use a scheme for transforming surface currents to highlight that the surface conductivity transforms in a way different from ϵ and μ. We use this surface conductivity transformation to demonstrate an example problem of reducing the scattering of the plasmon mode from sharp protrusions in graphene.

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Transformation optics [1,2] has proven a powerful technique to control the propagation of electromagnetic waves. The basic idea is that, under coordinate transformations, Maxwell's equations remain form-invariant, provided the material parameters are appropriately modified. Then the electromagnetic wave propagation in the transformed medium can be thought of as occurring in the original medium. Numerous applications of this technique have been proposed and demonstrated. Some examples are invisibility cloaks [3–5], waveguides with sharp bends [6], subwavelength image manipulation [7], etc.

With the recent discovery of two-dimensional materials such as graphene [8] and MoS_2 [9,10], there is enormous interest in studying their optical properties [11]. Such materials are usually characterized by surface conductivity, instead of volume conductivity, which characterizes three-dimensional materials. As such, it is expected that techniques of transformation optics, as usually applied, will have to be modified, to take into account the change in the dimensionality of the material parameter. To our knowledge, this is the first time that a full-transformation optics scheme involving surface conductivity has been considered. Although implementing transformation optics using spatial modulation of surface conductivity has been proposed in the past [12], we note that they do not address transformations that can take graphene out of the plane. In other words, they consider only flat graphene.

In this Letter, we will show how surface conductivity transforms under arbitrary coordinate transformations. We will find that the transformation rule is indeed different, compared to bulk conductivity. Then, we will present an example of how this surface conductivity transformation works, for the simple case of a two-dimensional transformation. We show how to reduce plasmon scattering from a triangular protrusion in graphene. It is indeed possible to implement such a surface conductivity transformation in graphene, using gate voltage [13] and chemical doping.

Let us consider the case of a two-dimensional material located between two dielectric materials. The source-free Ampère's Law is written in this case as

$$\nabla \times \mathbf{H} = -i\omega\epsilon_0\hat{\epsilon}_{\mathrm{bulk}}\mathbf{E} - i\omega\mathbf{P}_s|\nabla F(\mathbf{r})|\delta(F(\mathbf{r})), \quad (1)$$

where the equation of the surface $F(\mathbf{r}) = 0$ defines the geometry of the two-dimensional materials, $\hat{\epsilon}_{\mathrm{bulk}}$ is the permittivity of the surrounding three-dimensional materials, and $\mathbf{P}_s$ is the surface polarization of the two-dimensional material. The time derivative of the surface polarization gives rise to a surface current density:

$$\mathbf{J}_s = -i\omega\mathbf{P}_s = \sigma^{2D}\mathbf{E}_\parallel = \hat{\sigma}\mathbf{E}. \quad (2)$$

For the usual case of the interface of two bulk materials, this term is absent; however, for two-dimensional materials we need to retain this term in the derivation of the boundary conditions, due to the presence of the Dirac delta function in Eq. (1). Thus, in the case of a finite surface conductivity σ^{2D}, the boundary condition for the tangential magnetic field can be written in terms of a surface current [14]:

$$\hat{\mathbf{n}} \times \Delta\mathbf{H} = \mathbf{J}_\mathbf{s} = \hat{\sigma}\mathbf{E}, \quad (3)$$

where $\mathbf{J}_s$ is the surface current density, $\hat{\mathbf{n}}$ is the unit normal to the surface, $\hat{\sigma}$ is the surface conductivity tensor, and $\Delta\mathbf{H}$ is the difference between the magnetic fields on either side of the 2D material. For instance, an isotropic surface conductivity would be represented in terms of the basis $\{|t_1\rangle, |t_2\rangle, |n\rangle\}$, as $\hat{\sigma} = \sigma^{2D}(|t_1\rangle\langle t_1| + |t_2\rangle\langle t_2|)$. Here $|t_1\rangle$ and $|t_2\rangle$ are the two orthonormal local tangential vectors and $|n\rangle$ is the local-normal unit vector. Our aim here is to find the transformation rule for the $\hat{\sigma}$ tensor.

Based on Eqs. (1) and (2), the permittivity can be thought of as containing a Dirac delta function:

$$\hat{\epsilon} = \hat{\epsilon}_{\mathrm{bulk}} + \frac{i|\nabla F(\mathbf{r})|\delta(F(\mathbf{r}))}{\omega\epsilon_0}\hat{\sigma}. \tag{4}$$

Now, applying the usual transformation rule for permittivity, $\hat{\epsilon}' = \Lambda\hat{\epsilon}\Lambda^T/\det(\Lambda)$, to Eq. (4), and the standard rule for the change of variables in a delta function, we arrive at the result:

$$\hat{\sigma}' = \frac{\Lambda\hat{\sigma}\Lambda^T}{|(\Lambda^{-1})^T\hat{\mathbf{n}}|\det(\Lambda)}, \tag{5}$$

where $\hat{\mathbf{n}}(r)$ is the local surface normal given by $\nabla F(\mathbf{r})/|\nabla F(\mathbf{r})|$ and Λ is the transformation matrix $\Lambda_i^{i'} = \partial x^{i'}/\partial x^i$. The additional factor explicitly enters the surface conductivity tensor, because a compression in the plane normal to the two-dimensional material should produce no transformation of the surface conductivity, physically. But the $\det(\Lambda)$ factor does contain this compression factor. Therefore, surface conductivity further requires a multiplicative factor for the renormalization of the surface delta function. Equivalently, one could say that the normal unit vector, after transformation, does not remain a unit vector. Hence, the additional factor needs to be put in, to ensure that, in the transformed medium, $\mathbf{n}'$ is indeed a unit vector.

Taking a cue from the surface-plasmon polariton wave adapter proposed in [15,16], we illustrate that the surface conductivity transformation indeed works, by using the transformation shown in Fig. 1.

In the absence of any transformation optics, the plasmon mode propagating along the graphene sheet from the far left would suffer substantial scattering into the free space modes. Such radiative loss is typically dependent on the radius-of-curvature of the bump. For instance, if the graphene plasmon mode is highly confined, compared to the radius-of-curvature of the bump, then it is possible to achieve smaller radiative loss of the plasmon mode [17]. In our current formalism, however, we are able to tackle arbitrary radii of curvature. To subvert this scattering one can employ the well-known technique of transformation optics. This scheme would require us to modify the permittivity and permeability tensors in the region surrounding the sharp bump. However, this alone would not be enough to prevent scattering, since, as we mentioned earlier, the surface conductivity also needs to be transformed in a way that depends on the details of the transformation we wish to carry out.

Hence we consider three cases: (A) protrusion in graphene with no transformation optics employed; (B) transformation optics employed, but surface conductivity is not transformed; and (C) transformation optics employed for the surface conductivity, as well as the bulk parameters. The results are shown in Fig. 2. Finite element simulations in Fig. 2 were carried out using COMSOL Multiphysics, by employing a surface current boundary condition to represent the graphene. The surrounding media in the untransformed case is assumed to be a vacuum, for this example. However, we have performed tests, which are not presented here, with substrates of nonunity refractive indices, as well. For simplicity, we use only the imaginary part of the surface conductivity of graphene, at a doping level of $E_F = 0.5$ eV, at zero temperature. The excitation frequency for this test case is 0.25 eV, so the numerical value of the in-plane, untransformed surface conductivity is $\sigma = i1.46 \times 10^{-4}$ S.

Mathematically, the transformation in the four regions shown in Fig. 1 is given as follows:

$$x' = x, y' = y - \frac{\tan\beta}{\tan\alpha}|y| + (a - |x|)\tan\beta, z' = z. \tag{6}$$

Everywhere outside the four regions, there is no change. Note that we have chosen a linear map only for the purpose of demonstrating the main idea of surface conductivity transformation. The transformation we provided in Eq. (5) is valid, in general, beyond the linear approximation. In principle, other transformations can be employed, keeping in mind the material constraints. For instance, quasi-conformal maps [18], which have been applied in the context of plasmonics elsewhere [19], could be employed, or, in the case of rotationally symmetric bumps, it might be possible to design isotropic graphene-surface conductivity and the environment-permittivity profile using techniques similar to [20].

The Jacobian Λ is given by

$$\Lambda = \begin{bmatrix} 1 & 0 & 0 \\ -\mathrm{sgn}(x)\tan\beta & 1 - \mathrm{sgn}(y)\tan\beta/\tan\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{7}$$

Then the transformed bulk material parameters in the four regions are given, in the $\{|x\rangle, |y\rangle, |z\rangle\}$ basis, as follows:

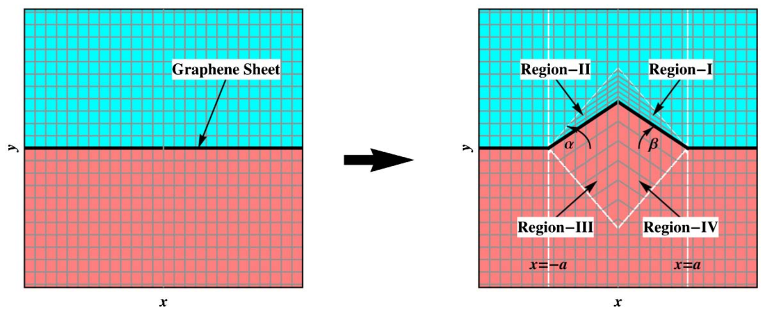

Fig. 1. Coordinate transformation, which compresses a triangular region toward the top and rarefies it at the bottom. A sharp protrusion in the graphene is produced at the center.

$$\epsilon', \mu' = \frac{\Lambda\Lambda^T}{\det \Lambda} = \frac{1}{1 - \mathrm{sgn}(y) \tan\beta / \tan\alpha} \begin{bmatrix} 1 & -\mathrm{sgn}(x)\tan\beta & 0 \\ -\mathrm{sgn}(x)\tan\beta & 1 - 2\,\mathrm{sgn}(y)\tan\beta/\tan\alpha + (\tan\beta/\sin\alpha)^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (8)$$

The new surface conductivity tensor $\hat{\sigma}'$ is expressed using Eq. (5), with $\hat{\mathbf{n}} = \hat{\mathbf{y}}$, as

$$\hat{\sigma}' = \frac{\Lambda\hat{\sigma}\Lambda^T}{|(\Lambda^{-1})^T\hat{\mathbf{y}}| \det \Lambda} = \sigma^{2D} \begin{bmatrix} \cos\beta & -\mathrm{sgn}(x)\sin\beta & 0 \\ -\mathrm{sgn}(x)\sin\beta & \sin\beta\tan\beta & 0 \\ 0 & 0 & \cos\beta \end{bmatrix}, \quad (9)$$

where σ^{2D} is the scalar surface conductivity of the untransformed graphene.

Now, from Eq. (9), it might appear that the surface conductivity tensor has off-diagonal components, which would be difficult to achieve experimentally. However, one must remember that the transformed tensor is given in the $\{|x\rangle, |y\rangle, |z\rangle\}$ basis. To get more physical insight, we go the $\{|t\rangle, |n\rangle, |z\rangle\}$ basis, where $|t\rangle$ is a unit vector, locally tangential to the graphene, and $|n\rangle$ is locally normal to the graphene surface. Since the z-direction is unchanged in this example, we keep the same unit vector in that direction. A basis change can be carried out using: $[\hat{\sigma}']_{tnz} = A[\hat{\sigma}']_{xyz}A^\dagger$, where A is the basis change matrix, composed of projections of the new basis vectors on the old basis vectors. In our case, graphene is situated in regions I and II, for which the A matrix is given by

$$A = \begin{bmatrix} \cos\beta & -\mathrm{sgn}(x)\sin\beta & 0 \\ \mathrm{sgn}(x)\sin\beta & \cos\beta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (10)$$

Then $[\hat{\sigma}']_{tnz}$ is given by

$$[\hat{\sigma}']_{tnz} = \sigma^{2D} \begin{bmatrix} \sec\beta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \cos\beta \end{bmatrix}. \quad (11)$$

Two things are apparent from the form of $[\hat{\sigma}']_{tnz}$ in Eq. (11). First, there is a geometrical scaling factor involved in the transformed conductivity tensor. In particular, for the untransformed case, the components $[\hat{\sigma}]_{tt}$ and $[\hat{\sigma}]_{zz}$ should both be equal to σ^{2D}. These geometrical factors can be understood in terms of surface current conservation, as pointed out in [21]. The surface current density in the tangential direction prior to the transformation is $J_{s,x} = \sigma^{2D}E_x$. After the transformation, it becomes: $J'_{s,t} = \sigma^{2D} \sec\beta(E'_x \cos\beta - \mathrm{sgn}(x)E'_y \sin\beta) = \sigma^{2D} \sec\beta(E_x \cos\beta) = J_{s,x}$. For the z-direction, we note that it is the surface current that needs to be preserved across the region $-a < x < a$. So we have: $I'_{s,z} = \int_{-a/\cos\beta}^{a/\cos\beta} J'_{s,z} \mathrm{d}x'_t = \int_{-a}^{a} J'_{s,z} \mathrm{d}x' / \cos\beta = \int_{-a}^{a} (\sigma^{2D}\cos\beta)E'_z \mathrm{d}x' / \cos\beta = \int_{-a}^{a} \sigma^{2D} E_z \mathrm{d}x = I_{s,z}$.

Second, it appears that the given transformation requires us to somehow make the graphene conductivity anisotropic, that is, $\hat{\sigma}'_{tt}$ and $\hat{\sigma}'_{zz}$ need to be different. Although it might be possible to achieve such anisotropic effects using strained graphene [22–25], in the present case of TM modes, the $\hat{\sigma}'_{zz}$ component does not matter, since the boundary condition for H'_z involves only the surface current in the $|t\rangle$ direction. Hence, this conductivity change can be easily implemented via electrostatic [26], or chemical doping. As far as bulk parameters namely ϵ', μ', are concerned, there have been numerous demonstrations of natural and artificial anisotropic materials in the terahertz range [27–30].

We have demonstrated the transformation rule for surface conductivity under arbitrary coordinate transformations. An additional factor related to the renormalization of the surface current needs to be included to maintain the form invariance of Maxwell's equations. We then presented an example problem of reducing scattering from a triangular protrusion in graphene, using the proposed method of surface conductivity transformation. This kind

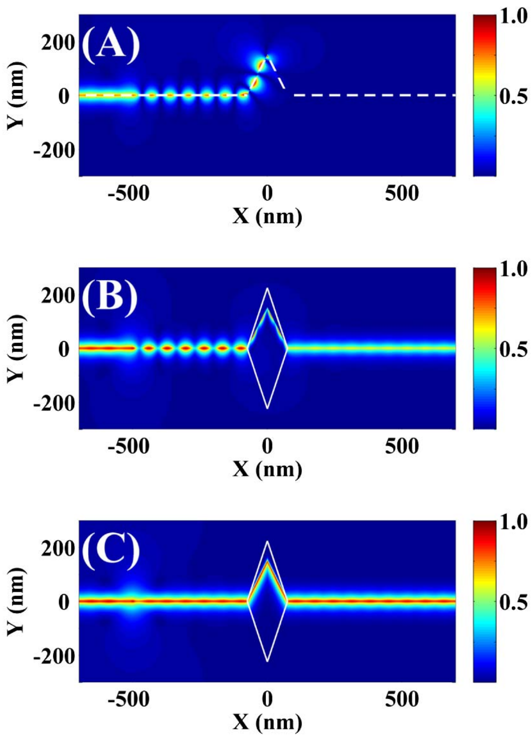

Fig. 2. Magnetic line current source is placed at (−500 nm, 2 nm). The normalized scattered field, $|\mathbf{H} - \mathbf{H}_{\mathrm{inc}}| / \max\{|\mathbf{H} - \mathbf{H}_{\mathrm{inc}}|\}$, is plotted here. (A) Protrusion in graphene with no transformation optics; (B) protrusion in graphene with transformation optics applied only to surrounding $\hat{\epsilon}$ and $\hat{\mu}$; and (C) protrusion in graphene with the full-transformation optics scheme applied to $\hat{\sigma}$, $\hat{\epsilon}$, and $\hat{\mu}$. In this example, $\alpha = \tan^{-1} 3$ and $\beta = \tan^{-1} 2$. In this example, the surrounding media in the untransformed case are assumed to be a vacuum.

of conductivity transformation would be useful for transformation optics applications involving two-dimensional materials.

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