

Continuous topological transition from metal to dielectric

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Metal and dielectric have long been thought as two different states of matter possessing highly contrasting electric and optical properties. A metal is a material highly reflective to electromagnetic waves for frequencies up to the optical region. In contrast, a dielectric is transparent to electromagnetic waves. These two different classical electrodynamic properties are distinguished by different signs of the real part of permittivity: The metal has a negative sign while the dielectric has a positive one. Here, we propose a different topological understanding of metal and dielectric. By considering metal and dielectric as just two limiting cases of a periodic metal-dielectric layered metamaterial, from which a metal can continuously transform into a dielectric by varying the metal filling ratio from 1 to 0, we further demonstrate the abrupt change of a topological invariant at a certain point during this transition, classifying the metamaterials into metallic state and dielectric state. The topological phase transition from the metallic state to the dielectric state occurs when the filling ratio is one-half. These two states generalize our previous understanding of metal and dielectric: The metamaterial with metal filling ratio larger/smaller than one-half is named as the "generalized metal/dielectric." Interestingly, the surface plasmon polariton (SPP) at a metal/dielectric interface can be understood as the limiting case of a topological edge state.

metamaterials | topology | plasmonics | Zak phase

From classical electrodynamics, metal and dielectric are dis-tinguished by permittivity with different signs. This basic understanding forms the basis of plasmonics (1-4). In the field of metamaterials, artificial properties are created by manipulating the subwavelength structure mixing metals and dielectrics to give novel properties such as negative refraction (5, 6). One of the simplest forms of metamaterials consists of alternate layers of metal and dielectric, which have shown interesting properties such as hyperbolicity in dispersion and have been exploited for superimaging applications (7). The properties of the layered metamaterial critically depend on the proportion of metal. Gradually varying the proportion of metal naturally leads to a continuous transition from solid metal to solid dielectric. At some ratio of metal to dielectric it is expected that there is an abrupt transition from metallic to dielectric behavior. The interface between metal and dielectric supports surface plasmon polaritons (SPPs) (4, 8, 9) and this is also true of interfaces between metallic and dielectric metamaterials.

Topology, a mathematical concept (10), has recently been an intensively researched topic in the field of photonics (11–17). A topological invariant is a quantized fingerprint that differentiates different materials systems, where the fascinating edge state exists at the interface between two bulk materials with different topological invariants (18–20). The topological invariant is like the sign of dielectric function that distinguishes metal and dielectric. Therefore, it is interesting to see whether metal and dielectric can be characterized with different topological invariants.

Here we generalize our previous understanding of metal and dielectric. These two matters are the limiting cases of a metaldielectric layered metamaterial, where a pure metal has a metal filling ratio $f_m = 1$ while a dielectric has $f_m = 0$. And the metal can continuously transform to a pure dielectric by varying f_m from 1 to 0. A topological invariant, the Zak phase (21, 22), is found to exist in this process and utilized to categorize the metamaterials with metallic state ($f_m > 0.5$) and dielectric state ($f_m < 0.5$). This classification generalizes the concept of metal to the layered metamaterial with $f_m > 0.5$, while the scope of the dielectric has been extended to the system with $f_m < 0.5$. The understanding of these generalized metallic and dielectric metamaterials gives the SPPs at the metal/dielectric interface an additional physical meaning: the limiting case of a topological edge state.

Results and Discussion

Continuous Transition from Metal to Dielectric. Fig. 1 illustrates how a metal continuously transitions into a dielectric, where the cyan region corresponds to the metal and the white region to the dielectric. Starting from a pure metal, we can deliberately cut it into unit cells consisting of many slabs with a period d. After that, we gradually decrease the filling ratio of the metal f_m (a pure metal has a filling ratio 1). When continuously decreasing the filling ratio f_m , the pure metal first transitions into a metal-dielectric layered system that has more metal ($f_m > 0.5$). By further reducing f_m , we arrive at a critical point where the ratio of the metal is the same as that of the dielectric; i.e., $f_m = 0.5$. After this point, continuous decreasing of the metal filling ratio leads to the dielectric-rich case ($f_m < 0.5$). In the limit, the metal filling ratio f_m goes down to 0, which corresponds to a pure dielectric.

Significance

We extend the concept of metals and dielectrics to the "generalized metal/dielectric" by treating a pure metal or dielectric as the limiting case of a metal-dielectric layered metamaterial. Specifically, the metamaterial with metal filling ratio larger than one-half shares the same topological invariant as a pure metal and thus exhibits some metallic behaviors. In contrast, the dielectric-rich metamaterial and a pure dielectric are topologically equivalent and display dielectric properties. The topological edge state exists between the generalized metal and dielectric, giving the surface plasmon polariton (SPP) an additional physical meaning: the limiting case of a topological edge state.

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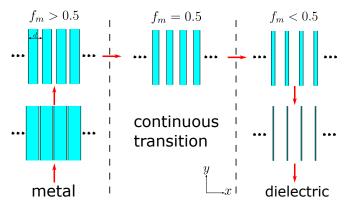


Fig. 1. Schematic for the continuous transition from metal to dielectric. By continuously decreasing the metal filling ratio f_m , the pure metal first transforms into a metal-rich case with $f_m > 0.5$. Further decreasing the filling ratio, we arrive at the half-way point $f_m = 0.5$. After that, the system enters into the dielectric-rich case, with a filling ratio $f_m < 0.5$. In the limit of $f_m \rightarrow 0$, the system becomes a pure dielectric. Note that the cyan region corresponds to the metal and the white region to the dielectric.

This kind of transition from a pure metal to a pure dielectric links metal and dielectric in a continuous manner so that metal and dielectric can be understood as two limiting states of a metal-dielectric system. In *Topological Transition and Zak Phase*, we study the topological properties during this continuous transition.

Topological Transition and Zak Phase. To characterize the topological property of this periodic system, the Zak phase is used as a topological invariant during this continuous transition. Note that the unit cell has an inversion symmetry such that the Zak phase of this one-dimensional periodic system can be quantized as π or 0 (21). This requirement of an inversion symmetry can be realized by choosing the center of the metal or the dielectric as the unit cell center. Here we put the metal in the cell center without loss of generality. Also, a Drude model is used for the metal

 $(\varepsilon_m = 1 - \frac{\omega_p^2}{\omega^2}$ with $\omega_p = 8.95 \text{ eV}/\hbar$) (23), while vacuum ($\varepsilon_d = 1$) is used for the dielectric.

To obtain the Zak phase of this periodic slab system as it transforms from metal to dielectric, we need first to calculate the corresponding band structure. For this one-dimensional photonic crystal, we have a Bloch k-vector K in the x direction and a continuous k-vector k_y in the y direction. The dispersion relation of this periodic slab system can be obtained from the transfer matrix method (24) and is written as (*SI Appendix*)

$$2\cos(Kd) = 2\cosh(f_m|k_y|d)\cosh((1-f_m)|k_y|d) + (\varepsilon + 1/\varepsilon)\sinh(f_m|k_y|d)\sinh((1-f_m)|k_y|d),$$
[1]

which determines the dispersion surface $\omega(k_y, K)$.

The band structure relating frequency ω and K is calculated and summarized in Fig. 2. Note that the band structure in Fig. 2 is a cross-section of two dispersion surfaces, where the k-vector k_y is chosen randomly as 1/d. Then, the Zak phase of each band can be calculated by integration in the first Brillouin zone $-0.5 < Kd/2\pi < 0.5$ (20, 21, 25). We can also derive the Zak phase by analyzing the symmetry of the eigenmodes at the center and edge of the Brillouin zone $(K=0 \text{ and } K=\pm\pi/d)$ (21, 26) (SI Appendix). For a given band, if the symmetries of the eigenmode at K=0 and $K=\pm\pi/d$ are different, the Zak phase of this band is quantized as π . On the contrary, the band possesses a Zak phase 0 if the symmetries at K=0 and $K=\pm\pi/d$ are the same. Following these procedures, we calculate the Zak phase for all of the bands, which are labeled in Fig. 2*A*–*E*.

By calculating the Zak phase, we can study how this topological invariant evolves when a metal continuously transforms into a dielectric. Starting from the nearly pure-metal case ($f_m = 0.999$) in Fig. 2A, both lower and upper bands have a Zak phase π . When decreasing the metal filling ratio to 0.9, we observe that the band gap becomes smaller, but the Zak phase remains

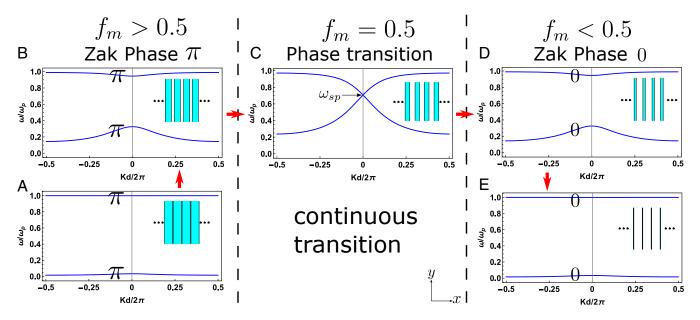


Fig. 2. Evolution of band structure and Zak phase on continuously changing the metal filling ratio f_m . (A) For a nearly pure metal case ($f_m = 0.999$), two bands with Zak phase π are separated with a gap. (B) On reducing the filling ratio to 0.9, the gap gets smaller but the Zak phase remains unchanged. (C) The band gap closes at singular point $f_m = 0.5$ where a topological phase transition happens. (D) The band gap reopens after passing through the singular point, and the Zak phase becomes 0 ($f_m = 0.1$). (E) The band gap becomes larger when further decreasing f_m to 0.001, while the Zak phase stays at 0.

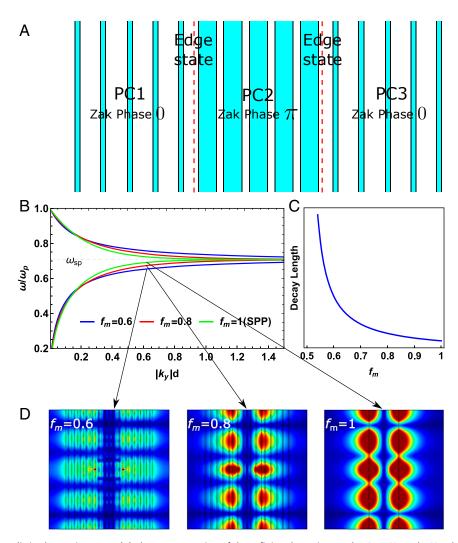


Fig. 3. Edge state for a realistic plasmonic system. (*A*) The system consists of three finite photonic crystals PC1, PC2, and PC3, where PC2 has a filling ratio $f_m > 0.5$ while PC1 and PC3 have a complementary filling ratio $1 - f_m$. (*B*) Dispersion relation of the edge state with different filling ratios. (*C*) Decay length of the edge state as a function of the filling ratio f_m . (*D*) Mode profile of excited edge states with different f_m , which is numerically calculated in Comsol with a damping $\Gamma = 65.8$ meV/ \hbar in the metal.

unchanged as π . As a topological invariant, the Zak phase is preserved during this continuous transition until the filling ratio f_m decreases to 0.5. At the half-filling ratio, when $f_m = 0.5$, the band gap closes at surface plasmon frequency $\omega_{sp} = \omega_p / \sqrt{1 + \varepsilon_d}$. This is a transition point after which the Zak phase changes from π to 0 abruptly. If we keep decreasing the filling ratio f_m , the Zak phase stays as 0 until we reach a pure dielectric. In particular, we observe that when $f_m \to 0$ or $f_m \to 1$, both lower and upper bands become flat, where the lower band approaches $\omega = 0$ while the upper band approaches $\omega = \omega_p$, forming a wide gap in between. Note that we have used quasistatic approximation in the band structure calculation, where only the electrostatic mode is considered, and the electromagnetic mode is neglected. To sum up, we have given metal and dielectric a topological property: The metal $(f_m = 1)$ is topologically equivalent to a periodic slab system with $f_m > 0.5$ as they share the same Zak phase π , while the dielectric $(f_m = 0)$ is topologically equivalent to a periodic slab system with $f_m < 0.5$ whose Zak phase is 0. This is the main result of this paper.

In the above calculation of the Zak phase, the metal/dielectric considered is lossless, i.e., a Hermitian system (27). When the loss is present, especially in the metal, we end up with a non-Hermitian system. For a non-Hermitian system, both left and

right eigenstates should be considered, which are generally not equal (28). However, we demonstrate these two eigenstates are the same in our system and further show that the Zak phase of our metal-dielectric slab system is still quantized as π or 0 in the quasistatic limit despite non-Hermiticity (*SI Appendix*). This means the topological properties of our system are robust to the loss.

Topological Edge State. From the phase transition in Fig. 2, we learn that two periodic slab systems with a metal filling ratio $f_m > 0.5$ and $f_m < 0.5$ are characterized with different topological invariants. According to the bulk-edge correspondence (12, 13, 20), a topological edge state is expected to exist in the energy gap at the interface between these two layered systems. To investigate this topological edge state, we study a realistic system shown in Fig. 3*A*, which consists of three photonic crystals: the left one with Zak phase 0 (photonic crystal [PC]1), the middle one with Zak phase π (PC2), and the right one with Zak phase 0 (PC3). Each of these bulk materials is composed of five unit cells and they form two interfaces of interest, marked with red dashed lines. The dispersion relation of the edge state localized on these two interfaces can be calculated for different filling ratios shown in Fig. 3*B*, where the filling ratio of PC2 is chosen as f_m while the

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two crystals on either side, PC1 and PC3, are both complementary to PC2 with filling ratio $1 - f_m$. On increasing f_m , the filling ratio of PC2 increases, while that of PC1 and PC3 decreases. In the limit of $f_m \rightarrow 1$, the PC1/PC2/PC3 system in Fig. 3A reduces to a single metal slab surrounded by a dielectric. By calculating the dispersion relation for the edge state, one observes that there exists a gapless edge state within the gap of corresponding bulk materials (see *SI Appendix* for the projected bulk band of different filling ratio f_m). Comparing the dispersion relation of the PC1/PC2/PC3 system with that of a metal slab having the same thickness as the bulk PC2, we can observe that the edge-state dispersion relation asymptotically approaches the SPP dispersion. Therefore, we conclude that the SPP is a limiting case of the topological edge state. This is another important result of this paper.

Finally, we study the mode configuration for different filling ratios with finite-element solver Comsol Multiphysics. By positioning a dipole source at the two interfaces, the edge state can be excited, as shown in Fig. 3D. By comparing the field profile for $f_m = 0.6$, $f_m = 0.8$, and $f_m = 1$, we can observe the mode getting more and more localized and enhanced at the interface when increasing f_m . A filling ratio of $f_m = 1$ corresponds to the single metal slab case and gives the smallest decay length of the edge state. When the filling ratio f_m is decreased, the decay length of the edge state becomes larger until $f_m \rightarrow 0.5$, where the decay length diverges, and the edge state becomes a bulk mode. This divergence behavior of the edge state can also be understood with effective medium theory, from which the metal-dielectric photonic crystal can be effectively modeled as an anisotropic material described as (6, 29)

$$\varepsilon_{\parallel} = f_m \varepsilon_m + (1 - f_m) \varepsilon_d$$

$$\varepsilon_{\perp} = \frac{\varepsilon_m \varepsilon_d}{f_m \varepsilon_d + (1 - f_m) \varepsilon_m},$$
[2]

where ε_{\parallel} and ε_{\perp} correspond to the effective permittivity parallel and normal to the metal–dielectric interface, respectively. For an edge state with a given k_y , the corresponding decay length inside the anisotropic medium is $1/\sqrt{\frac{\varepsilon_{\parallel}}{\varepsilon_{\perp}}k_y^2}$ (*SI Appendix*). This decay length increases when the filling ratio decreases and eventually diverges when $f_m \rightarrow 0.5$ (Fig. 3C).

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Conclusion

We assign a topological classification to metals and dielectrics by considering metal and dielectric as two limiting cases of a one-dimensional photonic crystal consisting of alternating layers of metal and dielectric slabs. The Zak phase of the system undergoes an abrupt transition between 0 and 1 at the critical filling ratio $f_m = 0.5$. This topological transition offers us a different understanding of the electromagnetic properties of metals and dielectrics: A metal is topologically equivalent to the layered metamaterial with $f_m > 0.5$ while a dielectric is topologically equivalent to this system with $f_m < 0.5$. Finally, the SPP can be understood as the limiting case of a more generalized edge state at the interface between metallic and dielectric metamaterials. Our increased understanding of metals and dielectrics leads to the concept of "generalized metal" and "generalized dielectric," which gives the material design a much higher degree of freedom.

Materials and Methods

For a detailed description of methods, see SI Appendix.

Calculation of Dispersion Relation. The transfer matrix method is used in the calculation of band dispersion for periodic layered metamaterials. We choose magnetic field H_z as the eigenfield, which in the periodic slab system follows the Bloch condition. By using the Bloch theorem in the transfer matrix method, we obtain the band dispersion of the metal–dielectric layered metamaterial in Eq. 1. Similarly, we calculate the transfer matrix for the whole PC1/PC2/PC3 system in Fig. 3, from which the edge-state dispersion relation can be obtained.

Calculation of Zak Phase. The Zak phase of a band is calculated by analyzing the symmetry of eigenfield H_z at the center and the edge of the first Brillouin zone, which is consistent with our numerical integration of the Berry connection in the first Brillouin zone.

Data Availability. All of the data are included in this paper.

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