Course Name: Introduction to Microwave and Optical Metamaterials
Professor Name: Dr. Debabrata Sikdar
Department Name: Electronics and Electrical Department
Institute Name: Indian Institute of Technology, Guwahati
Week-9
Lecture-44

Lec 44: Metamaterials Based Nanoscale Optical Cavities and Active Hyperbolic Metamaterials

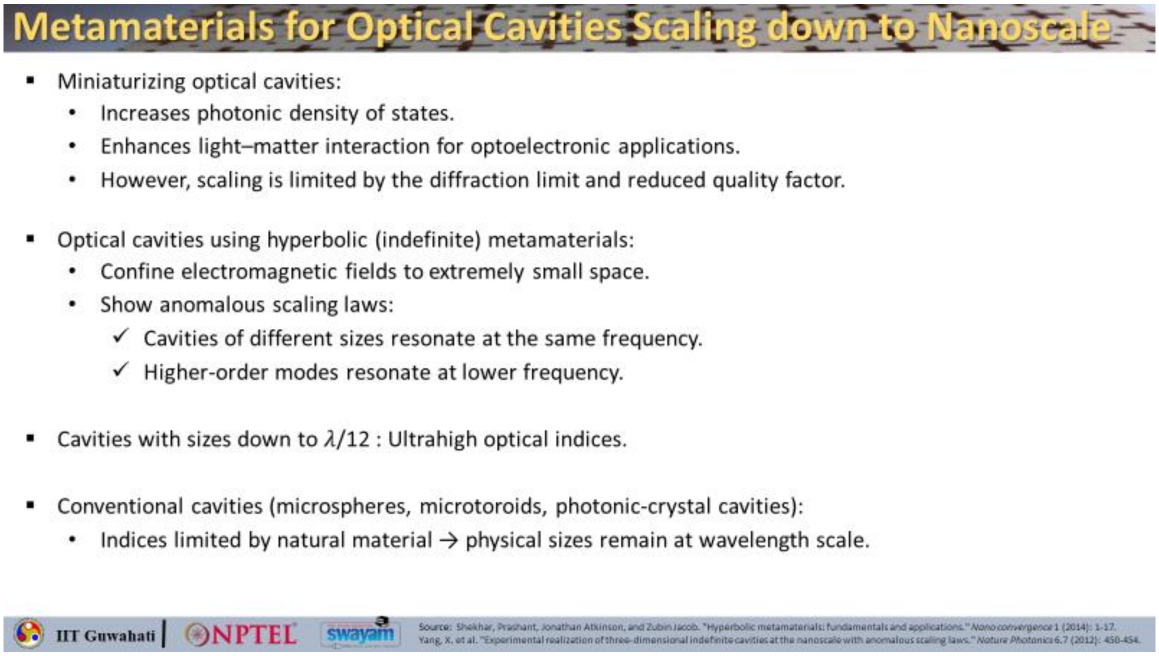
Hello everyone, welcome to Lecture 44 of the online course on Introduction to Microwave and Optical Metamaterials. Today's lecture will be on nanoscale optical cavities based on metamaterials, and we will also discuss some active hyperbolic metamaterials.

Lecture Outline

- Metamaterials for Optical Cavities Scaling down to Nanoscale
- Design of Metamaterials Based Nanoscale Optical Cavities
    - Hyperbolic Metamaterials for Optical Cavities
    - Permittivity and Dispersion Relation for Hyperbolic Metamaterials
    - Total Internal Reflection Mechanism
- Active Hyperbolic Metamaterials
- Applications of Active Hyperbolic Metamaterials

So, here is the lecture outline, we will continue our discussion of how metamaterials can be used for optical cavities that can be scaled down to nanoscale. We will discuss the design of metamaterials-based nanoscale optical cavities. We will cover hyperbolic metamaterials for optical cavities and discuss their permittivity and dispersion relation. And also, the mechanism for total internal reflection that allows it to work as a cavity.

After that, we will discuss active hyperbolic metamaterials and what the applications of active hyperbolic metamaterials are. Now, we have seen that hyperbolic metamaterials enable interesting applications due to their hyperbolic dispersion, right?



And one of those could be towards miniaturizing the optical cavities that will increase the photonic density of states. which, in turn, will increase the light-matter interactions very useful for optoelectronic applications. However, in conventional cavities, the scaling is typically limited by the diffraction limit of light.

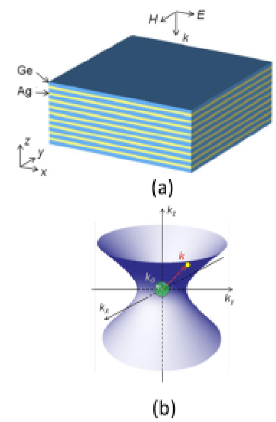
and it reduces the quality factor. So, you can think of optical cavities made of indefinite or hyperbolic metamaterials that can confine electromagnetic waves. Field in an extremely small space by, you know, overcoming the diffraction limit barrier. So, it also shows some anomalous scaling laws, something like, you know, the cavities of different sizes can be made to resonate. at different frequencies and also the higher order mode will be seen to resonate at lower frequency.

This is something completely opposite that happens with conventional cavities, okay. You will also see that you can make cavities with sizes down to lambda by 12. So, that means you are basically going to achieve ultra-high optical indices. So, in conventional cavities such as microspheres, microtoroids, and photonic crystal cavities, the index is basically limited by the natural material. and that also defines the physical size of the cavity, which remains typically on the wavelength scale, but because with metamaterials you can Achieve very extraordinary optical indices; that is how you can also change the overall physical size of the cavity.

Design of Metamaterials Based Nanoscale Optical Cavities

Hyperbolic metamaterials for optical cavities

- The metamaterial structure is made of alternating thin layers of silver (Ag) and germanium (Ge) (As shown in figure 1.(a)).
- When the multilayer period ≪ wavelength, the structure behaves as an effective medium (Maxwell-Garnett theory applies).
- The metamaterial's permittivity tensor is uniaxial:
  - The real parts of principal components can have different signs.
- This creates a 3D hyperboloid iso-frequency contour (IFC) (Figure 1.(b)).
  - A spherical IFC of air (radius $k_0 = 2\pi/\lambda$) is for comparison.



(b)

Figure 1.: (a) Schematic of multilayer hyperbolic metamaterial structure and (b) its hyperboloid IFC.

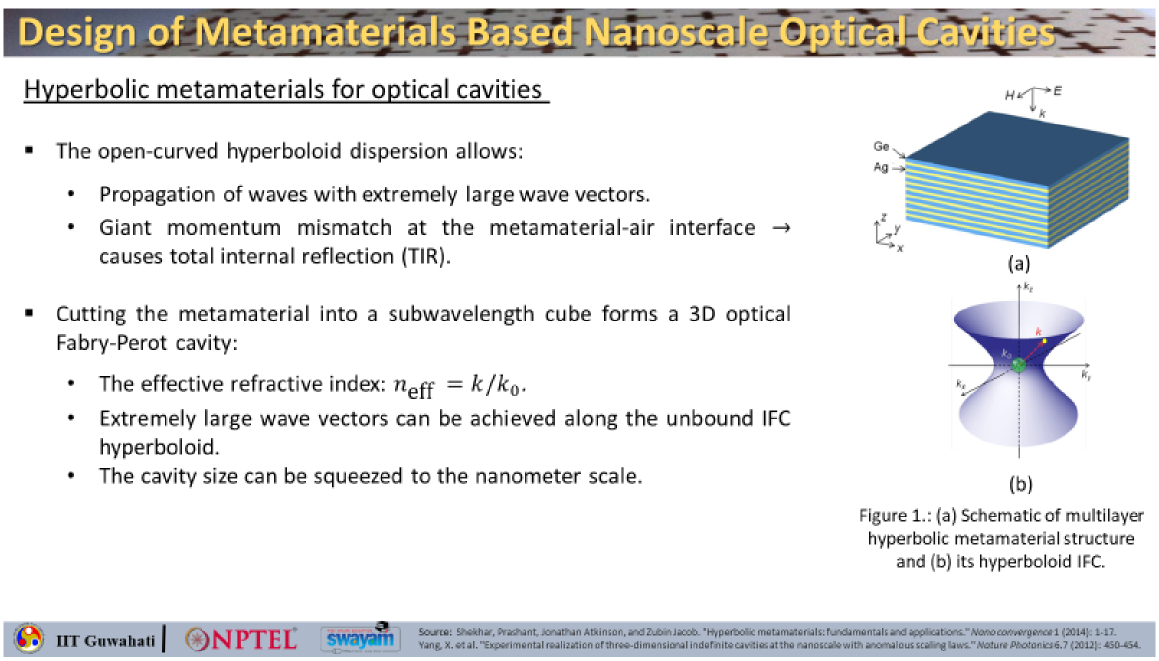
Source: Shekhar, Prashant, Jonathan Atkinson, and Zubin Jacob. "Hyperbolic metamaterials: fundamentals and applications." *Nano convergence* 1 (2014): 1-17.
Yang, X. et al. "Experimental realization of three-dimensional indefinite cavities at the nanoscale with anomalous scaling laws." *Nature Photonics* 6.7 (2012): 450-454.

So, here the metamaterial structure basically consists of alternating layers of thin silver and germanium. So, as you can see here, this is the direction of k light propagation. This is the electric field direction and this is the magnetic field direction, right. The electric field is generally considered parallel to the interface between the metal and the dielectric layers. Now, we have to consider the period of this multilayer, which is much smaller than the wavelength.

The period is nothing but the thickness of the germanium plus the thickness of the silver layer. Because that is the unit cell that is being repeated periodically in one direction, right? So, when the multilayer period is sub-wavelength or much smaller than the wavelength of the light it is interacting with, the structure basically behaves as an effective medium, and it will be safe to use the Maxwell-Garnett theory. For estimating the effective permittivity along the parallel and perpendicular directions, which we have seen a couple of times by now. So, this metamaterials permittivity tensor will be uniaxial because along the two parallel directions, they will have the same. So, x and y will experience the same kind of permittivity.

So, it will be epsilon parallel, and along the z direction, you will have different permittivity, which is epsilon. Now, because it is a metal-dielectric kind of interface, you will see that one will be positive and the other one will be negative. And that is when, you know, the principal components have different signs; you get hyperbolic dispersion curves, right? So, this basically creates a type 2 hyperboloid. Iso-frequency contour is right and for comparison, you can also see that there is a small spherical isofrequency contour shown here for air.

Where the radius is in the k-space, the radius is k naught, that is, 2 pi by lambda, okay. So, you can see this isofrequency contour of this multilayer metamaterial, which is basically taken from this dispersion relation shown here. blue surface right and the yellow dot here is located on this hyperboloid that shows the resonating wavelength k. That is inside the cavity, okay? So, you can see that this is much larger than you know, the k0 indicating that you know in this kind of material. You can have an ultra-high effective refractive index, which will be given by n effective as k by k0, okay.



So, the open curved hyperbolic dispersion also allows waves with extremely large wave vectors to propagate. Okay, which means there will be a large momentum mismatch at the metamaterial-air interface, and that will lead to total internal reflection, right? So, by cutting the metamaterial into sub-wavelength size cubes, what can you make? You can make a three-dimensional fabric parallel cavity kind of structure, where the effective refractive index can be given as k by k naught as we have seen ok. So, because of this extremely large wave vector k, that is coming from this unbounded isofrequency contour hyperboloid. So, the cavity size this will be very very high and that will make sure that the cavity can be squeezed to very small size or nanometer scale right.

Design of Metamaterials Based Nanoscale Optical Cavities

Permittivity and dispersion relation for hyperbolic metamaterials

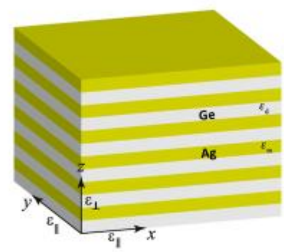
- The multilayer metamaterial can be modeled as a homogeneous effective medium.
  - Its anisotropic permittivity tensor components are calculated using Maxwell-Garnet theory.

- Permittivity equations:

$$\varepsilon_{\|}(\varepsilon_x = \varepsilon_y) = p\varepsilon_{\mathrm{m}} + (1-p)\varepsilon_{\mathrm{d}}$$

$$\varepsilon_{\perp}(\varepsilon_z) = \frac{\varepsilon_m \varepsilon_d}{p\varepsilon_{\mathrm{d}} + (1-p)\varepsilon_{\mathrm{m}}}$$

Where: p : filling ratio of metal, ε_{m} : permittivity of metal and ε_{d} : permittivity of dielectric.



- Silver's optical properties described based on the Drude model:

$$\varepsilon_{\mathrm{Ag}}(\varepsilon_{\mathrm{m}}) = \varepsilon_{\infty} - \frac{\omega_p^2}{\omega^2 + i\omega\gamma}$$

where, parameters: $\varepsilon_{\infty} = 5.0$

Plasma frequency $(\omega_p) = 1.38 \times 10^{16}\,\mathrm{rad/s}$, and Collision frequency $\gamma = 5.07 \times 10^{13}\,\mathrm{rad/s}$.

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Source: Shekhar, Prashant, Jonathan Atkinson, and Zubin Jacob. "Hyperbolic metamaterials: fundamentals and applications." Nano convergence 1 (2014): 1-17.
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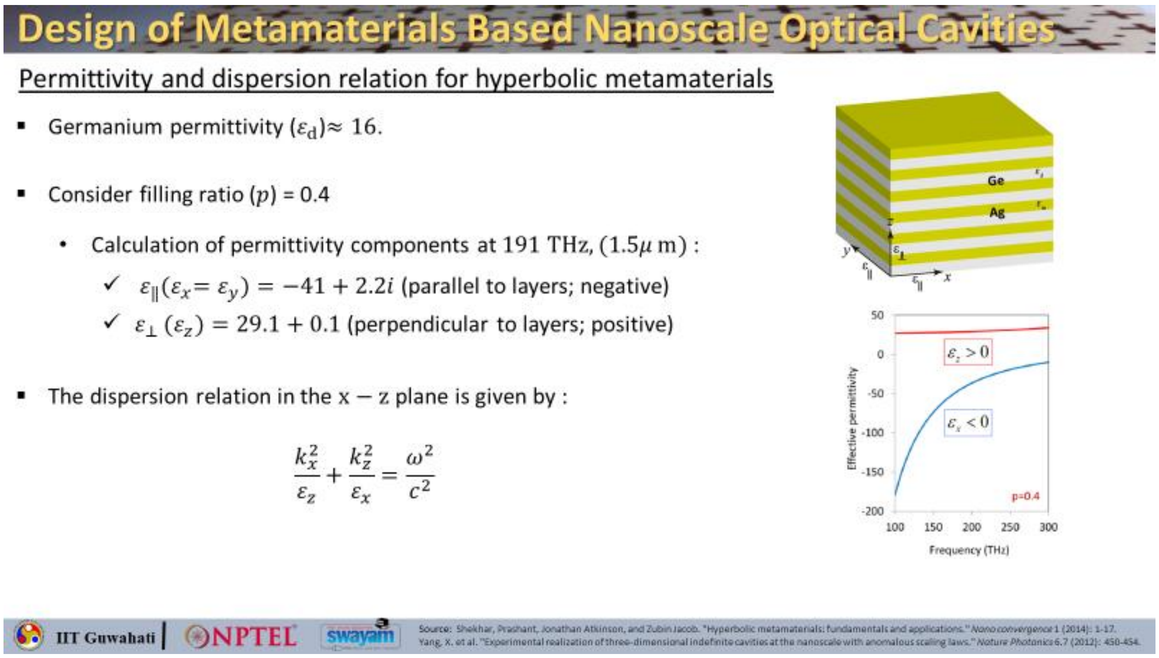
So, now let's look into the permittivity and dispersion relation for hyperbolic metamaterials with this particular example where silver and germanium layers are basically alternating.

So, we have learned that you can model this using the Maxwell-Garnett equation, okay. So, you can use this particular equation, epsilon parallel ($\varepsilon_{\|}$), that will be along the x and y axes. So, you can also write it as $\varepsilon_{\|}(\varepsilon_x = \varepsilon_y) = p\varepsilon_{\mathrm{m}} + (1-p)\varepsilon_{\mathrm{d}}$. What will be p? p is basically the filling fraction of metal right.

So, 1 minus p will be the filling fraction of the dielectrics ok. So, epsilon perpendicular can also be written as epsilon z (ε_z) because that is along the z direction. that is $\varepsilon_{\perp}(\varepsilon_z) = \frac{\varepsilon_m \varepsilon_d}{p\varepsilon_{\mathrm{d}} + (1-p)\varepsilon_{\mathrm{m}}}$. Now, if you take p equal to half, that is when you know the two-layer thicknesses are of the same size. The same thicknesses, then you can have a simplified version of this equation, right? So, this is a generic form and this is why it is important.

Because you will see that in this particular equation, you are also using a metallic permittivity epsilon m. So, because you are using silver, you can use the Drude model to describe the optical properties of silver. So, you can use this formula, epsilon Ag ($\varepsilon_{\mathrm{Ag}}$), which is your epsilon m here, that can be written as $\varepsilon_{\mathrm{Ag}}(\varepsilon_{\mathrm{m}}) = \varepsilon_{\infty} - \frac{\omega_p^2}{\omega^2 + i\omega\gamma}$. So, epsilon infinity is the background permittivity, which is 5 for silver. The plasma frequency is 1.38 times 10 to the power of 16 radians per second, and the collision frequency gamma.

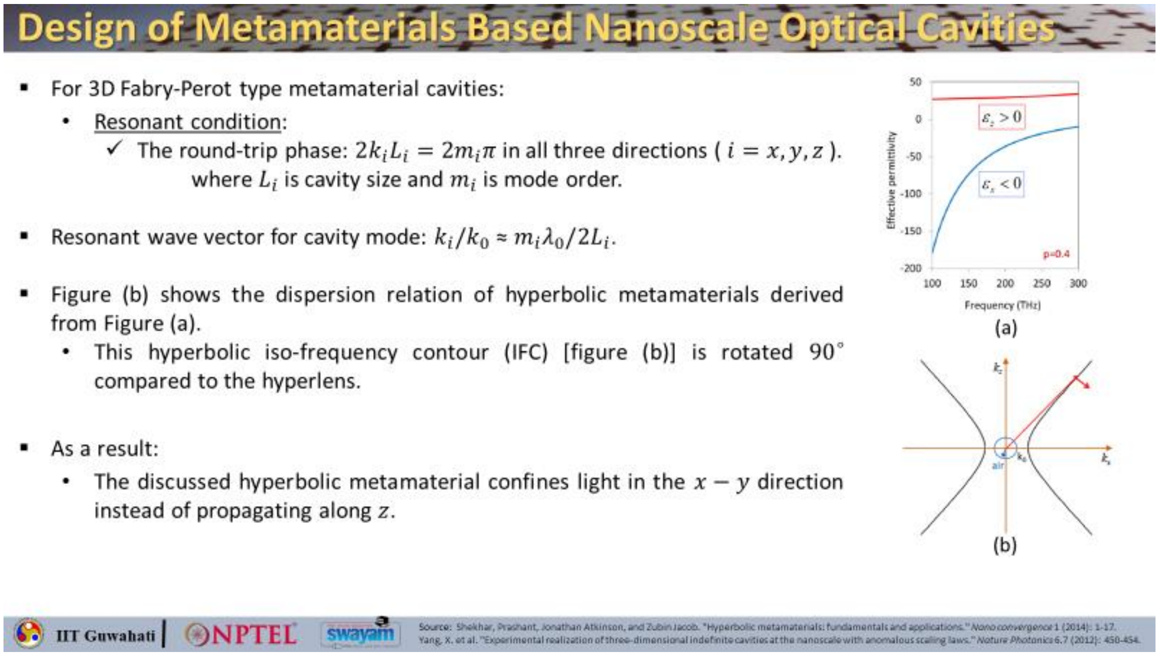
That is given as 5.07 times 10 to the power of 13 radians per second. So, with this, you can put it here, and you can calculate the values.



So, for that, you also need to know what the permittivity of germanium is; that is, your dielectric permittivity is taken as 16.

So, let us take an example where the filling fraction is 0.4; okay, that is, the metal filling fraction is 0.4. So, if you calculate the permittivity components at a given frequency, say 191 terahertz, which corresponds to 1.5 micrometer vacuum wavelength. You will see that epsilon parallel, which is epsilon x or epsilon y, comes out to be minus 41 plus 2.2 i. So, that is basically the permittivity along the layers, and it is coming out to be negative. And the perpendicular one is coming out to be 29.1 plus 0.1i. So, the i is missing, okay. So, that is basically positive permittivity, right? So, this ensures that. So, this is the plot that shows you the variation. So, we are considering only 191. So, that is somewhere here; okay, that value is shown here, okay.

So, this particular dispersion relation, which is plotted in the xz plane, can be written as: $\frac{k_x^2}{\varepsilon_z} + \frac{k_z^2}{\varepsilon_x} = \frac{\omega^2}{c^2}$.



Now, for the three-dimensional Fabry-Perot type metamaterial cavity, the resonant condition is that the round-trip phase, which is $2k_iL_i$, should be equal to an integral multiple of 2 pi; that is, you can write it as $2m_i\pi$. And that should happen in all three directions.

So here I will be x, y, and z. So, L_i is basically the cavity size, and m_i is representing the mode order. Now the resonant wave vector for the cavity mode can be written as $k_i/k_0 \approx m_i\lambda_0/2L_i$, right. So, here k_0 is nothing but 2 pi divided by λ_0 . So, you can actually use this to understand the resonant wave vector for the cavity mode. In this particular figure, it basically shows you the dispersion relation in k space for the hyperboloid.

or hyperbolic metamaterials that is shown here right which has got this kind of effective permittivities. So, what is noticeable here is that the hyperbolic isofrequency contour is basically rotated by 90 degree with respect to those we have seen for the hyperlens right. So, as a result, you can see that you know this is in kx and this is in kz. So, this is basically in the xz-plane. So, you can understand that this particular hyperbolic metamaterial can confine light in the xy direction instead of propagating along the z-direction.

Design of Metamaterials Based Nan[scale Optical Cavities [

Total internal reflection mechanism of Optical cavities:

- Figure 5.(a) illustrates the 3D hyperboloid IFC of hyperbolic metamaterials supports:
  - Large wave vectors in all directions (x, y, z).
  - k_z can be comparable to k_x or k_y.
- Cutting the indefinite medium into small cubes forms 3D Fabry-Perot cavities:
  - Total internal reflection (TIR) occurs at the air–metamaterial interfaces.
- The hyperbolic IFC:
  - Is open (not closed) → propagating modes in certain directions are forbidden.
  - Results in direction-dependent TIR conditions.

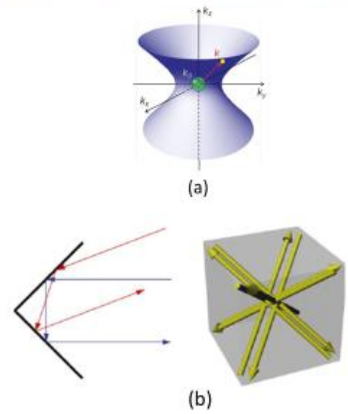


Figure 5.: Schematic of TIR mechanism to construct cavity

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Source: Shekhar, Prashant, Jonathan Atkinson, and Zubin Jacob. "Hyperbolic metamaterials: fundamentals and applications." *Nano convergence* 1 (2014): 1-17.
Yang, X. et al. "Experimental realization of three-dimensional indefinite cavities at the nanoscale with anomalous scaling laws." *Nature Photonics* 6.7 (2012): 450-454.

So, the figure (a) shows you the 3D hyperboloid isofrequency contour for this kind of hyperbolic metamaterial. So, this also tells you about the large wave vectors that are supported in all three directions. And you can see that, you know, the kz can be comparable to kx and ky, right? So, what is important here? Then you can basically cut the infinite medium into small cubes, and that will form a 3D fabric of pairs of cavities, right? So, how does it work? They work on the basis of total internal reflection that will occur at the air metamaterial interface. And you will see that the hyperbolic isofrequency contours here are the open ones. So, they are not closed; okay, that means the propagation is forbidden in some direction, okay.

So, that also results in varying the total internal diffraction condition based on the direction of propagation. Basically, it tells you about the schematic of the TIR mechanism, which is useful for constructing the cavity. So, this is what is happening at the different corners. So, this metamaterial and the air interface will support total internal reflection mainly based on the huge difference between the supported wave vectors. So, this also results in direction-dependent total internal reflection conditions.

Design of Metamaterials Based Nanoscale Optical Cavities

Total internal reflection mechanism of Optical cavities:

- Figure schematically illustrates how TIR occurs in metamaterial based optical cavities.
- TIR behavior:
  - Top/bottom facets (parallel to multilayer):
    - ✓ No air mode matches the in-plane momentum (k_p) of the metamaterial.
    - ✓ Total reflection for all allowed incident angles.
  - Side walls:
    - ✓ TIR critical angle $\theta_c = \arctan\left(\sqrt{\frac{\varepsilon_p}{\varepsilon_v(\varepsilon_p - 1)}}\right)$
    - ✓ From condition $k_v > k_0$ based on dispersion relation.

    Where ε_p and ε_v values are estimated using the effective medium approximation.

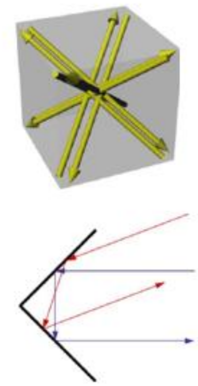

Figure: Schematic of TIR mechanism to construct cavity

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So, we will establish that dependency here. For the top and bottom facets, which are basically parallel to the multilayer, you will see that No mode in air matches the parallel momentum (k_p) in this indefinite medium. So, these facets will basically reflect light from all allowed incident angles. So, there is no issue with the top and the bottom one, right? Now, for the sidewalls, the total internal reflection that there is a critical angle involved that is θc, you can calculate this as $\theta c = \arctan\left(\sqrt{\frac{\varepsilon p}{\varepsilon_v(\varepsilon_p - 1)}}\right)$. So, here it indicates that this is coming from the condition that your kv is greater than k0.

So, what is kv? It is basically the vertical wave vector; you can also call it kz, okay? But here we are just telling you about kv; v stands for vertical in this case, okay? So, in this equation, what you see, epsilon p, is basically the effective permittivity that is parallel to the multilayer. So, it is epsilon x or epsilon y. Epsilon v is basically the vertical permittivity, or you can say the effective permittivity. That is perpendicular or vertical to the. So, these values can be estimated using effective medium approximation.

And after that, you can calculate what the total internal reflection's critical angle is. So, any angle that is above the critical angle will result in total internal reflection, and that is applicable to the side walls of the cavities. So, with that we understood the mechanism behind the hyperbolic metamaterials that can be used for making sub-deep wavelength nanoscale cavities.

Active Hyperbolic Metamaterials

- Conventional HMMs:
  - Made of alternating metallic and dielectric multilayers.
  - Provide a fixed hyperbolic dispersion over a broad spectral band (UV to infrared).
  - Dispersion properties are predetermined during fabrication by material choice and filling fraction.
- Limitation:
  - The hyperbolic dispersion is fixed and cannot be tuned after fabrication.
- Need for tunability:
  - Future reconfigurable photonic devices require hyperbolic dispersion that can be actively tuned across a wide spectral range.
- Solution:
  - Incorporate functional materials into HMMs to enable tunable hyperbolic dispersion without altering components or filling fraction.

 Source: Choudhury, Pankaj K., ed. "*Metamaterials: technology and applications*" CRC Press, 2021

Now, we will move on to discussing active hyperbolic metamaterials. Now, until now, we have seen conventional hyperbolic metamaterials that are made of alternating metal-dielectric multilayers.

We have seen that they could provide fixed hyperbolic dispersion over a broad spectral range, typically from UV to infrared. And these dispersion properties are predetermined during the fabrication by the choice of the material. And also, the choice of thickness, which is the filling fraction. So, what are the limitations? So, this hyperbolic dispersion remains fixed, and you cannot alter it after the fabrication is complete. So, normally in any kind of dynamic application, there is a need for tunability, right? So, if you think of future reconfigurable photonic devices that will require tunable hyperbolic dispersion, which can be actively tuned across a wide spectral range.

So, you can think more about conventional hyperbolic metamaterials where you can incorporate some functional materials into those hyperbolic metamaterials that will enable you to tune hyperbolic dispersion without altering the composition or the physical structure.

Applications of Active Hyperbolic Metamaterials

- Tunable optical properties of HMMs enable a range of potential applications.

- Active HMMs can be used in different spectral bands for:
  - Reconfigurable sensing
  - Supercollimation of THz light
  - THz modulators

1. Reconfigurable sensing:
   - Reconfigurable biosensing is demonstrated using an active Sb_2S_3–TiN HMM.
   - The technique uses the Goos–Hänchen (G-H) shift, which measures lateral displacement of a reflected beam near the coupling angle at the interface of two media.
   - The bulk plasmon-polariton (BPP) mode in the HMM is excited using the prism coupling principle.

Tunable optical properties of hyperbolic metamaterials enable a range of potential applications that we will briefly see in this lecture. So, active hyperbolic metamaterials can be used in different spectral bands.

They can be used for reconfigurable sensing. They can be used for super collimation of terahertz light, which is useful for terahertz modulators. So, we will take up some of these examples. The first one is reconfigurable sensing. So, reconfigurable sensing is demonstrated using an active hyperbolic metamaterial for highly sensitive biosensing of small molecules via ghost hand chain shift. Okay, that is basically using active; this is called antimony trisulphide hyperbolic metamaterial.

So, the technique here uses the Goos-Hanchen shift. In short, you can call it the G-H shift, which basically measures the lateral displacement of the reflected beam. Near the coupling angle at the interface of two media, right? We will show you an example in the following slides. So, the bulk plasmon-polariton, which is called the BPP mode in the hyperbolic metamaterial, gets excited using the prism coupling mechanism.

Applications of Active Hyperbolic Metamaterials

1. Reconfigurable sensing:
   - Experimental setup:
     - A p-polarized 632.8 nm light (in the hyperbolic region of the HMM) is used.
     - Prism coupling excites the bulk plasmon polariton (BPP) mode in the HMM.
     - The BK7 prism (n = 1.5) ensures momentum matching since HMM has a lower effective index. (figure 6)
   - Key observations (when switching Sb_2S_3 from amorphous to crystalline):
     - The effective index of the HMM decreases.
     - Resulting changes:
       - ✓ Minimum reflected intensity at resonance angle decreases.
       - ✓ Narrower reflection spectrum linewidth.
       - ✓ Slight shift in coupling angle.

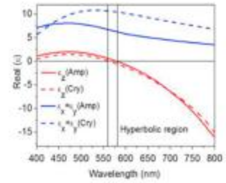

Figure 6.: Real parts of uniaxial permittivity components of Sb2S3-TiN HMM when Sb_2S_3 is in the amorphous and crystalline phases

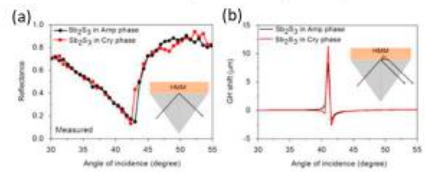

Figure 7.: (a) Excited BPP mode of Sb2S3-TiN HMM for both phases of Sb2S3, (b) Calculated tunable G-H shift of HMM

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So, we will discuss how the experimental setup looks.

So, you can use p-polarized light, which is a TM-polarized wavelength, with a typical wavelength of say 632.8 nanometers. This is a red wavelength, and you can use it in the hyperbolic region of the hyperbolic metamaterial. And then you use prism coupling, which can excite the bulk plasmon polariton mode within this hyperbolic metamaterial. So, this bulk plasmon polariton basically refers to a type of metamaterial structure.

This kind of BPP-HMM basically tells you about a type of metamaterial structure that can. exhibit both hyperbolic dispersion and support the propagation of these bulk plasmon polariton modes. So, the prism that you are using for coupling can be made of BK7 glass. okay which has got a refractive index of 1.5 that is used to ensure a momentum matching, because your HMM has a lower refractive index, as you can see here.

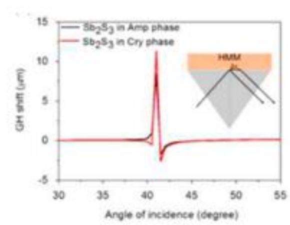
So, this particular plot shows you the real part of the uniaxial permittivity of the different components that are used. In this metamaterial, which is made of antimony trisulphide and titanium nitride. So, the different colors basically show you that the red ones tell you about, you know, the antimony tri-sulphide in amorphous and the other one shows when they are in the crystalline phase. So, this is basically epsilon z, the vertical permittivity, and this shows you the epsilon x or y, which is basically the parallel permittivity. Now, what you see here is the wavelength range, and beyond this particular wavelength, it is becoming negative; that means you can consider this region as your hyperbolic region where kind of permittivity constant is one permittivity is negative the other permittivity is positive.

So, this is the typical hyperbolic region in which you will be interested, right? Now, if you use this and this particular setup shows you the experimental setup that is got this prism which is made of BK7 glass. So, once you do that, okay? So, it tells you that you keep varying the incident angle and you keep measuring the reflectance angle. Or reflectance from this side only at this particular angle, you will see that the reflection dips, okay. And what are these two graphs? These are again the antimony tri-sulphides considered to be in either the amorphous phase or the crystalline phase.

They morally very closely give you a similar kind of dip. So, that dip actually indicates excitation of the BPP mode, okay. So, that energy is basically coupled to the plus-one polaritons. So, this minimum reflected intensity decreases at the resonance angle, which you can also see from here.

Applications of Active Hyperbolic Metamaterials

- Tunable Goos–Hänchen (G-H) Shift in Sb_2S_3–TiN HMM:
    - Enhanced G-H shift occurs at the BPP mode excitation angle, determined by the phase derivative at the coupling angle.
    - Figure shows maximum G-H shift where phase difference changes sharply.
    - Tunability of the G-H shift is enabled by switching Sb_2S_3 between amorphous and crystalline phases.
- The G-H shift scheme enables high refractive index sensitivity and can detect small biomolecules at extremely low concentrations.
- Improvement potential:
    - Use longer wavelengths and higher-index prisms to enhance tunable range.
- The HMM-based plasmonic platform is envisioned to detect small molecules (e.g., exosomes) from bodily fluids.



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So, here you can actually see that the G-H shift also occurs maximally at this particular angle of around 41 or 42 degrees. So, it also results in a narrower reflection spectrum linewidth.

So, the excited mode is confined to the fundamental BPP mode, which is a low k mode of This antimony trisulphide and titanium nitride hyperbolic metamaterial is okay. The phase singularity at the coupling angle which you can see here ok can be actively tunable by non-violet volatile phase change of this antimony trisulphide. That means when the antimony trisulphide can change between the amorphous and crystalline phases, that is when You can change this wavelength, and that will actually give you the shift in the properties, right? So, the phase singularity at the coupling angle can be actively tuned, okay, by this antimony trisulphide. As the TE and TM polarized light phase difference shows a sharp singularity at this particular angle, okay. So, this is how you are seeing this tunable, you know, Guzhanchen shift in this kind of metamaterial, right? So here again, the two graphs tell you about the shift in this wavelength because of the change in the phase of.

Antimony trisulfide. So, the red one is the crystalline phase; the other one is the amorphous phase, right? So, we can observe that this enhanced G-H shift, or Goos-Hansen shift, occurs at the BPP mode. The excitation angle is determined by the phase derivative at the correct coupling angle. So, this figure shows you the maximum shift that happens when the phase changes sharply, isn't it? So, the tunability of this G-H phase is enabled by the switching of this antimony tri-sulphide between the amorphous and the crystalline phase. So, this is how you can do active tuning. So, this GH shift scheme also enables high refractive index sensitivity and it can detect small biomolecules at extremely low concentrations.

So, what is the improvement potential? You can think of using longer wavelengths and a higher index prism. Okay, here to enable the tunable range of the shift. So, you can also think of a hyperbolic metamaterial-based plasmonic platform that can be used for detection of. Small molecules like exosomes are obtained from bodily fluids using this kind of mechanism. So, this tells you that you can also use active hyperbolic metamaterials for dynamically tunable systems.

So, with that, we conclude this lecture. So, if you have any queries regarding this lecture, you can drop an email to this email address. Mention the course name and the lecture number in the subject line. Thank you.