Graphene epsilon-near-zero plasmonic crystals

Marios Mattheakis

ACM NanoCom. 2019
Dublin, Ireland
Metamaterials

3D optical holography. Nat. Comm. 4 2013


Hyperbolic antennas shape radiation pattern. JAP 116 2014

Efficient waveguides. J. Optics 14 2012
Epsilon-Near-Zero (ENZ)

Tunneling through narrow channels. PRL 97 2006

Bending and Cloaking. Nat. Matt. 10 2011

Tailoring the radiation phase pattern. PRB 75 2007

On-chip zero-index. Nat. Phot. 9 2015
Plasmons in two-dimensional materials

**Graphene, a semi-metal:**
Becomes metal after doping
Large electrical conductivity
Tunable conductivity via doping
Reduced dimensions
Low optical losses

**Graphene plasmonics:**
Plasmons are charge oscillations
THz plasmons with tunable properties
Ultra-subwavelength plasmons


Outline

A systematic way to design ENZ plasmonic crystals based on two-dimensional metals.

ENZ appears as a Dirac (linear) dispersion in k-space

- Anisotropic dielectric host: ENZ condition
- Space-dependent host: Universality of ENZ and Dirac dispersion
- Frequency-dependent host: Extending the ENZ frequency window
- Effective permittivity for arbitrary plasmonic crystal of 2D metals
Plasmonic Crystal

Periodic arrangement of dielectric/metal slabs

2D metals are embedded periodically in an anisotropic dielectric host

The metals carry surface current \( J = \sigma \vec{E}_z \)

**Motivation:**
Can we design tunable metamaterials with desirable effective permittivity?
Maxwell Equations

Transverse Magnetic (TM) polarization

Transversal Field

\[-i \frac{\partial}{\partial z} \Psi = \mathcal{M} \cdot \Psi \quad \Leftrightarrow \quad -i \frac{\partial}{\partial z} \begin{pmatrix} E_x \\ H_y \end{pmatrix} = k_0 \eta_0 \begin{pmatrix} 0 & \frac{1}{k_0^2} \frac{\partial}{\partial x} \frac{1}{\varepsilon_z} \frac{\partial}{\partial x} \\ \frac{\varepsilon_z}{\eta_0} & 0 \end{pmatrix} \begin{pmatrix} E_x \\ H_y \end{pmatrix}.\]

Longitudinal Field

\[E_z = \frac{i \eta_0}{k_0 \varepsilon_z} \frac{\partial H_y}{\partial x}, \quad k_0 = \omega / c, \quad \eta_0 = \sqrt{\mu_0 / \varepsilon_0}.

Propagation along z direction (plasmons)

\[\Psi(x, z) = \Psi(x) e^{ik_z z}, \quad k_z \Psi = \mathcal{M} \Psi.\]
Dispersion Relation

Assume periodicity along x direction (Bloch waves)

\[ D(k_x, k_z) = \cos(k_x) - \left[ \cosh(\kappa d) - \frac{\xi d}{2} \sinh(\kappa d) \right] = 0 \]

\[ \kappa^2 = \frac{\varepsilon_z}{\varepsilon_x} \left( k_z^2 - k_0^2 \varepsilon_x \right) \]

Plasmonic Thickness
(twice the decay length)

\[ \xi = \frac{i\sigma}{\omega \varepsilon_z} \]

Wang et. al. PRL 112 2012
Effective dielectric function

dense grid: $d \ll \lambda$

$$\frac{k_z^2}{\varepsilon_x} + \frac{d}{(d - \xi)\varepsilon_z} k_x^2 = k_0^2$$

**effective medium**

$$\frac{k_z^2}{\varepsilon_x^{\text{eff}}} + \frac{k_x^2}{\varepsilon_z^{\text{eff}}} = k_0^2$$

$$\varepsilon_z^{\text{eff}} = \frac{d - \xi}{d} \varepsilon_z$$

$$\varepsilon_x^{\text{eff}} = \varepsilon_x$$

ENZ condition

$$d = \xi \implies \varepsilon_z^{\text{eff}} = 0$$

✓ Dirac dispersion yields ENZ behavior

✓ Systematic method for designing ENZ metamaterials

MM et. al. PRB 94 2016
ENZ behavior (simulation)

- 40 graphene layers embedded in MoS$_2$ host ($\varepsilon_x=3.5$, $\varepsilon_z=13$, $d=20.8$ nm).
- Drude model for graphene conductivity.
- $\lambda_0=12$ μm (THz regime).
- 2D magnetic dipole source.

\[ \sigma(\omega) = \frac{ie^2\mu_e}{\pi\hbar^2(\omega + i/\tau)} \]

Ultra fast phase transitions
No dispersion
No phase delay

MM et. al. PRB 94 2016
ENZ behavior (simulation)

- 40 graphene layers embedded in MoS$_2$ host ($\epsilon_x=3.5$, $\epsilon_z=13$, $d=20.8$ nm).
- Drude model for graphene conductivity.
- $\lambda_0=12$ $\mu$m (THz regime).
- 2D magnetic dipole source.

$$\sigma(\omega) = \frac{ie^2\mu_c}{\pi\hbar^2(\omega + i/\tau)}$$

Ultra fast phase transitions
No dispersion
No phase delay

$\text{MM et. al. PRB 94 2016}$
Numerical EM wave simulations

- 40 graphene layers embedded in MoS$_2$ host ($\varepsilon_x=3.5$, $\varepsilon_z=13$, $d=20.8$ nm).
- Drude model for graphene conductivity.
- $\lambda_0=12$ μm (THz regime).
- 2D magnetic dipole source.
A systematic way to design ENZ plasmonic crystals based on two-dimensional metals.

ENZ appears as a Dirac (linear) dispersion in k-space

- Anisotropic dielectric host: ENZ condition
- Space-dependent host: Universality of ENZ and Dirac dispersion
- Frequency-dependent host: Extending the ENZ frequency window
- Rigorous formulation for arbitrary plasmonic crystals with 2D metals
Universal behavior of a Dirac dispersion

Dirac dispersion and ENZ is a universal property of plasmonic crystals consisting of 2d metals in host with space-dependent permittivity.

Universal condition for ENZ

\[ d_0 = \xi_0 \left[ \int_0^1 f(x)dx \right]^{-1}, \quad \frac{\varepsilon_{\text{eff}}}{\varepsilon_{z,0}} = \xi_0 \left( \frac{1}{d_0} - \frac{1}{d} \right) \]

\[ \varepsilon_z(x) = \varepsilon_{z,0} f(x/d), \quad f(x) > 0 \]

\[ \xi_0 = -\frac{i\sigma}{\omega \varepsilon_{z,0}} \]

Introduce an extra degree of freedom for tuning the dielectric properties.

Maier, MM et al., PRB 97, 2018
Universal behavior of a dispersive Dirac cone

Parabolic profile

\[ \varepsilon_z(x) = \varepsilon_{z,0} \left[ 1 + 6\alpha \frac{x}{d} \left( 1 - \frac{x}{d} \right) \right], \]

Maier, MM et al., PRB 97, 2018
Universal behavior of a dispersive Dirac cone

Double well profile

\[ f_{dw}(x) = 1 - 3.2x + 13.2x^2 - 20x^3 + 10x^4 \]
Outline

A systematic way to design ENZ plasmonic crystals based on two-dimensional metals.

ENZ appears as a Dirac (linear) dispersion in k-space

- Anisotropic dielectric host: ENZ condition
- Space-dependent host: Universality of ENZ and Dirac dispersion
- **Frequency-dependent host: Extending the ENZ frequency window**
- Rigorous formulation for arbitrary plasmonic crystals with 2D metals
Expanding the ENZ frequency window

Very narrow frequency window with ENZ properties

\[ \varepsilon = 2 \]
Lorentz dispersive host

Add a new Dirac point expanding ENZ frequency range

\[ \varepsilon(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{\omega_0^2 - \omega^2 + i\omega\Gamma} \]

\[
\begin{align*}
\varepsilon_\infty &= 11.2 \\
\varepsilon_s &= 2.6 \\
\Gamma &= 0 \\
\omega_0 &= 1\text{eV} \quad (f = 242.8\text{THz})
\end{align*}
\]
Multi-Oscillator Lorentz dispersive host

Add more Dirac points and expanding more the ENZ window

\[ \varepsilon(\omega) = \varepsilon_\infty + \sum_{i}^{N} \frac{g_i \omega_{0i}^2}{\omega_{0i}^2 - \omega^2 + i\omega \Gamma_i}, \]

MM et. al. ACM NanoCom 2019
A systematic way to design ENZ plasmonic crystals based on two-dimensional metals.

ENZ appears as a Dirac (linear) dispersion in k-space

- Anisotropic dielectric host: ENZ condition
- Space-dependent host: Universality of ENZ and Dirac dispersion
- Frequency-dependent host: Extending the ENZ frequency window
- Rigorous formulation for arbitrary plasmonic crystals with 2D metals
General formula for the effective medium

A rigorous formulation for the effective dielectric function

Arbitrary shape of a 2D material as the building element
Periodic structure in one, two, or three dimensions
Finite and edge state effects (surface + line currents)
Finite number of structural periods
Spatial & frequency-dependent host permittivity

Choose your 2D element: planar, ribbon, tube

Maier, MM, et al. RSPA 2019
Conclusion

- A systematic way to design crystals with ENZ behavior
  - Tuning dynamically the optical properties
  - Dirac dispersion indicates ENZ behavior
- Universality of Dirac dispersion and ENZ for 2D plasmonic crystals with spatial-dependent host
- Expand the ENZ frequency window with Lorentz dispersive host
- A rigorous formulation for a general case of plasmonic crystal structure: A general ENZ condition

mariosmat@g.harvard.edu
https://scholar.harvard.edu/marios_matthaiakis
A promising direction in engineering

Machine Learning for designing new metamaterials

Scheme:
- Set target properties
- Define a periodic structure
- Choose the building elements
- Let ML to design the optimal configuration

Kitai et al. ArxiV 1902.06573

Flatland multilayer heterostructures

Geim et al. Nature 499 2019
Acknowledgments

EFRI 2-DARE NSF
Grant No. 1542807

ARO MURI
Award No. W911NF-14-0247

ACM NanoCom Proceedings:
Graphene epsilon-near-zero plasmonic crystals

Co-authors:
  Matthias Maier
  Wei Xi Boo
  Efthimios Kaxiras

mariosmat@g.harvard.edu
https://scholar.harvard.edu/marios_matthaiakis
Supplementary Material
General Investigation (maps)

- Combinations of $\mu_c$ and $\lambda$ leading to PDP & ENZ ($\xi$ is plotted in nm).
- A structure with arbitrary $d$ can be fabricated and then with suitable choice of $\mu_c$ and $\lambda$ we achieve ENZ behavior.

\[ \frac{L}{d} = \sqrt{\frac{2}{\varepsilon_z}} \sqrt{\frac{\text{Im}[\sigma_s]}{\text{Re}[\sigma_s]}} \frac{1}{k_0 d} \]

The propagation distance \(L/d\) of a plasmonic mode for all $\lambda$, $d$ and $\mu_c$ combinations leading to ENZ.

Effective permittivity for $\lambda$ & $\mu_c$ combinations and fixed period $d=20\text{nm}$.

- Dashed lines indicate the ENZ regime.
- Low losses in the ENZ region.
- Very negative $\varepsilon$ achieved but accompanied with high losses.
Assuming that Graphene carries surface current \( J = \sigma E_z \).

Periodicity: The eigenmodes are Bloch waves and arranged in bands.

\[
H_y^+(x) = H_y^-(x - d)e^{ik_x d}
\]

\[
F(k_x, k_z) = \cos(k_x d) - \left[ \cosh(\kappa d) - \frac{\xi \kappa}{2} \sinh(\kappa d) \right] = 0
\]

- Assume very dense grid: \( \kappa d \ll 1 \)
- Around Brillouin center: \( k_x \sim 0 \)

- \( d > \xi \): Weak Plasmon Coupling \( \rightarrow \) Elliptic Band
- \( d = \xi \): Critical Plasmon Coupling \( \rightarrow \) Two Linear Bands
- \( d < \xi \): Strong Plasmon Coupling \( \rightarrow \) Hyperbolic Band
Effective dielectric function

Real part

Imaginary part

\( \lambda (\mu m) \)

\( \mu_c \) (eV)

\( \lambda (\mu m) \)

\( \mu_c \) (eV)
Tunable EM properties

ENZ condition

Effective permittivity

(a)

(c)
Universal behavior of a dispersive Dirac cone

Dirac dispersion and ENZ is a universal property of plasmonic crystals consisting of 2d metals in host with space-dependent permittivity

General dispersion relation:

\[
D[k] = \det \begin{bmatrix}
    \mathcal{E}_1(\mathbf{d}) & \mathcal{E}_2(\mathbf{d}) \\
    \mathcal{E}'_1(\mathbf{d}) & \mathcal{E}'_2(\mathbf{d})
\end{bmatrix} \\
- e^{ik_xd} \begin{bmatrix}
    1 \\
    -i(\sigma/\omega)\kappa(k_z) \\
    0 \\
    \mathbf{1}
\end{bmatrix} = 0.
\]

Universal condition for ENZ

\[
d_0 = \xi_0 \left[ \int_0^1 f(x)dx \right]^{-1}, \quad \frac{\varepsilon_{\mathbf{z}}^{\text{eff}}}{\varepsilon_{\mathbf{z},0}} = \xi_0 \left( \frac{1}{d_0} - \frac{1}{d} \right).
\]
Multilayer Metamaterial


Negative refraction. APL 2013
Numerical EM wave simulations (vids)

- 40 graphene layers embedded in MoS$_2$ host ($\varepsilon_x=3.5$, $\varepsilon_z=13$, $d=20.8$ nm).
- Drude model for graphene conductivity.
- $\lambda_0=12$ μm (THz regime).
- 2D magnetic dipole source.

Weak plasmon coupling

Strong plasmon coupling

M. Mattheakis et. al. PRB 94 (2016)
Numerical EM wave simulations (vids)

- 40 graphene layers embedded in MoS$_2$ host ($\varepsilon_x=3.5$, $\varepsilon_z=13$, $d=20.8$ nm).
- Drude model for graphene conductivity.
- $\lambda_0=12$ μm (THz regime).
- 2D magnetic dipole source.

M. Mattheakis et. al. PRB 94 (2016)
Numerical EM wave simulations (vids)

- 40 graphene layers embedded in MoS$_2$ host ($\varepsilon_x=3.5$, $\varepsilon_z=13$, $d=20.8$ nm).
- Drude model for graphene conductivity.
- $\lambda_0=12$ μm (THz regime).
- 2D magnetic dipole source.

COMSOL simulations

M. Mattheakis et. al. PRB 94 (2016)
ENZ properties

Wave propagation with no dispersion and with no phase delay
Propagation through narrow channels
Bending over arbitrary angles
Ultra fast phase transitions
Hiding objects (cloaking)