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ABSTRACT

One notable issue in low terahertz (THz) applications is to achieve sources with higher output power than the state of the art. One possible solution to the foregoing problem is to amplify the electromagnetic field emitted by already accessible THz generators. Here, we study the quantum Čerenkov effect as a possible explanation for low-THz amplification, which has been found experimentally elsewhere. Specifically, the emission of surface plasmons from traveling electrons in mono-dimensional graphene, mediated by charge–field interaction, is shown to provide in-plane electromagnetic radiation down to THz and mm-wave frequencies. We focus on a structure consisting of a graphene layer between metal electrodes, which enhance the field confinement and lead to a linearization of the plasmon dispersion in the frequency domain. When compared to a non-confined plasmonic radiation, the above-mentioned configuration shows emission rates ten times larger, which make it promising for THz amplification.

The terahertz (THz) band lies in a "gap" between high-millimeter and infrared optical frequencies. In this range, amplification can be achieved at either signal or optical level by standard approaches, such as traveling-wave,[1,2] Fabry–Pérot resonant amplification,[3,4] terahertz monolithic integrated circuits,[5] high electron mobility transistors,[6,7] and THz radiation by fast carrier dynamics in semiconductors after photoexcitation.[8,9] However, the aforementioned technologies have shown strong limitations in providing sufficient gain at THz frequencies, in terms of costs, losses, bandwidth, and scalability. In order to bypass these limitations, alternative solutions have been proposed for an amplification mediated by surface plasmons, which can be relatively broadband and spatially confined near a 2D surface.[10] Recent studies achieved, indeed, plasmon amplification through electron pumping[11] and proposed the possibility to obtain amplifiers with metal–graphene structures.[12] Therefore, graphene has been assumed as a reference material for two main factors: (i) its extremely high theoretical carrier mobility and velocity,[13] two essential elements for high-frequency charge–light interaction; and (ii) its electromagnetic (EM) response, which has been already extensively studied, can be described by widely used models.[14] In addition, screening effects, charge density, and, consequently, plasmon dispersion can be easily tuned by applying an external electrostatic bias. Moreover, it was recently demonstrated that, in graphene, the dynamic conductivity can be negative in certain ranges of plasmon frequencies, providing a positive and large amplification coefficient.[1,15] Semiclassical models, such as the hydrodynamic approach (based on the assumption of 2D relativistic electron liquid), seem to be suitable for non-ballistic regimes and long propagation lengths (few to tens of micrometers), where charges have a drift velocity in the range of 10^5 m/s.

However, the THz amplification mechanism is not yet completely understood. Indeed, different agents are possibly involved and still need to be investigated, such as the role played by interband/intraband transitions and by the group and phase velocities of the EM fields. Charge ballisticity at a sub-micron scale is also to be investigated, with proper comparison to the non-ballistic case, since THz amplification can be mediated by electron–phonon scattering and charge transfer between different sideband energy minima or valleys.[16,17] All these considerations can be extended to 2D materials based on transition metal dichalcogenides (TMDs) and monochalcogenides (TMMs). These share several features with graphene, such as a reduced insertion loss and strong coupling effects under external excitation,[18] large-scale high-quality film growth (mm to cm-scale), and the possibility to be transferred into different substrates.[19]

In the present work, we explore the quantum Čerenkov emission to explain charge coupling with THz plasmons in graphene mono-layer. This theoretical interpretation of EM amplification, is mostly suitable for coherent transport at ballistic or sub-micrometric scale, where the velocity of the propagating charges is assumed to be the Fermi velocity ($v_F = 10^6$ m/s). To observe low-THz emission, we propose a device where graphene is embedded in a metal-confined structure. This choice extends the frequency range for Cerenkov radiation in comparison to previous publications,[20,21] which investigate plasmon emission only at infrared wavelengths. Our main achievements are given by (i) a rigorous description of the Čerenkov effect (ČE), based on the Fermi golden rule,[22] for the case under study, which is easily extendable to arbitrary multilayer structures, and (ii) the analysis of the main characteristics of coherent light emission in the low-THz range of frequencies.

The spatial confinement by metallic plates is proved to be an effective method to modify the dispersion and achieve high degrees of field confinement for a graphene plasmon (GP).[23] Let us consider a structure, as depicted in Fig. 1, composed of a single layer of graphene between a parallel plate metal lines filled with dielectric. Assuming $\varepsilon_{A,B}$ and $d_{A,B}$ to be the permittivity and thicknesses of the dielectrics above and below the graphene layer, respectively, it is possible to define C_s as in (1) which represents the effective capacitance of the structure per unit area

$$C_s = \frac{1}{2}\left(\frac{\varepsilon_A}{d_A} + \frac{\varepsilon_B}{d_B}\right). \quad (1)$$

In the assumption of small signals, no losses and small thicknesses compared to plasmon wavelength, by analyzing the transverse resonance (see supplementary material Note 1), it is possible to obtain the dispersion relation $q(\omega)$ given by the following equation:

$$q^2(\omega) = \frac{\pi\hbar^2}{e^2|E_F|}\left(\frac{\varepsilon_A}{d_A} + \frac{\varepsilon_B}{d_B}\right)\omega^2 = \frac{2\pi\hbar^2 C_s}{e^2|E_F|}\omega^2, \quad (2)$$

where e is the unit charge, $\hbar$ is the reduced Planck constant, and E_F is the Fermi level of the graphene. The phase velocity, defined in (3), is constant and, therefore, the high-confined plasmon is non-dispersive.

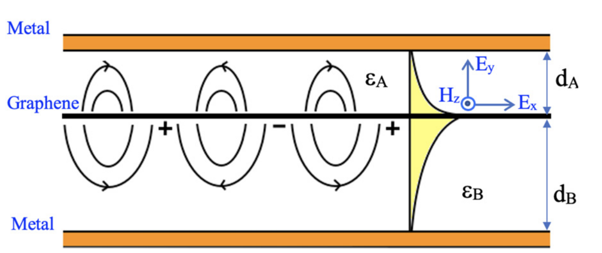

FIG. 1. Structure under study composed of a graphene layer between two metal plates at distances d_A and d_B. The structure is filled with dielectrics of permittivity ε_A and ε_B, respectively.

$$v_p = \frac{\omega}{q} = \frac{e}{\hbar}\sqrt{\frac{|E_F|}{2\pi C_s}}. \quad (3)$$

Assuming a Drude-like conductivity as in Refs. 24 and 25, it is possible to introduce the losses in (2) assuming a finite relaxation time of the carriers (τ), mainly due to phonon scattering. Therefore, calculating the propagation length of the GP, as the ratio between the real and the imaginary part of q, gives $\gamma = \Re q/\Im q \simeq 2\omega\tau$ (see supplementary material Note 1). The analytical calculations have been compared to numeric simulations, as shown in Fig. 2, and provide a good approximation for the range of frequencies which are involved in this work. Consider now a charge traveling in a graphene layer with energy E_i, the spontaneous emission of plasmon photons with frequency ω and momentum q can be calculated from the Fermi's golden rule, as already established in the literature.[20–22] In the limit of low losses, the GP emitted from a charged carrier is given by the following equation:

$$\Gamma = \frac{2\pi}{\hbar}\int_{-\infty}^{\infty} |M_{\mathbf{k}_i \to \mathbf{k}_f + \mathbf{q}}|^2 \delta(E_i - \hbar\omega - E_f)\frac{d^2\mathbf{q}}{(2\pi)^2/S}\frac{d^2\mathbf{k_f}}{(2\pi)^2/S}, \quad (4)$$

where $M_{\mathbf{k}_i \to \mathbf{k}_f + \mathbf{q}}$ is the matrix element (see supplementary material Note 3) of the transitions from an initial state k_i to a final state k_f and S is the surface of the sample. The matrix element is calculated assuming $d_A = d_B = d$ and adapting the energy normalization of the GP to the structure under study (see supplementary material Note 2). The emission rate for a frequency between ω and $\omega + d\omega$ in an angle between θ and $\theta + d\theta$ can be obtained by the following equation (see supplementary material Note 4):

$$\Gamma_{\omega,\theta} = \frac{4\alpha c}{\pi^2 \bar{\varepsilon}_r v_p}\left|\frac{E_i}{\hbar\omega} - 1\right|\left(1 - e^{-2qd}\right)^{-1}\int_0^{2\pi} |\zeta|^2 \cdot \frac{|\cos\theta/\gamma|}{\left(\frac{v_p}{v_F}\frac{E_i}{\hbar\omega} - \frac{v_p}{v_F}\left|\frac{E_i}{\hbar\omega} - 1\right|\cos\phi - \cos\theta\right)^2 + |\cos\theta/\gamma|^2} \cdot \frac{|\sin\theta/\gamma|}{\left(\frac{v_p}{v_F}\left|\frac{E_i}{\hbar\omega} - 1\right|\sin\phi + \sin\theta\right)^2 + |\sin\theta/\gamma|^2} d\phi, \quad (5)$$

where α is the fine-structure constant, c is the speed of light, ε_r is the average permittivity of the dielectrics, v_F is the Fermi velocity in graphene, and ζ is the coefficient of the interaction between charges and photons obtained by (S17) for intraband and interband transitions,

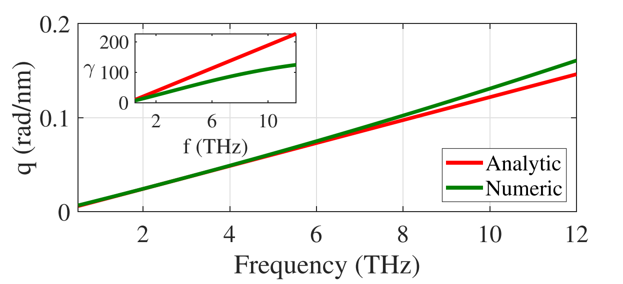

FIG. 2. Comparison of the graphene plasmon wavenumber calculated by introducing the losses in (2) (line) and by the numeric solver (green). (Inset) propagation length factor γ for both analytic and numeric computations.

respectively. In the case of no losses, all the plasmonic radiation is emitted at two specific angles $\pm\theta_C$, defined by the following equation (see supplementary material Note 5):

$$\cos\theta_C = \frac{v_p}{v_F}\left[1 - \frac{\hbar\omega}{2E_i}\left(1 - \frac{v_F^2}{v_p^2}\right)\right]. \quad (6)$$

These angles are the quantum Čerenkov angles and are composed of the sum of two term: (i) the ratio between the phase velocity of the wave and the charge velocity ($v = v_F$) and (ii) the quantum correction term due to the fact that carriers in graphene presents energies comparable with the ones of the emitted photons. If the charge energy is much larger than $\hbar\omega$, it is possible, indeed, to recover the classical formula. Since carriers in graphene move at high speed and the plasmon phase velocity is rather slow, the Čerenkov condition is achieved, and the GP emission is possible. The presence of confinement plates reduces, furthermore, both the groups and phase velocities, and it increases the total emission rate. However, the total rate is reduced by the introduction of losses. A finite scattering time allows emission even at angles different from (6) and it broadens the radiation around the Čerenkov angles.

In Figs. 3(a) and 3(b), we show the spreading of the emission rate at a Fermi level of 0.05 eV and an initial carrier energy of 0.10 eV for a relaxation time of 1.5 and 0.5 ps, respectively. As shown, for lower energy losses (higher τ value), most of the emission is localized in the direction of the Čerenkov angle. By reducing the scattering time, the rate values decrease, and the radiation is spread in a wider range of angles. In Fig. 3(d), we compared the emission at 1 THz for different loss factors. Assuming $\tau = 0.1$ ps, the peak emission at $\theta = \theta_C$ is more than one order of magnitude lower compared to $\tau = 1.5$ ps.

Analyzing the behavior of Γ with respect to the initial carrier energy, it is interesting to note that this is proportional to the radiation cut-off frequency. This effect is made clear from Fig. 3(d) that shows the emission rate assuming an identical situation to the one in Fig. 3(a), but with E_i ten times lower. Assuming different initial energy values, at a fixed frequency of 1 THz, as shown in Fig. 3(e), it is possible to notice that, by lowering the E_i, the radiation angle of the emitted EM field tends to zero since the quantum correction term in (6) becomes dominant and the module of the cosine becomes larger than 1. From (6), considering the aforementioned condition, we can obtain a formula for the cut-off frequency, (7), that clearly shows the dependency on the initial energy of the carrier and on the plasmon phase velocity

$$f_{cutoff} = \frac{2E_i}{h}\frac{v_p}{v_p + v_F}. \quad (7)$$

Assuming a fixed C_s, the phase velocity, from (3), is proportional to $\sqrt{E_F}$. Increasing the Fermi level on the graphene sheet has, therefore, the effect of increasing the cut-off frequency up to the limit $2E_i/h$, which purely depends on the carrier energy. Figures 4(a)–4(c) show Γ for a $E_i = 0.05$ eV and a Fermi level of 0.10, 0.02, and 0.002 eV, respectively, and the red line represents the cut-off frequency obtained from (7). As shown, the electrochemical potential is also involved in the emission rate. The maximum value, indeed, grows inversely with E_F, since an increase in the plasmon phase velocity reduces the photon momentum and, therefore, more carriers can contribute to the emission. In Fig. 4(d), we plotted the Čerenkov angle as a function of the Fermi level and the frequency of the emitted photon. For a certain frequency, by tuning the Fermi level, it is possible, indeed, to orient the

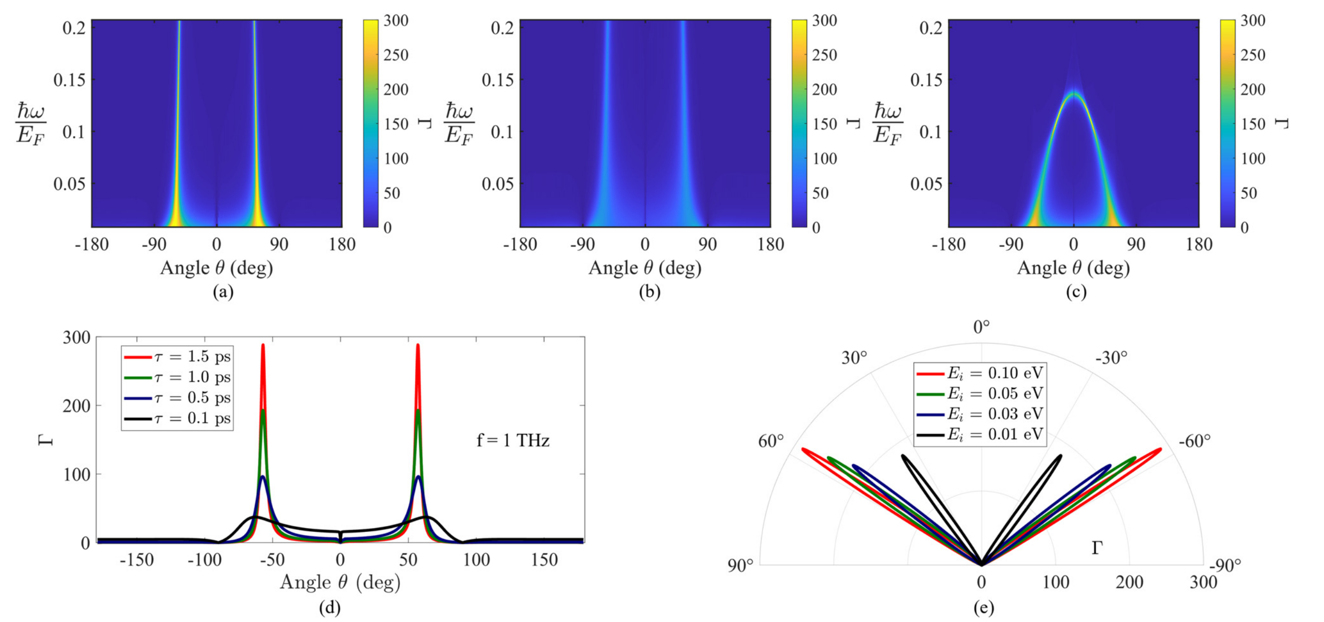

FIG. 3. (a) and (b) GP emission rate at a Fermi level of 0.05 eV, an initial carrier energy of 0.10 eV, and a relaxation time of 1.5 and 0.5 ps, respectively. (c) GP emission rate for $E_F = 0.05$ and $E_i = 0.01$ eV, assuming a τ of 1.5 ps. (d) Comparison of the emission rate at a frequency of 1 THz as a function of the angle for different scattering times. (e) Polar emission diagram at 1 THz for different initial energy of the carrier.

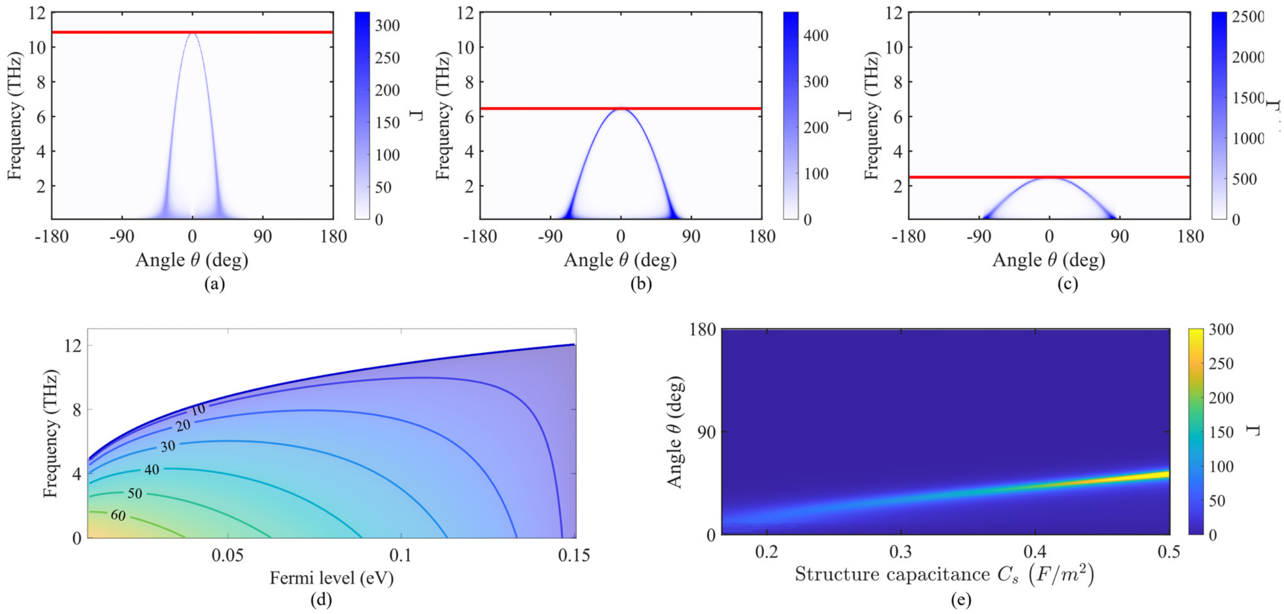

FIG. 4. GP emission rate considering a carrier energy of $E_i = 0.05$ eV with (a) E_F 0.10, (b) $E_F = 0.02$, and (c) $E_F = 0.002$ eV. The red line represents the cut-off frequency from (7). (d) Čerenkov angle as a function of the Fermi level and the frequency assuming E_i 0.05 eV. (e) GP emission rate for different C_s values.

peak of radiation, at a specific angle. This is an interesting result since it makes the emission direction potentially controllable.

Let now consider the effect of the structure properties on the Čerenkov GP emission. The capacitance C_s, that has been introduced in (1), has two main positive effect on the plasmon: (i) slow down the phase and group velocities of the wave and (ii) confine the electromagnetic energy in the out-of-plane direction. The first has the clear purpose to increase the range of charge velocities that allows Čerenkov effect, the second has the effect of increasing the field intensity and, therefore, the emission rate. As shown in Fig. 4(e), assuming a constant frequency of 1 THz, lower capacitance values decrease the maximum Γ and broaden the emission rate around θ_C. Therefore, a larger C_s should be desirable. However, a high capacitive behavior reduces the cut-off frequency and the ability to control the emission angle. Indeed, if the capacitance is doubled, double values of the Fermi level are required to achieve the same control as in Fig. 4(d). Moreover, if the plates are too near, the EM field may induce charges on the metals, enhancing the losses.

It is noted that the photon emission rates are in the order of 100, as opposed to the emission of the order of 10^{-5}, calculated from the Frank–Tamm formula[26] for classical ČE, assuming the same wave and particle velocities, at 1 THz. The quantum Čerenkov effect in graphene arises as a promising possible means to obtain high frequency EM amplification. Even though this work studied the spontaneous emission from charges with energy E_i, by setting the carrier energy, e.g., by applying a DC bias, it is possible to achieve much higher emission rates. To achieve high output-power sources, it will be necessary (i) to have a stable photon emission and (ii) to confine the radiation in a rather sharp angle. This last point is fundamental to couple efficiently the GP with a grating to exchange energy with an external EM wave. The total emission rate per unit time can be obtained by integrating (5) in the whole low-THz band. Figure 5 shows the total emission rate, as a function of the angle, for different E_i values. This rate is in the order of 10^{15} s^{-1}, which corresponds to a time constant of femtoseconds. These values are few orders of magnitude higher than the electron relaxation time, which in this work is assumed to be in the order of picoseconds. This is an important result since it shows that Čerenkov photon emission is more probable than carriers scattering and, in principle, allows a highly stable source of emission.

In this contribution, we analyzed the graphene plasmon emission, in the low-THz band, by quantum Čerenkov effect in a confined structure. The proposed architecture could provide an effective way to transfer DC power from accelerated charges to high-frequency electromagnetic waves, to achieve THz amplification. We discussed the possibility to control the radiation angle by shifting the Fermi level through electrical doping. Moreover, input guidelines have been provided for

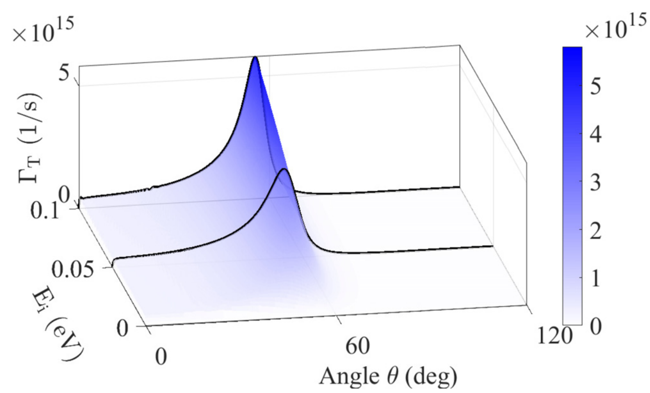

FIG. 5. Total emission rate per unit time in the low-THz band, as a function of the angle, for different E_i values.

design, in particular, considering the impact of the device "effective capacitance" on the GP emission. According to our analysis, we believe that the quantum Čerenkov effect could play a relevant role in the future development of THz amplifiers and powerful sources.

See the supplementary material for the full calculations to obtain the dispersion of the confined plasmon, the matrix element as well as the emission rate in the presence of losses, and the Čerenkov angle.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Gian Marco Zampa: Conceptualization (equal); Data curation (lead); Formal analysis (lead); Methodology (equal); Software (lead); Visualization (lead); Writing – original draft (equal). **Davide Mencarelli:** Conceptualization (lead); Data curation (supporting); Formal analysis (supporting); Funding acquisition (lead); Methodology (equal); Supervision (lead); Validation (lead); Visualization (supporting); Writing – original draft (equal). **Elaheh Mohebbi:** Validation (supporting); Visualization (supporting). **Eleonora Pavoni:** Validation (supporting); Visualization (supporting). **Luca Pierantoni:** Validation (supporting); Visualization (supporting). **Emiliano Laudadio:** Validation (supporting); Visualization (supporting).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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