基于石墨烯可调和增强太赫兹渡越辐射研究

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摘要 太赫兹辐射具有量子能量低、信噪比高、频率宽等一系列特殊性质, 在各个领域都具有相当重要的应用前景, 随着太赫兹技术的发展以及应用领域的拓展, 迫切需要性能各异的大赫兹辐射源. 基于光子学和电子学相结合产生辐射的方法弥补了传统电子学方法产生的辐射功率高但频率低和传统光子学方法频率高但功率低的缺点, 解决了太赫兹源遇到的难题. 本文根据石墨烯表面等离子体波位于太赫兹波段的独特性, 采用经典电磁理论, 研究电子注以任意角入射石墨烯时产生太赫兹渡越辐射的场分布和光谱角分布; 通过MATLAB数值计算, 分析了渡越辐射的辐射特性, 以及入射角度、介质和石墨烯电导率对所产生的渡越辐射的影响, 利用光谱角分布更直观地展现了渡越辐射能量的特点. 石墨烯电导率的可调节特性和这种特殊的边界条件, 为研究可调太赫兹辐射源提供了灵活的选择和便捷的处理方式.

关键词 太赫兹源, 石墨烯, 渡越辐射, 电导率

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1 引言

在电磁波谱中, 太赫兹波所处电磁波谱中位置决定了其兼有微波与红外线的特点^[1,2], 因而具有极大的应用前景. 目前太赫兹波的主要应用有: 安检成像、医疗诊断、食品安全检测、太赫兹通讯与雷达^[3-11]等. 石墨烯是一种奇特的二维碳原子六角形晶格材料^[12,13], 能激励出太赫兹波段表面等离子体波^[14-16]. 石墨烯在太赫兹波段、红外波段能支持表面等离子体波的传输. 在等离子体波局域性^[17]、电导率可调^[18-20]等方面, 石墨烯具有更明显的优势.

电子注激励石墨烯产生表面等离子体波^[19,21-24]的同时将产生渡越辐射^[25,26], 该辐射位于太赫兹波段. 本文采用经典电磁理论研究电子注以任意角入射石墨烯表面时所激发的渡越辐射, 并借助MATLAB数值计算研讨辐射场随入射角、电导率、基底介质的变化特性, 以及光谱角分布的特征.

2 基于石墨烯渡越辐射的理论研究

2.1 物理建模

石墨烯渡越辐射的模型如图1所示, 石墨烯位于两

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种半无限大介质的界面上, 运动带电粒子从介质I(如真空)穿过石墨烯进入介质II, 为了便于理论分析, 带电粒子注在均匀介质中运动时不计能量损耗和对石墨烯的损伤^[27]. 图1中介质 I 和介质 II 的相对介电常数分别为 ε_I 和 ε_{II} , 相对磁导率分别为 μ_I 和 μ_{II} , 电子运动速度为

$$\mathbf{v} = \{0, v_y, -v_z\} = v\{0, \cos\alpha, -\sin\alpha\}. \quad (1)$$

令 $\mathbf{v}$ 处于 yoz 平面内, v 为相应速度矢量的模, α 为 $\mathbf{v}$ 与 y 轴的夹角, θ , φ 分别是波矢 $\mathbf{k}$ 在柱坐标系中与 z 轴的夹角、在 xoy 平面的投影与 x 轴的夹角.

由式(1)中 $\mathbf{v}$ 坐标分解形式可知, 其 x 轴分量为0, 简化了理论模型. 实际上, 选择适当的坐标系, 可使得任意方向入射的电子注速度的 x 轴分量始终为0.

2.2 电子注自身电磁场的解

对于各向同性介质, 联立麦克斯韦方程的复数形式并借助矢量恒等式可以得到电场的偏微分方程:

$$\begin{aligned} \nabla^2 \mathbf{E}_0(\mathbf{r}, \omega) + \frac{\omega^2}{c^2} \varepsilon_r \mathbf{E}_0(\mathbf{r}, \omega) \\ = \frac{1}{\varepsilon_0 \varepsilon_r} \nabla \rho(\mathbf{r}, \omega) - i\mu\omega \mathbf{J}(\mathbf{r}, \omega), \end{aligned} \quad (2)$$

其中, $\mathbf{J}(\mathbf{r}, \omega)$ 为电流密度, $\rho(\mathbf{r}, \omega)$ 为电荷密度, $\mathbf{r}$, ω 分别为位移矢量和角频率, μ 为磁导率, ε_0 和 ε_r 分别为真空介电常数和介质的相对介电常数.

方程(2)的解具有如下形式:

$$\mathbf{E}_0(\mathbf{k}, \omega) = \frac{iq}{\varepsilon_0 \varepsilon_r} \delta(\omega - \mathbf{k} \cdot \mathbf{v}) \frac{\mu_r \varepsilon_r \omega \mathbf{v} - c^2 \mathbf{k}}{c^2 k^2 - \mu_r \varepsilon_r \omega^2}. \quad (3)$$

为了与被激励出的辐射场加以区分, 令 $\mathbf{k}=\mathbf{Q}$, 其中 $\mathbf{Q}$ 为电子注自身场的波矢量, 对式(3)进行逆傅里叶变

图 1 (网络版彩图)物理模型
Figure 1 (Color online) Schematic model.

换, 可以得出:

$$\begin{cases} \mathbf{E}_{0//}(\mathbf{Q}_{//}, z, \omega) = -\frac{iq}{\varepsilon_0 \varepsilon_b} \frac{1}{v_z} \frac{\mu_b \varepsilon_b \omega \mathbf{v}_y - c^2 \mathbf{Q}_{//}}{c^2 Q^2 - \mu_b \varepsilon_b \omega^2} e^{ik_z^b z}, \\ \mathbf{E}_{0z}(\mathbf{Q}_{//}, z, \omega) = -\frac{iq}{\varepsilon_0 \varepsilon_b} \frac{1}{v_z} \frac{\mu_b \varepsilon_b \omega \mathbf{v}_z - c^2 \mathbf{k}_z^b}{c^2 Q^2 - \mu_b \varepsilon_b \omega^2} e^{ik_z^b z}, \\ \mathbf{H}_{0\phi}(\mathbf{Q}_{//}, z, \omega) = -\frac{iqc^2}{v_z} \frac{\mathbf{k}_z^b \cdot \mathbf{v}_{//} - \mathbf{Q}_{//} \cdot \mathbf{v}_z}{c^2 Q^2 - \mu_b \varepsilon_b \omega^2} e^{ik_z^b z}, \end{cases} \quad (4)$$

其中下标 b 表示介质类型(介质 I 或 II), 令 $a=k_z$,

$$a = \frac{\omega - \mathbf{k}_{//} \cdot \mathbf{v}_{//}}{v_z}, \text{ 则 } \mathbf{Q} = \mathbf{Q}_{//} + \mathbf{k}_z = \mathbf{Q}_{//} + a\mathbf{e}_z.$$

以上就是电子注的电磁场在介质 I 和 II 中的通解形式, 其中 q 可以是正电荷也可以是负电荷, 如果是负电荷(比如电子), 则在计算时需要带上负号.

2.3 电子注激发石墨烯产生的渡越辐射场分布

在线性理论和类Drude模型下, 石墨烯的电导率为^[22]

$$\begin{cases} \sigma = \frac{e^2 E_F}{\pi \hbar^2} \frac{\tau^{-1} + i\omega}{\omega^2 + \tau^{-2}}, \\ E_F = \hbar v_f \sqrt{\pi n_s}, \end{cases} \quad (5)$$

式中, τ 为载流子弛豫时间, E_F 为费米能, n_s 为载流子浓度, v_f 为载流子速度.

电子注激发石墨烯将在介质 I 和 II 中产生渡越辐射, 由于渡越辐射电场的散度为0, 因此可得渡越辐射场在介质 I 和 II 中分别具有如下形式:

$$\begin{cases} \mathbf{E}_{r//}^I(\mathbf{k}_{//}, z, \omega) = A^I e^{ik_z^I z} \mathbf{e}_{//}, \\ \mathbf{E}_{rz}^I(\mathbf{k}_{//}, z, \omega) = -\frac{k_{//}^I}{k_z^I} A^I e^{ik_z^I z} \mathbf{e}_z, \\ \mathbf{H}_{r\phi}^I(\mathbf{k}_{//}, z, \omega) = \frac{\varepsilon_0 \varepsilon_I \omega}{k_z^I} A^I e^{ik_z^I z} \mathbf{e}_\phi, \\ \mathbf{E}_{r//}^{II}(\mathbf{k}_{//}, z, \omega) = A^{II} e^{ik_z^{II} z} \mathbf{e}_{//}, \\ \mathbf{E}_{rz}^{II}(\mathbf{k}_{//}, z, \omega) = -\frac{k_{//}^{II}}{k_z^{II}} A^{II} e^{ik_z^{II} z} \mathbf{e}_z, \\ \mathbf{H}_{r\phi}^{II}(\mathbf{k}_{//}, z, \omega) = \frac{\varepsilon_0 \varepsilon_{II} \omega}{k_z^{II}} A^{II} e^{ik_z^{II} z} \mathbf{e}_\phi, \end{cases} \quad (6)$$

式中的参数 A^I 和 A^{II} 为待定参数, 且 $\mathbf{k}_{//} = \mathbf{Q}_{//}$.

这两种场必须满足以石墨烯为界面的边界条件为

$$\begin{cases} \mathbf{n} \times (\mathbf{E}^I - \mathbf{E}^{II}) = 0, \\ \mathbf{n} \times (\mathbf{H}^I - \mathbf{H}^{II}) = \sigma \mathbf{E}_{//}^I, \end{cases} \quad (7)$$

其中, $\mathbf{E}^I = \mathbf{E}_0^I + \mathbf{E}_r^I$, $\mathbf{E}^{II} = \mathbf{E}_0^{II} + \mathbf{E}_r^{II}$, $\mathbf{H}^I = \mathbf{H}_0^I + \mathbf{H}_r^I$,
 $\mathbf{H}^{II} = \mathbf{H}_0^{II} + \mathbf{H}_r^{II}$.

通过系列化简, 可得待定系数为如下形式:

$$\begin{cases} A^I = \frac{\sigma a_0^I - (b_0^I - b_0^{II}) + a_r^I(a_0^I - a_0^{II})}{a_r^I - a_r^{II} - \sigma}, \\ A^{II} = \frac{\sigma a_0^{II} - (b_0^I - b_0^{II}) + a_r^I(a_0^I - a_0^{II})}{a_r^I - a_r^{II} - \sigma}, \end{cases}$$

其中,

$$\begin{aligned} a_0^I &= -\frac{iq}{\varepsilon_0 \varepsilon_1 v_z} \frac{1}{c^2 Q^2 - \mu_1 \varepsilon_1 \omega^2} \frac{\mu_1 \varepsilon_1 \omega v_y - c^2 Q_{//}}{v_z}, \\ a_0^{II} &= -\frac{iq}{\varepsilon_0 \varepsilon_{II} v_z} \frac{1}{c^2 Q^2 - \mu_{II} \varepsilon_{II} \omega^2} \frac{\mu_{II} \varepsilon_{II} \omega v_y - c^2 Q_{//}}{v_z}, \quad a_r^I = \frac{\varepsilon_0 \varepsilon_1 \omega}{k_z^I}, \\ b_0^I &= -\frac{iq c^2}{v_z} \frac{v_y k_z^I - v_z Q_{//}}{c^2 Q^2 - \mu_1 \varepsilon_1 \omega^2}, \\ b_0^{II} &= -\frac{iq c^2}{v_z} \frac{v_y k_z^{II} - v_z Q_{//}}{c^2 Q^2 - \mu_{II} \varepsilon_{II} \omega^2}, \\ a_r^{II} &= -\frac{\varepsilon_0 \varepsilon_{II} \omega}{k_z^{II}}. \end{aligned}$$

当参数 A^I 和 A^{II} 的分母为零时, 所对应的 $\mathbf{k}_{//}$ 为石墨烯表面等离子波的波矢; 当参数 A^I 和 A^{II} 的分母不为零时, $\mathbf{k}_{//}$ 为渡越辐射的波矢. 从上面参数可知, 渡越辐射的电磁场分布与电子注的速度和入射角有非常大的关系, 同时也与石墨烯的电导率以及介质基底有关. 可见, 通过调节电子注、石墨烯和介质可以得到不同的辐射分布.

最后, 经过傅里叶逆变换, 可将渡越辐射在 $\mathbf{k}$ 空间的分布变换到 $\mathbf{r}$ 空间中.

2.4 渡越辐射的光谱角分布

辐射场表达式在描述辐射能量方面的能力有限且不够直观, 而单位辐射角、单位角频率的光谱角分布更能描述辐射场的能量在空间中的分布. 单个运动电子的渡越辐射光谱角分布公式为

$$\begin{aligned} \frac{d^2 W(\mathbf{r}, \omega)}{d\Omega d\omega} &= \frac{1}{16 \varepsilon_r \varepsilon_0 c \pi r^2} k^2 \sigma(\omega)^2 |A^I|^2 \\ &\times \left[\left(\cos \theta \cos \varphi + \frac{k_{//}^I}{k_z^I} \right)^2 \right. \\ &\left. + \left(\cos \theta \sin \varphi - \frac{k_{//}^I}{k_z^I} \right)^2 + \sin^2 \theta \right]. \end{aligned} \quad (8)$$

3 渡越辐射的数值计算

3.1 渡越辐射场分布特性

本文利用 MATLAB 对渡越辐射场进行数值计算并分析辐射场电场分布的特性. 假设电子注从真空中以任意角入射到石墨烯上, 取参数 $q = -e$, $\mu_I = \mu_{II} = 1$, $\varepsilon_I = 1$, 电子电压 3 keV, 根据常规石墨烯的参数^[15], 取载流子浓度 $5 \times 10^{15} \text{ m}^{-2}$ 、速度 $1 \times 10^6 \text{ m s}^{-1}$ 和弛豫时间 $2.5 \times 10^{-13} \text{ s}$, 由式(5)可得到石墨烯的费米能 $E_F = 0.0825 \text{ eV}$.

(1) 电子注入射角对激发的渡越辐射的影响

当石墨烯两侧均为真空且电子入射角 α 为 90° (垂直入射) 时, 对应激发的渡越辐射场电场分布图如图2(a)所示 (以 5 THz 为例). 图2(b) 为 5 THz 辐射场的幅值随入射角的变化. 由图可知, 石墨烯上下两侧的渡越辐射沿石墨烯平面对称分布, 且石墨烯两侧的辐射均为双瓣状, 有一定的辐射角; 随着电子入射角的增大, 辐射场的强度会增加. 当垂直入射时, 辐射场最强.

当介质 II 不为真空时, 取其相对介电常数 $\varepsilon_{II} = 4$, 而其他参数保持不变, 入射角 α 为 90° 的辐射场的分布图如图3所示. 由图3(a)与图2(a)相比可知, 有介质情况下石墨烯两侧的辐射强度都明显增强了; 变化最明显的是石墨烯下侧的辐射角和辐射集中度, 由于介质中波长变短, 所以辐射分布更密集.

为了体现石墨烯对渡越辐射的增强作用, 图3(b)给出了有无石墨烯两种情况下辐射场的幅值随入射角的变化. 随着电子入射角度的增加, 两种情况下的辐射场幅值都保持上升的趋势, 但是在有石墨烯的情况下, 渡越辐射明显增强.

(2) 介电常数变化对渡越辐射的影响

其他条件不变的情况下, 当垂直入射且 ε_{II} 为 7 时, 辐射场分布如图4(a)所示. 图4(b) 为 5 THz 辐射场的幅值随介质相对介电常数的变化.

结合 ε_{II} 为 1 (如图2(a)) 和 4 (如图3(a)) 的辐射场情况, 不难发现, 当介电常数增加时, 在下半区域内, 辐射能量集中在一个较小锥角里, 且辐射更趋于前向辐射. 由图4(b) 可知随着介电常数的增大, 电场幅值变化的大致趋势也是增大的; 不过, 介电常数在 1–3 这个区间时, 电场最值变化比较迅速, 之后趋于平缓.

(3) 石墨烯导电率对渡越辐射的影响

在太赫兹波段, 石墨烯电导率随频率的变化如

图 2 (网络版彩图)石墨烯两侧均为真空时 5 THz 的辐射电场 E_{rz} 随入射角的变化图. (a) 入射角 $\alpha=90^\circ$ 时的情形; (b) E_{rz} 幅值随入射角 α 变化的曲线

Figure 2 (Color online) Distribution of the electric field E_{rz} of the transition radiation with the electron incidence angle of (a) $\alpha=90^\circ$, and (b) the amplitude of E_{rz} with the incident angle α , in the case of vacuum on the two sides of graphene layer.

图 3 (网络版彩图)石墨烯下层介质 $\epsilon_{II}=4$ 时 5 THz 的辐射场随电子入射角的分布图. (a) 入射角为 $\alpha=90^\circ$ 时的情形; (b) 有无石墨烯情况下 E_{rz} 幅值随入射角 α 变化的曲线图

Figure 3 (Color online) Distribution of the electric field of the transition radiation with (a) the electron incidence angle of $\alpha=90^\circ$ and (b) the amplitude of E_{rz} varies with incident angle α in the presence or absence of graphene, with the medium $\epsilon_{II}=4$ under graphene layer.

图5(a)所示. 随着频率的增加, 总体上电导率在下降^[23]. 垂直入射时, 辐射电场最大值随频率的变化如图5(b)所示, 随着频率增加, 辐射场幅值先快速增加, 而后趋于平缓, 有微微下降趋势.

(4) 石墨烯载流子速度和浓度对渡越辐射的影响

由式(5)可知, E_F 随载流子浓度和速度增加而递增, 且电导率随着 E_F 的增大而增大, 通过调节载离子浓度和速度可以调节 E_F , 进而达到调节石墨烯电导率的目的, 如图6(a)所示. 因此, 可以通过调节载流子浓度和速度改变辐射场. 由图6(b)可知, 辐射场随着随载流子浓度、速度的增加而增加. 鉴于石墨烯的电导率可以通过改变掺杂与基底、载流子浓度、外置偏压、石墨烯形态等方式^[28-30]得以调控, 因此可以得到可调的太赫兹辐射源.

3.2 光谱角分布特性

(1) 渡越辐射的光谱角分布随入射角的变化

取频率为 2 THz, 电子注电压 U 为 3 keV, $\epsilon_{II}=4$, 当单个电子的入射角 α 分别为 0.01° (近似于平行) 和 90° (垂直入射) 时, 对应的界面上的光谱角分布如图7所示.

在图7(a)中, 光谱角分布表明, 辐射场主要集中在界面附近, 没有出现明显的前向($\theta=0^\circ$)或后向($\theta=\pi$)辐射; 同时也表明, 近乎平行入射依然会激发渡越辐射. 在图7(b)中, 出现了明显的前向和后向辐射. 经比较, 光谱角分布的强度随着入射角的增大而增大.

(2) 渡越辐射的光谱角分布随电子注能量的变化

当垂直入射时, 并保持其他参数不变, 渡越辐射光谱角分布随电子注电压的变化如图8所示, 图8(a)和(b)

图 4 (网络版彩图)辐射场随介电常数的分布图. (a) $\varepsilon_{II}=7$ 时场分布图; (b) 电场幅值随 ε_{II} 变化图

Figure 4 (Color online) Distribution of the electric field of the transition radiation with dielectric constant of medium II, (a) $\varepsilon_{II}=7$ and (b) the amplitude of the electric field with ε_{II} , respectively.

图 5 (网络版彩图)石墨烯电导率对渡越辐射的调制. (a) 电导率随频率的变化; (b) 辐射场幅值随频率的变化

Figure 5 (Color online) Modulation of the transition radiation by graphene conductivity. (a) Conductivity varies with the frequency; (b) the amplitude of the radiation field varies with the frequency.

图 6 (网络版彩图)电导率随费米能变化(a)和 E_{rz} 的幅值随载流子浓度和密度变化的曲线(b)

Figure 6 (Color online) (a) Curve of Fermi energy with conductivity; (b) curve of the amplitude of E_{rz} with carrier concentration and velocity.

图 7 (网络版彩图)光谱角分布随入射角度的变化. (a) 入射角为 0.01° ; (b) 入射角度为 90°

Figure 7 (Color online) Spectral angular distribution as a function of incident angle with (a) the electron incidence angle of $\alpha=0.01^\circ$ and (b) $\alpha=90^\circ$.

图 8 (网络版彩图)光谱角分布随电子注电压的变化. (a) 电压为1 keV; (b) 电压为100 keV

Figure 8 (Color online) Spectral angular distribution as a function of the voltage with (a) the voltage of $U=1$ keV and (b) $U=100$ keV.

的电压分别为1和100 keV. 由图8可知, 光谱角分布随电子注电压增大, 且辐射的集中度增加, 倾向于前向入射.

4 结论

本文从经典电磁理论出发, 推导了电子注入射到石墨烯上产生的太赫兹渡越辐射及其光谱角分布. 通过数值计算, 详细分析了渡越辐射随电子注入射角、介质基底、石墨烯电导率的变化特性以及光谱角分布随入射角度的变化. 研究发现渡越辐射的分布非常奇特: 太赫兹辐射具有明显的双瓣结构, 这种结构会随着入射角增大而趋于轴对称, 并且辐射强度随入射角的增大而增强; 介质基底会影响介质中辐射的传播特

性, 随着介电常数的增大, 辐射锥角将变小并趋向于前向辐射; 石墨烯能大幅度增强辐射强度, 特别是在介质中的前向辐射. 由于石墨烯电导率与表面等离子体波频率或辐射频率是相关的, 且石墨烯的电导率可以通过外加偏置电压和掺杂来调节, 同时介质、电子注能量、入射角都方便调控, 这为开发可调太赫兹辐射源提供更便捷的途径. 在实验中, 可以采用扫描电子显微镜的电子束激发石墨烯并检测产生的渡越辐射. 高能量、大电流密度电子注会对石墨烯及其基底材料造成损伤, 而扫描电子显微镜的电压和电流便于调节, 其电压通常在1–30 kV范围内, 电流在nA– μ A范围内, 在这种电压和电流环境下, 电子束的能量较低, 可以防止石墨烯及其基底材料被损伤. 本文研究有助于发展高效、便利、经济的太赫兹辐射源.

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Study of tunable and enhanced transition radiation from graphene in terahertz band

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Terahertz (THz) radiation has many special properties, such as low quantum energy, high signal-to-noise ratio and wide frequency, so that it possesses important application prospects in various fields. With the development of THz technology and its application fields, it is an urgent need to develop all types of terahertz source. It is as well-known that the radiation generated by traditional electronics methods has high power with low frequency, while by traditional photonics method has relatively high frequency with low power. Fortunately, the method of generating radiation based on the combination of photonics and electronics can overcome the above disadvantages, so it can solve the problem encountered by the terahertz source. In this paper, the integrated method by using electron beam to excite surface plasmon waves and generate transition radiation is adopted to obtain terahertz waves. Although the output power by this method is not remarkably high, the method is flexible and easy to implement. Due to the merit of graphene plasmon in THz band, a physical model of a moving electron incidence on a monolayer graphene at arbitrary angle is established in this paper to generate transition radiation in THz band. The field of the transition radiation is fully deduced by Maxwell's equations combined with the special boundary conditions due to graphene's conductivity. Then the expression of spectral-angular distribution is also derived in order to show the radiation energy characteristic more intensively in three-dimensional space. The characteristic of the radiation is numerically calculated by MATLAB. We focus on the transition radiation generated by a charged particle with a moderate energy and explain some contributions to the radiation, such as the incident angle, the conductivity or the Fermi level in graphene and the substrate dielectric characteristic. The pattern and intensity of the radiation field are numerically analyzed in the upper and lower half-spaces. We plot the figures of field distribution and the spectral angular distribution related to these variables mentioned above to analyze their influences on the radiation. In the case of the normal incidence, the transition radiation exhibits strong symmetry and considerably more intensive than that at grazing and oblique incidence. The results of the spectral angular distribution display that the radiation intensity increases strongly with the incident angle, and that the radiation energy focuses in backward and forward directions in the case of normal incidence. This study summarizes that the parameter adjustment mechanism is favorable for the performance of terahertz source. Since the conductivity of graphene can be adjusted by applying a bias voltage and doping, the radiation frequency and intensity can be tuned by the conductivity of graphene. Meanwhile, the substrate, electron energy and incident angle are conveniently controlled, therefore a more flexible way is obtained to develop tunable terahertz radiation sources.

terahertz source, graphene, transition radiation, conductivity

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