Lieb莫尔光子晶格及其光子学特性研究

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摘　要：受到电子学领域双层扭曲石墨烯的启发,莫尔光子晶格的多种莫尔构型被证明具有光子局域等特性。将两个相同周期的 Lieb 子晶格旋转角 36.87°叠加构造了 Lieb 莫尔晶格,并基于平面波展开法计算了其能带结构。结果表明,相比于常规的 Lieb 晶格,Lieb 莫尔晶格的无量纲化光子禁带宽度最高可增加 0.25,并且禁带中心发生了蓝移,因而更适合在光通信领域的应用。数值计算结果表明在 Lieb 莫尔晶格的能带结构中还具有平带,其特性可通过改变介质柱的几何参数进行调控,最高平整度可达到 0.001 872 2。通过计算平整度最高时的电场分布,发现了局域的现象。基于 Lieb 晶格的莫尔构型可为光子晶体研究提供新的方法,也为研究复杂光子晶体结构提供新的平台。

关键词：光子晶体;光子莫尔晶格;平面波展开法;禁带;电场局域

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0　引言

莫尔现象在自然和日常生活中非常常见,比如明媚的阳光反射在窗帘上产生的水波样条纹、用相机拍摄液晶显示器时出现的条纹等。莫尔结构是两个相同周期性结构叠加而成的复合结构,并且基于莫尔结构的检测技术被广泛应用。近年来,曹原等[1]关于石墨烯的"魔角"的研究掀起了微观领域中电子莫尔结构的研究热潮[2-4],二维材料莫尔结构的非平凡电子特性也使得其具有奇异的光学特性,例如双层 α-MoO₃莫尔结构的色散曲线在魔角下的可调拓扑过渡[5]。

然而,天然二维材料构成的莫尔结构,因其子晶格是固有的原子晶格,所以难以调控。近年来,基于人工子晶格（如金属超材料、光子晶体等）构造的莫尔晶格结构引起了研究者重视,如采用金属超材料形成的表面等离激元莫尔晶格,可诱导产生强圆二向色性的光场[6]。理论研究表明,采用光子晶体构造的光子莫尔晶格表现出比子晶格更宽的禁带以及更平的能带[7-10],实验上光子莫尔晶格可以采用多种方式产生,如叶芳伟等[11-12]提出的在光折变晶体中通过光强诱导方法构造光子莫尔晶格,实现了空间光孤子的调控。曾健华等[13]提出在相干原子气体中基于电磁诱导产生光子莫尔晶格。马仁敏等[14]基于半导体多量子阱膜叠加的方法设计了光子魔角激光器。因此,光子莫尔晶格具有宽禁带以及平带特性,旋转角提供更多的调控自由度,是一种极具前景的新型光子学研究平台。

光子禁带和平带是光子晶体的两个重要特性。宽禁带的光子晶体可用于低阈值激光器[15]、光学晶体管[16]和光波导[17]等领域。平带范围内的光子群速度极小,能引发光子的局域,因此具有平带特征的光子晶体在光致发光增强[18]和慢光产生[19]等领域应用广泛。目前研究的由四方晶格[11,13]、六方晶格[8-9,11]等构成的莫尔光子晶格中均发现具有平带特征,但四方、六方等晶格自身的平带特征并不明显。因此,由自身具有平带特征的子晶格（如 Lieb、Kagome 晶格等）构成的光子莫尔晶格可能具有突出的平带特性。

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Lieb晶格是一种常见的具有平带特征的光子晶体结构[20-22],因此基于Lieb晶格的莫尔结构也被期望具有更宽的禁带和更平的光子能带。本文通过旋转两个Lieb子晶格构造出周期性Lieb莫尔晶格,通过数值计算研究了Lieb莫尔晶格的光子禁带和平带特性,并通过改变填充系数和介质材料调控其光子禁带,为实现宽光子禁带、超平带光子晶体提供一种新的途径。

1 Lieb莫尔晶格的构造

在本文中,Lieb晶格结构由介质柱和空气间隙构成。采用一组基矢$(\boldsymbol{a}_0, \boldsymbol{b}_0)$描述未旋转Lieb子晶格的坐标,如图1(a),$\boldsymbol{a}_0 = \sqrt{2}\,\alpha_1\boldsymbol{l}, \boldsymbol{b}_0 = \sqrt{2}\,\alpha_1\boldsymbol{j}$,随着两个子晶格之间旋转角的改变,形成的莫尔晶格的晶格常数也会变化。当旋转角为某些特定角度时,两个子晶格的某些节点会重合,形成具有周期性的莫尔结构,这些特定的角度称为可公度角,用一组整数(m, n)定义可公度旋转角度θ为

$$\theta = 2\arctan\left(\frac{n}{m}\right)\left(\frac{b_0}{a_0}\right) \tag{1}$$

图1(b)为旋转角为36.87°的莫尔晶格的示意图($n=1, m=3$)。未旋转的子晶格的基矢乘以旋转矩阵 $\boldsymbol{M}(\theta) = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$ 即可得到旋转后子晶格的基矢。

图1(a)中的红色圆点表示未旋转的Lieb晶格(其晶格常数为α_1)中的介质柱A,顺时针旋转36.87°后得到的介质柱B记为绿色圆点,介质柱A和B组合构成莫尔晶格,如图1(b)所示。该莫尔超元胞包含了27个介质柱,晶格常数为α_2,保留了原本Lieb晶格四方晶格的几何特征。介质柱A和B的介电常数分别记为ε_1和ε_2,半径分别记为r_1和r_2,背景介质为真空。根据理论计算,还存在其他的可公度角,但是由于形成的莫尔晶格的超元胞中介质柱数目太多,本文仅研究旋转角为36.87°的Lieb莫尔晶格。

(a) Unrotated Lieb lattice   (b) Supercell of Moire lattice with rotation angle θ=36.87
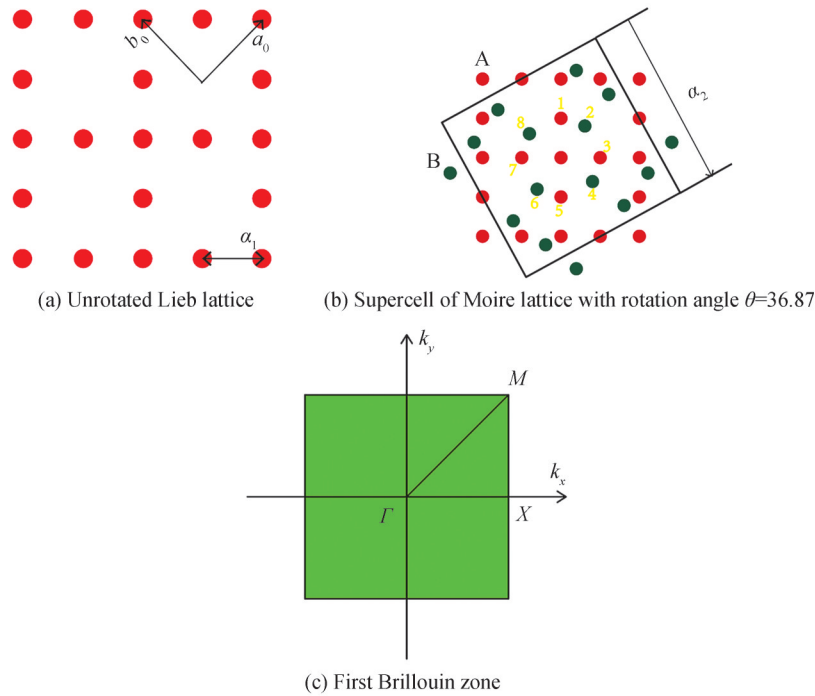

(c) First Brillouin zone

图1 Lieb莫尔晶格的构造方法
Fig. 1 Construction method of Lieb Moire lattice

2 Lieb莫尔晶格的光子能带特征

本节中Lieb子晶格和莫尔晶格的介质材料均为GaAs。为了对比子晶格和莫尔晶格的特性,设Lieb子晶格和形成的莫尔晶格的晶格常数相等,即$\alpha_1 = \alpha_2 = \alpha = 2\sqrt{5}$ μm。能带结构图采用无量纲的坐标,计算结

果能够方便地进行比例变换，有利于应对不同具体数值的情况。根据几何关系可知，Lieb结构的填充系数为$f_1=3\pi r_1{}^2/S_1$，莫尔晶格的填充系数为$f_2=27\pi r_2{}^2/S_2$，S_1和S_2表示结构单元胞面积，其中$S_1=4\alpha_1^2$，$S_2=\alpha_2^2$。

采用平面波展开法（Plane Wave Method，PWM）[23]计算TM模式下光子晶体的能带结构，沿着第一布里渊区内三个高旋转对称点Γ、M、X采样（见图1(c)），$f_1=f_2=0.10$的计算结果如图2所示。因为光子能量正比光子频率，因此这种色散关系图也被称为能带结构图。将能带结构图中最宽的禁带定义为主禁带，在图2中用灰色区域表示。Lieb晶格的主禁带宽度为0.074，禁带中心为0.285，如图2(a)；莫尔晶格的主禁带宽度为0.148，禁带中心为1.849，如图2(b)。在相同的填充系数下，Lieb莫尔晶格的禁带比Lieb晶格的禁带更宽。

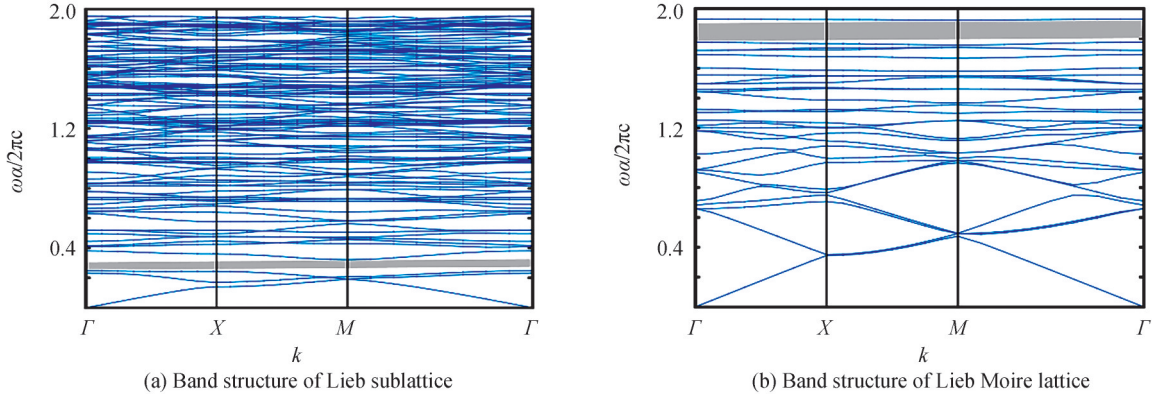(a) Band structure of Lieb sublattice (b) Band structure of Lieb Moire lattice

图2　填充系数为0.1时Lieb子晶格和Lieb莫尔晶格的能带结构图
Fig. 2　Band structures of Lieb sublattice and Lieb Moire lattice with filling factor of 0.1

Lieb晶格和莫尔晶格的禁带中心波长分别为15 691.7 nm、2 418.6 nm，属于红外波段。Lieb莫尔晶格的光子禁带相比于Lieb子晶格发生了蓝移，主要因为在相同的晶格常数条件下，莫尔晶格中的介质柱数目更多，为了保证相同的填充率，具有较小介质柱直径的莫尔晶格形成了较大介电常数的对比度。在光通信及其他实际应用中，典型的波长是800 nm到1 600 nm，因此莫尔晶格的禁带更靠近实际应用的波段，具有更高的应用价值。因为计算结果以无量纲形式表示，所以可以通过介质柱大小和晶格常数之比的变换获得所需波段的禁带。

为了研究介质柱直径对禁带特征的影响，得到优化的禁带宽度，对Lieb晶格和莫尔晶格的填充系数进行了扫描，将不同情况下的能带特征进行整理得到的禁带特征图如图3所示。图3(b)显示莫尔晶格最宽的主禁带宽度为0.212，远大于Lieb晶格最宽的主禁带宽度0.076（见图3(a)），对应的填充系数分别为0.153和0.120。将填充系数分别固定在禁带宽度最大时，相应的能带结构图如图3(c)和图3(d)。Lieb晶格的主禁带宽度最宽时对应的禁带中心位于0.275，而莫尔晶格的主禁带宽度最宽时对应的禁带中心为1.703，具有明显的蓝移特征。

Lieb莫尔晶格的平带特征如图3(d)所示。Lieb莫尔晶格中存在三条平带，分别为第15带、第22带、第27带（图中标号为1、2、3）。为了表征光子平带的特征，定义光子带的平整度F为[24]

$$F=\frac{\omega_t-\omega_b}{\omega_t+\omega_b} \tag{2}$$

式中，ω_t和ω_b分别为光子带的顶部和底部频率。F值越小，表明光子带的平整度更高。图3(d)中三条平带的F值分别为0.006 014 9、0.002 328 4、0.005 258 7，其中第22带具有最小的F值，即具有最高的平整度。对比图3(c)，Lieb晶格的平带最小的F值为0.0150，因此莫尔晶格平带的平整度远高于Lieb晶格。

介质柱的半径也影响光子带的特征，因此通过改变介质柱的半径对第22带的平整度进行了研究。计算结果如图4所示，当$r_1=0.038\ 0\alpha$时，F具有极小值0.001 872 2，此时平带对应的归一化频率为1.47。已经报道的四方、六方等光子莫尔晶格结构中均展示了平带以及超平带[8-9, 11, 13]，但未给出数值表征。对比已经报道的Kagome晶格[24]平带平整度（0.002），Lieb莫尔晶格的平带平整度更好，同时Lieb莫尔晶格的光子禁带更宽且具有更高的灵活性。

(a) Bandgap characteristic of Lieb lattice

(b) Bandgap characteristic of Lieb Moire lattice

(c) Band structure of Lieb sublattice

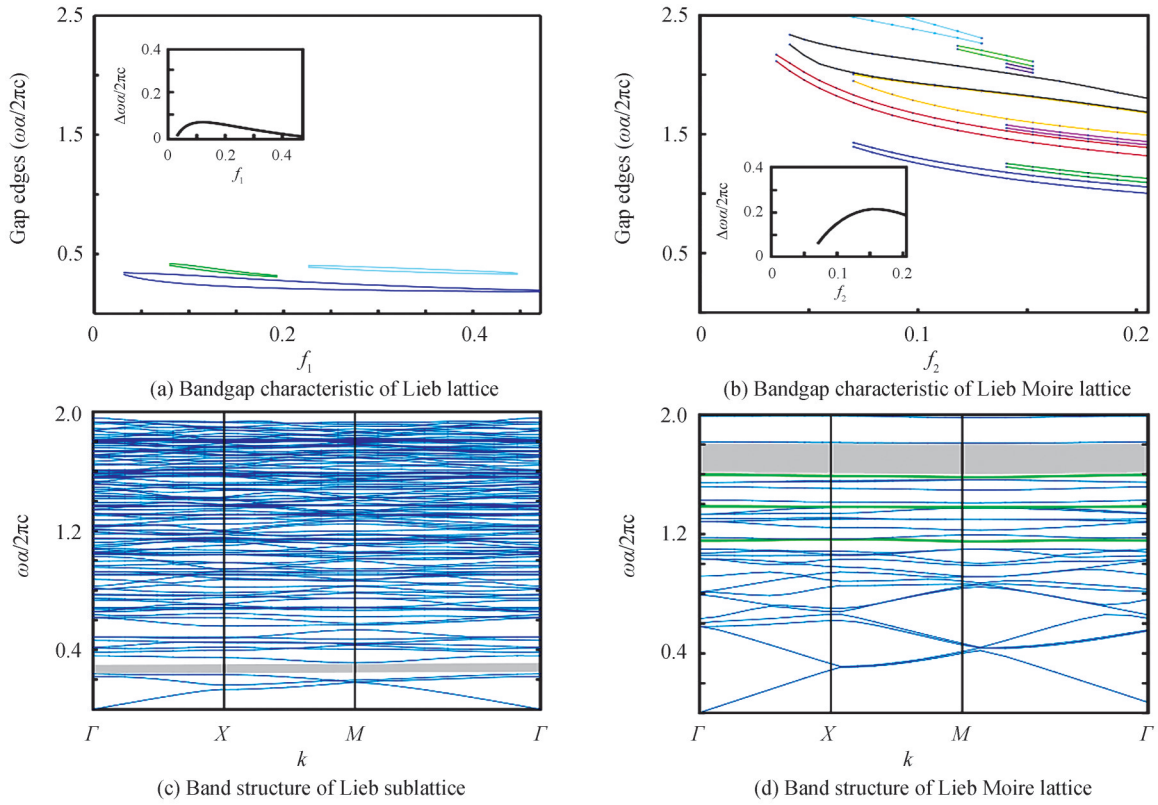(d) Band structure of Lieb Moire lattice

图 3　Lieb 晶格和 Lieb 莫尔晶格的禁带特征图和能带结构图（插图为主禁带宽度随填充系数变化的曲线）

Fig. 3　Bandgap characteristic diagrams and band structures of Lieb lattice and Lieb Moire lattice（the illustrations show the curves of the main bandgap width changing with the filling factor）
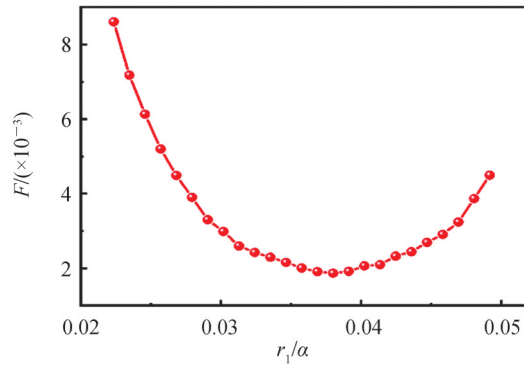

图 4　光子平带的平整度 F 随 r_1/a 变化曲线

Fig. 4　Flatness F of the photonic band varies with r_1/a

　　为了验证平带对电场局域的效果，计算了 22 能带在 Γ 点和 X 点的电场分布，初始的电场满足归一化规则：$\dfrac{1}{S}\displaystyle\int \mathrm{d}x^2 \varepsilon \left| E(x) \right|^2 = 1$，计算结果如图 5 所示。图 5 只显示了一个超元胞内的情况，电场被局限在中心一圈的介质柱上，对应于图 1(b) 中标号为 1~8 的八个"花瓣"形状，最高的光强 $|E(x)|^2$ 分别为 2.49 W/m² 和 2.54 W/m²。更高平整度的平带能导致更强的电场局域，强烈的局域在非线性光学、光电能量转换器件等方面具有广泛的应用前景，因此 Lieb 莫尔晶格将为这些研究提供一个新的途径和平台。

(a) Electric energy distributions at the Γ point

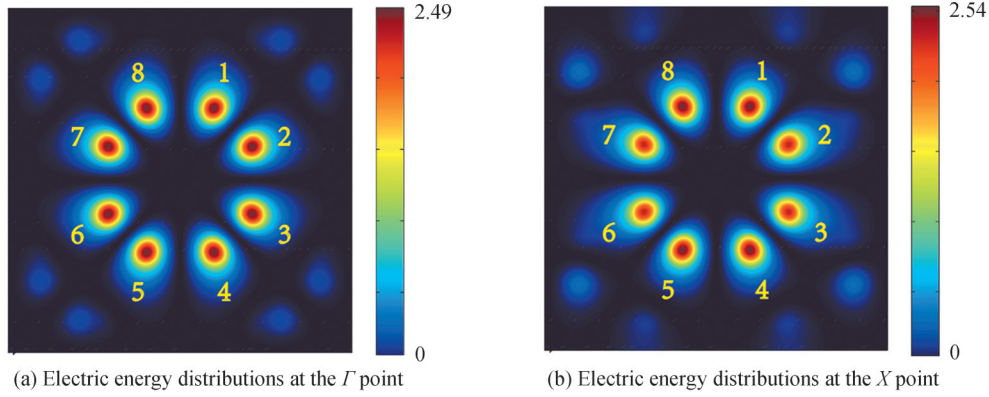(b) Electric energy distributions at the X point

图 5　平带的电场强度分布图

Fig. 5　Electric energy distributions of the flat photonic band

3　介质特性对 Lieb 莫尔晶格禁带的影响

研究不同介质材料的子晶格叠加形成的复合莫尔晶格的能带特征。选择两种实验中常用的介质材料：GaAs和SiO$_2$,两个子晶格重合点选用了GaAs介质柱,采用平面波展开法对莫尔晶格的禁带特征进行计算,结果如图 6(a)所示。

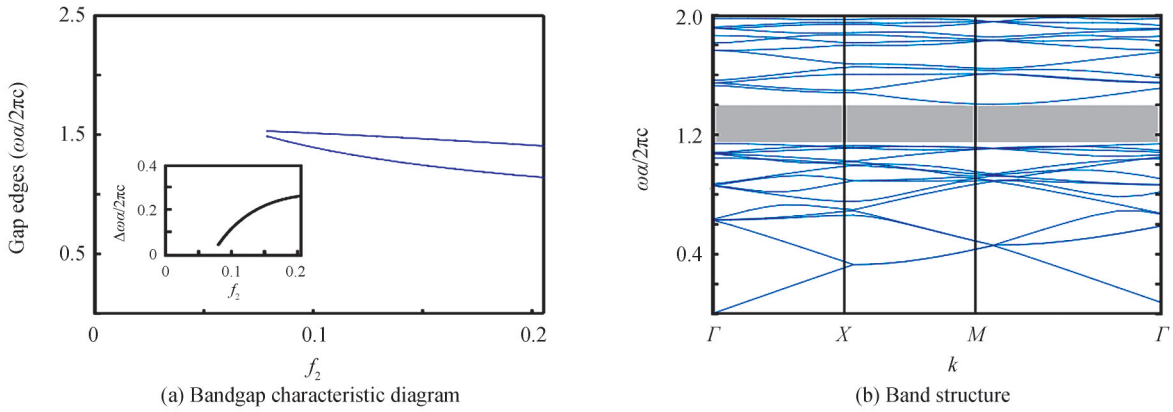
(a) Bandgap characteristic diagram

(b) Band structure

图 6　Lieb复合莫尔晶格的禁带特征图和能带结构图(插图为主禁带宽度随填充系数变化的曲线)

Fig. 6　Bandgap characteristic diagram and band structure of Lieb composite Moire lattice (the illustrations shows the curve of the main bandgap width changing with the filling factor)

由图 6(a)可知,Lieb复合莫尔晶格的禁带宽度随着填充系数的增大而增大。因为随着介质柱半径的增加,复合晶格结构出现了重叠的情况,因此在图 6(a)中,最大的填充系数为 0.205。图 6(b)给出了近极限情况下 Lieb 复合莫尔晶格的能带结构图,晶格的主禁带宽度为 0.265,禁带中心为 1.274。通过对比 Lieb 莫尔晶格(GaAs)和 Lieb 复合莫尔晶格(GaAs＋SiO$_2$)的禁带特征,证明了材料介电特性差异也能对莫尔结构的禁带进行调控。对比材料单选 GaAs 的 Lieb 莫尔晶格,Lieb 复合莫尔晶格的主禁带宽度得到了提升。禁带增宽的原因主要是两种介质引起的晶格结构对称性降低,减小结构的对称性是提高光子晶体禁带的有效手段[25-26]。

Lieb 复合莫尔晶格的两个子晶格介质柱的半径也可以作为一个调控参数,设定两个子晶格的介质柱半径关系为 $r_2＝0.5r_1$,此时对应的填充系数为 $f_3＝(15r_1^2＋12r_2^2)\pi/a_2^2$。两个子晶格重合点仍选用了 GaAs 介质柱。计算得到的不同半径条件下,晶格能带特征如图 7(a)和(b)所示。在不同半径的 Lieb 莫尔晶格(GaAs)中,当填充系数为 0.137时,主禁带最大;在不同半径的 Lieb 复合莫尔晶格(GaAs＋SiO$_2$)中,当填充系数为 0.170时,主禁带最大。最宽禁带条件下的能带结构如图 7(c)和(d)所示。在 $r_2＝0.5r_1$ 的 Lieb 莫尔晶格中,主禁带宽度为 0.167,禁带中心为 1.265。在 $r_2＝0.5r_1$ 的复合莫尔晶格中,主禁带宽度为 0.326,禁带中心为 1.246。Lieb 复合莫尔晶格的主禁带宽度得到了进一步的提升,这仍可以归因于子晶格介质柱半径的变化所
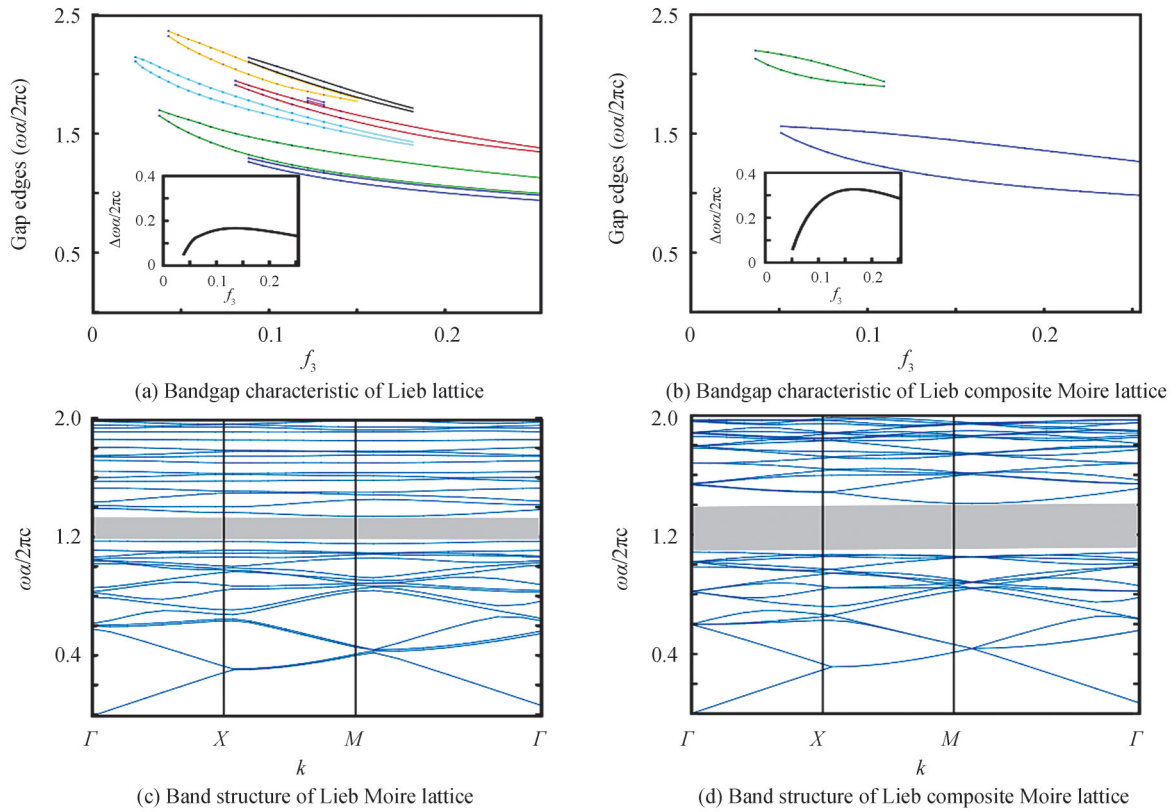
带来整体晶格对称性的降低。因此,通过改变介质柱 A 和 B 半径的相对大小,禁带宽度可以得到进一步提高。

图 7　$r_2=0.5r_1$ 时 Lieb 莫尔晶格和 Lieb 复合莫尔晶格的禁带特征图和能带结构图(插图为主禁带宽度随填充系数变化的曲线)
Fig. 7　Bandgap characteristic diagrams and band structures with $r_2=0.5r_1$ of Lieb Moire lattice and Lieb composite Moire lattice (the illustrations show the curves of the main bandgap width changing with the filling factor)

4　结论

　　本文通过两个 Lieb 子晶格的可公度旋转,构造了 Lieb 莫尔光子晶格,通过数值计算研究了该晶格结构的光子禁带特征与结构参数、材料特性之间的关系。计算结果表明在相同填充因子条件下,Lieb 莫尔晶格中禁带频率区间的宽度相比于子晶格有显著的增加。在 $r_1=0.038\ 0a$ 的 Lieb 莫尔晶格中,得到了平整度最高的平带。在 Lieb 复合莫尔晶格中,得到了最宽的带隙 0.326。通过莫尔配置,在原有晶格基础上实现了更平的平带和更宽的禁带结构,可为集成光子器件性能的优化提供新的平台。此外,莫尔结构引入了更多的结构参数和材料参数自由度,通过改变结构和材料参数,能够实现较大范围的光子禁带调控、丰富光子晶格结构的功能、扩展光子晶体的应用范围。

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Lieb Moire Photonic Lattice and Its Photonic Properties

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Abstract: Inspired by the two-layer twisted graphene in electronics, Moire photonic lattices are also of great interest to researchers. Various Moire photonic configurations have been shown to possess peculiar photonic properties. In this paper, the photonic characteristics of Lieb Moire lattices composed of two overlapping Lieb sublattices with different rotation angles are studied. It is found that two Lieb sublattices

can form a lattice with square characteristics when the rotation angle is 36.87°. Both the Lieb lattice and Lieb Moire lattice are composed of GaAs dielectric cylinders embedded in air. The radii of the cylinders of the two sublattices are r_2 and r_1 respectively. In order to compare their lattice properties, their lattice constants are set to be equal. With the same filling factor, the plane wave method is used to simulate the band structures of TM modes. According to numerical simulation, the Lieb Moire lattice has a wider photonic bandgap and a blueshift of the bandgap center than the conventional Lieb lattice, which is more suitable for optical communication applications. The main reason for the phenomenon is the change of dielectric contrast. To find the widest bandgaps, the filling factors of Lieb lattice and Lieb Moire lattice are further scanned, and the bandgap maps are obtained. The numerical simulation results show that the bandgap firstly increases and then decreases with the increasing filling factor, and the bandgap of Lieb Moire lattice is wider. At the same time, the photonic flat band properties are also observed. Three bands with very small gradients are observed in the band structure of Moire lattice, which are the 15th, 22nd and 27th bands. In order to indicate the characteristics of flat bands, the flatness is defined as F. Through calculation, the 22th band has the minimum F, meaning it has the highest flatness. By changing the size of the dielectric cylinders, the flatness of the flat band can be higher. The flat band can lead to localization of field near lattice. By calculating the intensity of electric field distribution at the Γ and K points in the 22th band with the highest flatness, it can be seen that the electric energies are obviously located tightly to the central rings of cylinders , which verifies the effective flatness of photon band. The flat band with higher flatness can lead to stronger localization of electric field, which has a wide application prospect in nonlinear optics, photoelectric energy conversion devices and so on. Changing the structural parameters and dielectric parameters of Lieb Moire lattice can further increase the width of bandgap. In order to obtain the optimized bandgap width, the materials are changed. The band characteristics of composite Moire Lieb lattice formed by the superposition of sublattices of different dielectric materials are also studied based on plane wave method. The dielectric material of the unrotated sublattice labelled as "A" was selected as GaAs, and the dielectric material of rotated sublattice labled as "B" was selected as SiO_2, and the superposition points of two sublattices were selected as GaAs. The dielectric cylinders are all embedded in air. It is proved that the composite Lieb Moire photonic lattice has a wider bandgap, which is mainly due to the reduced symmetry caused by the two kinds of materials. Then the radius relationship of the two sublattices is simply set as $r_2 = 0.5r_1$, and r_2 changes synchronously with r_1. The main bandgap width of the composite Lieb Moire photonic lattice is further increased, which can be attributed to the decrease in the overall lattice symmetry caused by the change of the radius. The Moire configuration based on Lieb lattice proposed in this paper provides a new method to improve the bandgap of photonic lattice, it provides a meaningful platform for studying the physical phenomena of flat band.

Key words：Photonic crystal；Photonic Moire lattice；Plane wave method；Bandgap；Localization of electric energy field

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