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Nonclassical Plane-crystallographic Groups and Their Applications II

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Abstract: Nonclassical periodic lattices are classified and enumerated via the nonclassical crystallographic groups (NCGs). Some of the nonclassical periodic lattices might be used to construct larger unit cells to explain the structures of so-called quasicrystals or other nonclassical crystalline substances.

Key words: nonclassical periodic lattices, nonclassical crystallographic groups, quasicrystals

Modern theory of ordinary solid matter is founded on the science of the classical crystallographic groups (CCGs), which is concerned with the enumeration and classification of the actual structures of various crystalline substances.[1] Mathematically, the CCGs delineate the crystal lattices (classical periodic lattices), and a lattice site (lattice point) may be associated with one atom or a group of atoms in a real corresponding crystal. In this paper, the nonclassical crystallographic groups (NCGs)[2] are used to classify some noncrystallographic periodic lattices with locally 5-, 8-, 10-, 12- and 14-fold symmetries.

1 Simple Nonclassical Periodic Lattices

In this section, the NCGs are used to classify and describe some simple nonclassical periodic lattices. They can construct complex periodic lattices to delineate nonclassical crystallographic structures which might appear in the real world.

(1) Group $G(2\pi/5, \beta, d_1, d_2)$. The lattices shown in Figs. 1(a) and 1(b) have locally 5-fold symmetry. The two lattices can be generated by the same NCG. In fact, the translations $T_{1\beta} = T_{12\pi/5} = (2a\cos(\pi/5), 0)$, $T_{2\beta} = T_{22\pi/5} = (2a\cos(\pi/5)\cos(2\pi/5), 2a\cos(\pi/5)\sin(2\pi/5))$; the rotation $R_\alpha = R_{2\pi/5}$ and the two generating sets $\{O, P\} = \{(0,0), (b\cos(\pi/5), b\sin(\pi/5))\}$ and $\{O, P\} = \{(0,0), (b, 0)\}$, where $b = a(\sqrt{5} - 1)/2$. Therefore the corresponding NCG is $G(2\pi/5, 2\pi/5, 2a\cos(\pi/5), 2a\cos(\pi/5))$; the corresponding NCLs can be denoted by

$L(2\pi/5, 2\pi/5, 2a\cos(\pi/5), 2a\cos(\pi/5))$; $(0, 0)$ $(b\cos(\pi/5), b\sin(\pi/5), \pi/5)$, $L(2\pi/5, 2\pi/5, 2a\cos(\pi/5), 2a\cos(\pi/5))$; $(0, 0)$, $(b, 0)$, $0)$.

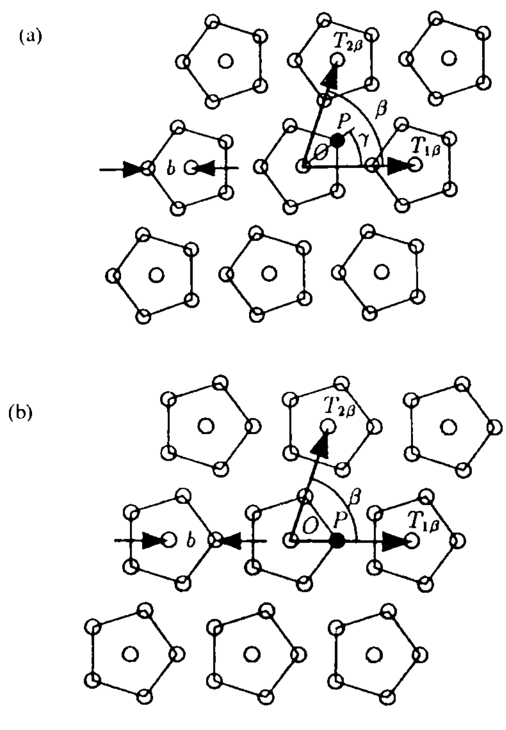

Fig. 1 Periodic lattice with locally 5-fold symmetry
(a) where $P = (b\cos(\pi/5), b\sin(\pi/5))$
(b) where $P = (b, 0)$

(2) Group $G(2\pi/8, \beta, d_1, d_2)$. From Figs. 2(a), 2(b), we can see two lattices with locally 8-fold symmetry. The same translations $T_{1\beta} = T_{1\pi/2} = (2a\cos(\pi/8), 0)$, $T_{2\beta} = T_{2\pi/2} = (0, 2a\cos(\pi/8))$, and rotation $R_\alpha = R_{2\pi/8}$ generate these lattices. The two generating sets are $\{O, P\} = \{(0,0), (a\cos(\pi/8), a\sin(\pi/8))\}$, $\{O, P\} = \{(0, 0), (b, 0)\}$, where $b = \sqrt{((2 - \sqrt{2})/2)}$.

Consequently, the corresponding NCG is $G(2\pi/8, \pi/2, 2a\cos(\pi/8), 2a\cos(\pi/8))$ and the corresponding NCLs are expressed by

$L(2\pi/8, \pi/2, 2a\cos(\pi/8), 2a\cos(\pi/8); (0, 0), (a\cos(\pi/8), (a\sin(\pi/8)), \pi/8)$, $L(2\pi/8, \pi/2, 2a\cos(\pi/8), 2a\cos(\pi/8); (0,0), (b,0), 0)$.

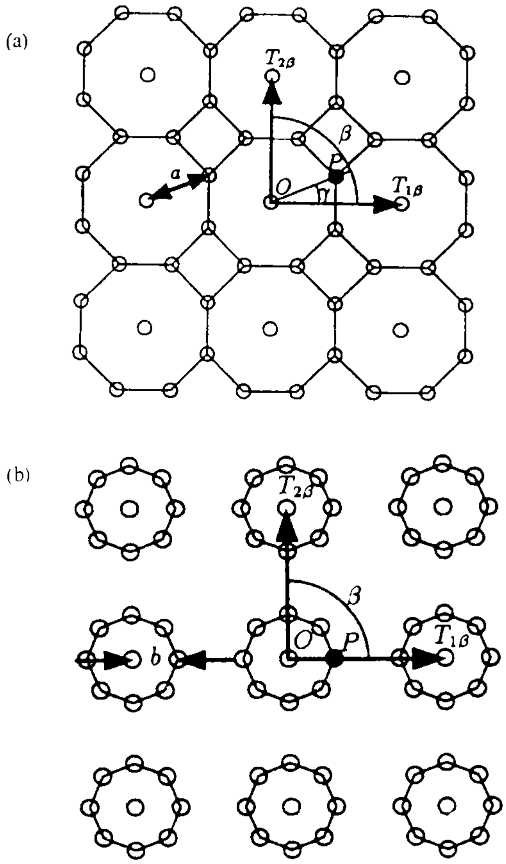

Fig.2 Periodic lattices with locally 8-fold symmetry
(a) $P=(a\cos(\pi/8), a\sin(\pi/8))$; (b) $P=(b,0)$

(3) Group $G(2\pi/10, \beta, d_1, d_2)$. The lattices shown in Figs. 3 and 4 have locally 10-fold symmetry.

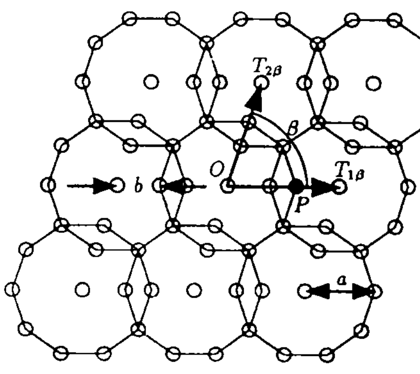

Fig.3 A periodic lattice with locally 10-fold symmetry where $P=(a,0)$

The lattices are also generated by the same NCG. The corresponding translations and rotation are $T_{1\beta} = T_{12\pi/5} = (2a\cos(\pi/5), 0)$, $T_{2\beta} = T_{22\pi/5} = (2a\cos(\pi/5)\cos(2\pi/5), 2a\cos(\pi/5)\sin(2\pi/5))$, and $R_\alpha = R_{2\pi/10}$. The three generating sets are $\{O, P\}=\{(0, 0), (a, 0)\}$, $\{O, P\}=\{(0, 0)\ (b, 0)\}$ and $\{O, P\}=\{(0, 0), (c\cos(\pi/10), c\sin(\pi/10))\}$, where $b=a(\sqrt{5}-1)/2$ and $c=a\sqrt{(5-2\sqrt{5})/5}$. Therefore the corresponding NCG is $G(2\pi/10, 2\pi/5, 2a\cos(\pi/5), 2a\cos(\pi/5))$. These lattices respectively belong to

$L(2\pi/10, 2\pi/5, 2a\cos(\pi/5), 2a\cos(\pi/5); (0,0), (a,0), 0)$,
$L(2\pi/10, 2\pi/5, 2a\cos(\pi/5), 2a\cos(\pi/5); (0,0), (b,0), 0)$,
$L(2\pi/10, 2\pi/5, 2a\cos(\pi/5), 2a\cos(\pi/5; (0,0), (c\cos(\pi/10), c\sin(\pi/10)), \pi/10)$.

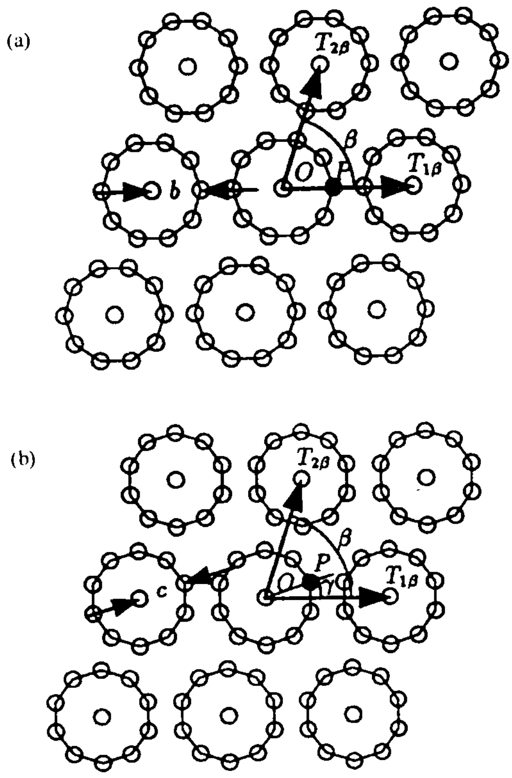

Fig.4 Periodic lattices with locally 10-fold symmetry
(a) $P=(b,0)$; (b) $P=(a\cos(\pi/10), c\sin(\pi/10))$

(4) Group $G(2\pi/12, \beta, d_1, d_2)$. In Figs. 5(a) and 5(b), the lattices have locally 12-fold symmetry which also correspond to the same NCG. The translations $T_{1\beta} = T_{1\pi/3} = (2a\cos(\pi/12), 0)$, $T_{2\beta} = T_{2\pi/3} = (2a\cos(\pi/12)\cos(\pi/3), 2a\cos(\pi/12)\sin(\pi/3))$, and the rotation $R_\alpha = R_{2\pi/12}$. The two generating sets are $\{O, P\}=\{(0,0), (a\cos(\pi/12), a\sin(\pi/12))\}$ and $\{O, P\}=\{(0, 0), (b, 0)\}$ where $b=2a\sin(\pi/12)$. Therefore the corresponding NCG is $G(2\pi/12, \pi/3, 2a\cos(\pi/12), 2a\cos(\pi/12))$; and the corresponding NCLs can be denoted by

$L(2\pi/12,\ \pi/3,\ 2a\cos(\pi/12),\ 2a\cos(\pi/12);\ (0,\ 0),\ (a\cos(\pi/12),\ a\sin(\pi/12)),\ \pi/12)$, $L(2\pi/12,\ \pi/3,\ 2a\cos(\pi/12),\ 2a\cos(\pi/12);\ (0,\ 0),\ (b,\ 0),\ 0)$.

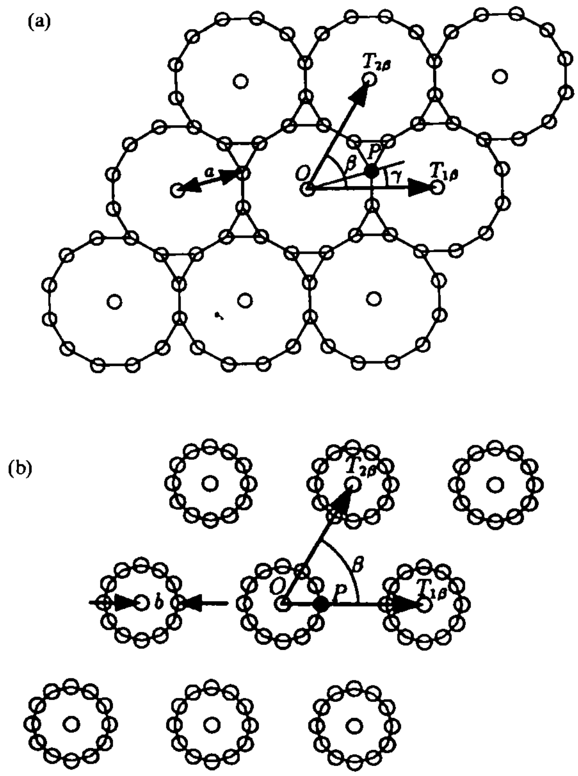

Fig.5 Periodic lattices with locally 12-fold symmetry
(a) $P=(a\cos(\pi/12),\ a\sin(\pi/12))$; (b) $P=(b,0)$

(5) Group $G(2\pi/14,\ \beta,\ d_1,\ d_2)$. From Figs.1 in Ref.[2] and 6(a), we can see two lattices with locally 14-fold symmetry. The same translations $T_{1\beta}=T_{13\pi/7}=(2a\cos(\pi/14),0)$, $T_{2\beta}=T_{23\pi/7}=(2a\cos(\pi/14)\cos(3\pi/7),\ 2a\cos(\pi/14)\sin(3\pi/7))$, and rotation $R_\alpha=R_{2\pi/14}$ generate them. The two generating sets are $\{O,\ P\}=\{(0,0),\ (a\cos(\pi/14),\ a\sin(\pi/14))\}$, and $\{O,\ P\}=\{(0,0),\ (b,0)\}$ where $b=a\sin(\pi/14)/\sin(\pi/7)$. The corresponding NCG and NCLs can be expressed via

$G(2\pi/14,\ 3\pi/7,\ 2a\cos(\pi/14),\ 2a\cos(\pi/14))$ and
$L(2\pi/14,\ 3\pi/7,\ 2a\cos(\pi/14),\ 2a\cos(\pi/14);\ (0,0),\ (a\cos(\pi/14),\ a\sin(\pi/14)),\ \pi/14)$,
$L(2\pi/14,3\pi/7,2a\cos(\pi/14),2a\cos(\pi/14);(0,0),(b,0),0)$.

2 Complex Nonclassical Periodic Lattices

Now we can use the direct sum of NCLs[2] to describe more complex nonclassical periodic lattices. First we introduce the following definitions.

Definition 1 For $n=1,\ 2,\ \cdots,\ m$, let $G_n(a_n,\ \beta_n,\ d_{1n},\ d_{2n})$, be NCL's. Then $G_1\oplus G_2\oplus\cdots\oplus G_m$ or

$$\prod_{n=1}^{m} G_n=\prod_{n=1}^{m} G_n(a_n,\beta_n,d_{1n},d_{2n}) \tag{1}$$

is called the direct sum of the NCG G_n's or a direct sum group. Every element in $\prod_{n=1}^{m} G_n$ has a form $(R_1,T)\oplus(R_2,T_2)\oplus\cdots\oplus(R_m,T_m)$ where $(R_n,T_n)\in G_n,\ 1\le n\le m$.

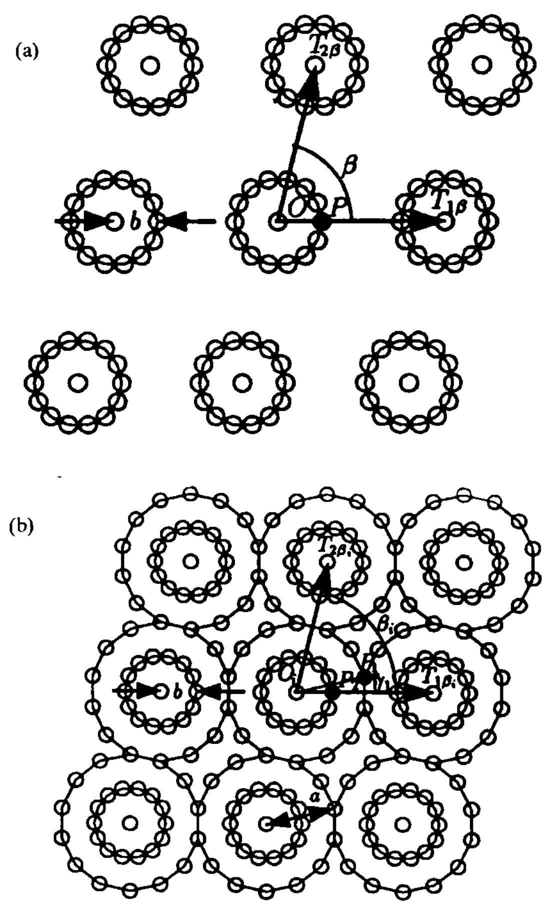

Fig.6 Periodic lattices with locally 14-fold symmetry
(a) $P=(b,0)$
(b) $P=(a\cos(\pi/14),\ a\sin(\pi/14))$, $P_2=(b,0)$, $\gamma_1=\pi/14$, $\gamma_2=0$

(1) Direct sum group $G(2\pi/14,\ 3\pi/7,\ d_{11},\ d_{21})\oplus G(2\pi/14,\ 3\pi/7,\ d_{12},\ d_{22})$. The lattice shown in Fig. 6(b), in fact, consists of Figs.1 in Ref.[2] and 6(a). Hence the corresponding direct sum group is $G(2\pi/14,\ 3\pi/7,\ d_{11},\ d_{21})\oplus G(2\pi/14,\ 3\pi/7,\ d_{12},\ d_{22})$ where $d_{ij}=2a\cos(\pi/14)$. This lattice can be expressed by

$L(2\pi/14,\ 3\pi/7,\ 2a\cos(\pi/14),\ 2a\cos(\pi/14);$
$(0,\ 0),\ (a\cos(\pi/14),\ a\sin(\pi/14),\ \pi/14)\oplus$

$L(2\pi/14,\ 3\pi/7,\ 2a\cos(\pi/14),\ 2a\cos(\pi/14);\ (0,0),\ (b,\ 0),\ 0)$.

(2) Direct sum group $G(2\pi/8,\ \pi/2,\ d_{11},\ d_{21}) \oplus G(2\pi/8,\ \pi/2,\ d_{12},\ d_{22})$. The lattice with locally 8-fold symmetry shown in Fig. 7(a) is in fact the combination of the lattices given in Figs. 2(a) and 2(b). Therefore, for $i = 1, 2$, $\alpha = 2\pi/8$, $\beta_i = \pi/2$, $T_{1\beta i} = T_{1\beta} = (2a\cos(\pi/8), 0)$, $T_{2\beta i} = T_{2\beta} = (0,\ 2a\cos(\pi/8))$, $d_{1i} = d_{2i} = 2a\cos(\pi/8)$, $O_i = O = (0,0)$. $P_1 = (a\cos(\pi/8),\ a\sin(\pi/8))$, $\gamma_1 = \pi/8$. $P_2 = (b,\ 0)$, $\gamma_2 = 0$. The corresponding direct sum group is $G(2\pi/8,\ \pi/2,\ d_{11}, d_{21}) \oplus G(2\pi/8,\ \pi/2, d_{11}, d_{21})$;and the corresponding direct sum lattice is given by

$$L(2\pi/8, \pi/2,\ d_{11},\ d_{21};\ O_1,\ (a\cos(\pi/8),\ a\sin(\pi/8)), \pi/8) \oplus L(2\pi/8,\ \pi/2,\ d_{11},\ d_{21};\ O_2,\ (b,\ 0),\ 0).$$

(3) Direct sum group $G(2\pi/10,\ \beta,\ d_{21},\ d_{22}) \oplus G(2\pi/10,\ \beta,\ d_{11},\ d_{22})$. From Fig. 7(b), we can see that the lattice with locally 10-fold symmetry is generated by the lattices given in Figs. 3 and 4(a).

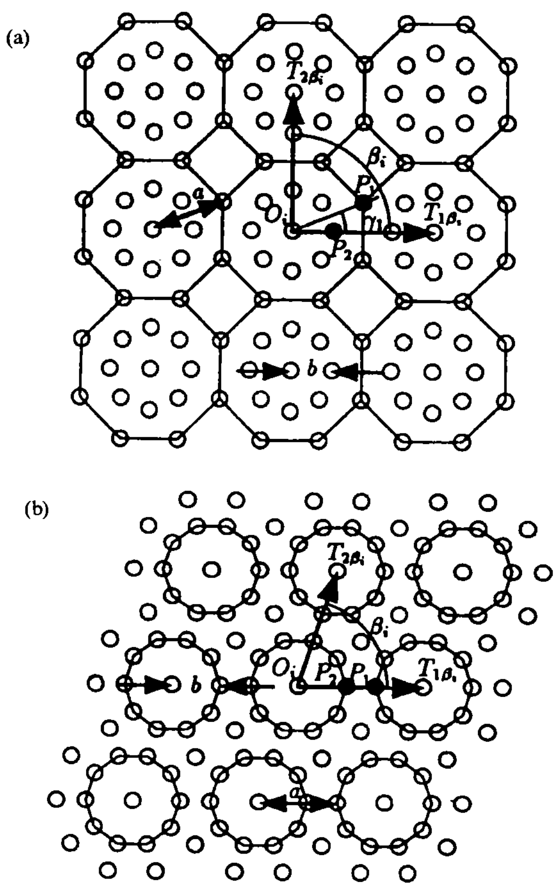

Fig.7 Direct sum lattice with locally 8-, 10-fold symmetry
(a) $P_1 = (a\cos(\pi/8),\ a\sin(\pi/8))$, $\gamma_1 = \pi/8$; $P_2 = (b,\ 0)$, $\gamma_2 = 0$.
(b) $P_1 = (a,\ 0)$, $\gamma_1 = 0$, $P_2 = (b,\ 0)$, $\gamma_2 = 0$ (10-fold)

Consequently, for $i = 1, 2$, $\alpha = 2\pi/10$, $\beta_i = 2\pi/5$, $T_{1\beta i} = T_{1\beta} = (2a\cos(\pi/5), 0)$, $T_{2\beta i} = T_{2\beta} = (2a\cos(\pi/5)\cos(2\pi/5),\ 2a\cos(\pi/5)\sin(2\pi/5))$, $d_{1i} = d_{2i} = 2a\cos(\pi/5)$, $O_i = O = (0,\ 0)$. $P_1 = (a,\ 0)$, $\gamma_1 = 0$. $P_2 = (b,\ 0)$, $\gamma_2 = 0$. $G(2\pi/10,\ 2\pi/5,\ d_{11},\ d_{21}) \oplus G(2\pi/10,\ 2\pi/5,\ d_{11},\ d_{21})$ is the corresponding direct sum group; and the direct sum lattice is expressed via

$$L(2\pi/10,\ 2\pi/5,\ d_{11},\ d_{21};\ O_1,\ (a,\ 0),\ 0), \oplus L(2\pi/10,\ 2\pi/5,\ d_{11},\ d_{21};\ O_2,\ (b,\ 0),\ 0).$$

(4) Direct sum group $G(2\pi/12,\ \beta,\ d_{11},\ d_{21}) \oplus G(2\pi/12,\ \beta,\ d_{12},\ d_{22})$. The lattice in Fig.8 (Also see Ref. [3]) is generated by the lattices shown in Figs. 5(a) and 5(b). The corresponding direct sum group is $G(2\pi/12,\ \pi/3,\ d_{11},\ d_{21}) \oplus G(2\pi/12,\ \pi/3,\ d_{11},\ d_{21})$ where $d_{11} = d_{21} = 2a\cos(\pi/12)$. The lattice belongs to class $L(2\pi/12,\ \pi/3,\ d_{11},\ d_{21};\ O_1,\ (a\cos(\pi/12),\ a\sin(\pi/12)),\ \pi/12) \oplus L(2\pi/12,\ \pi/3,\ d_{11},\ d_{21};\ O_2,\ (b,\ 0), 0)$.

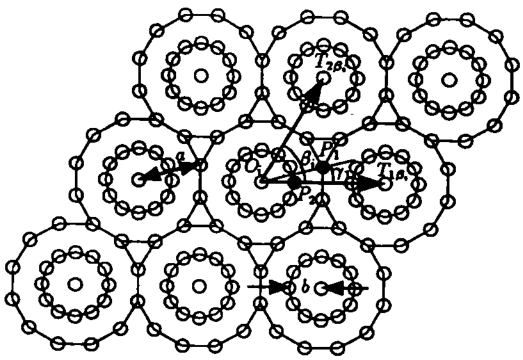

Fig.8 Direct sum lattice with locally 12-fold symmetry
$P_1 = (a\cos(\pi/12),\ a\sin(\pi/12))$, $\gamma_1 = \pi/12$, $P_2 = (b,\ 0)$, $\gamma_2 = 0$

Definition 2 $L(0,\ \beta,\ d_1,\ d_2,\ \phi,\ P,\ 0)$ denotes a parallelogram lattice generated via translations $T_{1\beta}$ and $T_{2\beta}$ acting on a point P. And the corresponding NCG is represented by $G(0,\ \beta,\ d_1,\ d_2)$.

More complex direct sum lattices.

(1) The direct sum lattice (Fig.7(a)) with a rectangular lattice generates a new direct sum lattice shown in Fig. 9(a). It can be denoted by (where $d_{1i} = d_{2i} = 2a\cos(\pi/8)$ and $O_i = (0,\ 0)$). $L(2\pi/8,\ \pi/2,\ d_{11},\ d_{21};\ O_1,\ (a\cos(\pi/8),\ a\sin(\pi/8)),\ \pi/8) \oplus L(2\pi/8,\ \pi/2,\ d_{12},\ d_{22};\ O_2,\ (b,\ 0),\ 0) \oplus L(0,\ \pi/2,\ d_{13},\ d_{23};\ \phi,\ (a\cos(\pi/8),\ a\cos(\pi/8)),\ 0)$.

(2) The lattice in Fig.4(b) and the direct sum lattice shown in Fig. 7(b) generate a new direct sum lattice (Fig.9(b)). This lattice belongs to the class (where $d_{11} = d_{21} = 2a\cos(\pi/5)$). $L(2\pi/10,\ 2\pi/5,\ d_{11},\ d_{21};\ (0,\ 0),\ (a,\ 0),\ 0) \oplus L(2\pi/10,\ 2\pi/5,\ d_{11},\ d_{21};\ (0,\ 0),\ (b,\ 0),\ 0) \oplus L(2\pi/10,\ 2\pi/5,\ d_{11},\ d_{21};\ (0,\ 0),\ (c\cos(\pi/10),\ c\sin(\pi/10)),\ \pi/10)$.

In conclusion, direct sum groups and direct sum lattices can describe and classify some nonclassical periodic lattices, in particular for those which have locally n-fold rotational symmetries.

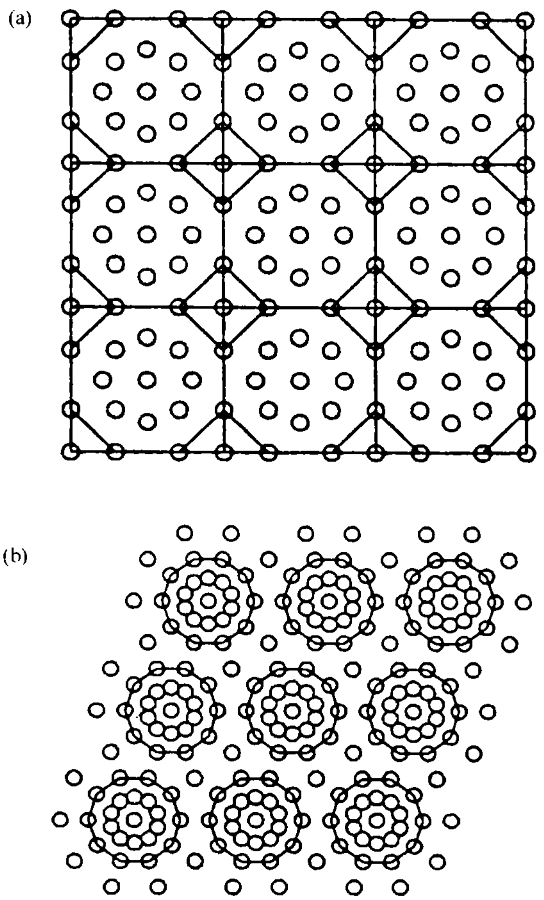

Fig.9 (a) Direct sum lattice with locally 8-fold symmetry; (b) Direct sum lattice with locally 10-fold symmetry

3 Discussion and Summary

A classical crystallographic G is generated via given translation mappings $T_{1\beta}$, $T_{2\beta}$ and a given rotation mapping R_α where $\alpha = 2\pi/n$ and n can only be equal to 2, 3, 4, and 6. However a nonclassical crystallographic group $G = G_1 \times G_2$ is a product group of $G_1$and G_2 where G_2 is a translation group G_1 is a rotation group generated via a rotation mapping R_α where $\alpha = 2\pi/n$ and n is any given positive number.

In a classical crystallographic lattice generated by a classical crystallographic group G, all lattice points are equivalent to each other and every lattice point is an n-fold center of rotation. Consequently, such a lattice point set can be produced by all group elements in G acting with the center O of the rotation, respectively. The lattice is unchanged under the action of the group elements. But in a nonclassical crystallographic lattice case, we need a generating set $Z = \{O, P\}$ consisting of an n-fold center O of the rotation and a point P which is not equivalent to point O. A nonclassical crystallographic lattice set is defined by all product group elements in G acting on the elements in the generating set Z, respectively. Lattices points in a simple nonclassical crystallographic lattice set are distinguished into two equivalent classes. One of them consists of n-fold center and quasicenters of the rotation. Many nonclassicalperiodic lattices can be described via direct sum of NCLs.

In a classical crystallographic lattice, the position of a lattice point is hardly expressed by the corresponding group elements. Whereas in a nonclassical crystallographic lattice, the positions of every lattice point can be clearly described via the "group element". In fact a lattice point has form $(R_\alpha^i, T_{2\beta}^k * T_{1\beta}^j)P$ or form $(R_\alpha^i, T_{2\beta}^k * T_{1\beta}^j)O$ where i, j, and k are integers.

Furthermore NCGs can describe infinite kinds of nonclassical periodic lattices. It might be expected that NCGs would provide a hopeful tool in studies of nonclassical periodic structures.

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