1 Introduction

lat file generates the lattice structure of a given systems. A lattice is constructed by three parameters: 1). lattice constant 2). primitive lattice vectors 3). sublattice vectors. Any lattice site is specified by four index $[n_1, n_2, n_3, s]$ which follows the rules: $\mathbf{r}_s^{n_1,n_2,n_3} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 + \mathbf{d}_s$, where $[n_1, n_2, n_3]$ are integers which specifies the unitcell and d_s specifies the sublattice vectors. If there are N sublattices in a unitcell, then s ranges from 1 to N. In this task, users have to input all necessary parameters and PiLab will search for the nearest neighbor sites of a sublattice in the $[n_1 = 0, n_2 = 0, n_3 = 0]$ unitcell up to n-th order.

2 Dictionary

2.1 Input

lat.Const This parameter sets the lattice constant of the system. The values of lat.Primitive and lat.Sublattice will automatically multiply this parameter during the calculation.

lat.Primitive This parameter sets the primitive lattice vectors. This parameter multiply lat.Const defines the $[\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]$ vectors. Each lattice vector is represented by a row vector x, y, z and different vectors are separated by a semicolon ";" as shown in Fig.1. If the system is two or one dimension, each row vector can be given by two or one dimension only. For example, the primitive lattice vector of a 2D graphene can be: $[-3/2, sqrt(3)/2; 3/2, sqrt(3)/2]$ ("sqrt" is the keyword of square root in Scilab). For 1D dimer chain, it can be [1]

lat.Sublatt This parameter sets the sublattice vectors. This parameter multiply lat.Const defines the $\mathbf{d}_s$ vectors. Also, different vectors are separated by semicolons ";".

lat.Order This parameter sets the order of neareat neighbor. For example, lat.Order=[2] means PiLab will search first and second order of nearest neighbor sites of each sublattice located in the $[n_1 = 0, n_2 = 0, n_3 = 0]$ unitcell.

2.2 Output

lat.recip_vec This variable gives you the reciprocal lattice vectors, $\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{a}_3}{\mathbf{a}_1\cdot(\mathbf{a}_2\times\mathbf{a}_3)}$, $\mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3\times\mathbf{a}_1}{\mathbf{a}_2\cdot(\mathbf{a}_3\times\mathbf{a}_1)}$, $\mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1\times\mathbf{a}_2}{\mathbf{a}_3\cdot(\mathbf{a}_1\times\mathbf{a}_2)}$. In Fig.3, PiLab gives you a 3x3 matrix. Each row vectors corresponds to a reciprocal lattice vector.

lat.surr_site(n) This variable gives you the surrounding neighbor sites of the n-th sublattice. For example, lat.surr_site(1) gives you the surrounding neighbor sites of sublattice 1 defined by the first row vector in lat.Sublatt. There are nine values of each row vector whose meaning is [order, distance, sublattice index, n_1, n_2, n_3, x, y, z]. The sublattice itself will always listed in the first row, so the order is always 0 and distance is always 0 too. Therefore, in Fig.1, the third row vector of lat.surr_site(1) means there is a first order neighbor site around sublattice 1. The distance between them is 0.5 and this neighbor site belongs to sublattice 2. It is located in the $[n_1 = -1, n_2 = 0, n_3 = -1]$ unitcell and its coordinate is [0,-0.5,0]. One should check this variable carefully to make sure the lattice structure is generated correctly. If not, you might pick wrong primitive lattice vectors or sublattice vectors.

```
lat.Const=[1]                    // lattice constant, 1x1 real
lat.Primitive=...                // Primitive vectors, (3x3/2x2/1x1)
[1/2,1/2,0;1/2,0,1/2;0,1/2,1/2]
lat.Sublatt=[0,0,0;1/2,1/2,1/2]  // sublattice position, (nx3/nx2/nx1/)
lat.Order=[1]                    // Nearest Neighbor Order, 1x1 integer

============= PiLib Variable =============
lat.recip_vec, @full, the reciprocal lattice vectors
ORDER=    0, SIZE=[    3,    3], TYPE=REAL

        1         2         3

   6.283185   6.283185  -6.283185
   6.283185  -6.283185   6.283185
  -6.283185   6.283185   6.283185

============= PiLib Variable =============
lat.surr_site(1),  @full, surrouding sites [order, dist, sublatt, n1, n2, n3, x, y, z]
ORDER=    0, SIZE=[    7,    9], TYPE=REAL

        1         2         3         4         5         6         7         8         9

   0.000000  0.000000  1.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   1.000000  0.500000  2.000000 -1.000000 -1.000000  0.000000 -0.500000  0.000000  0.000000
   1.000000  0.500000  2.000000 -1.000000  0.000000 -1.000000  0.000000 -0.500000  0.000000
   1.000000  0.500000  2.000000 -1.000000  0.000000  0.000000  0.000000  0.000000  0.500000
   1.000000  0.500000  2.000000  0.000000 -1.000000 -1.000000  0.000000  0.000000 -0.500000
   1.000000  0.500000  2.000000  0.000000 -1.000000  0.000000  0.000000  0.500000  0.000000
   1.000000  0.500000  2.000000  0.000000  0.000000 -1.000000  0.500000  0.000000  0.000000

============= PiLib Variable =============
lat.surr_site(2), @full, surrouding sites [order, dist, sublatt, n1, n2, n3, x, y, z]
ORDER=    0, SIZE=[    7,    9], TYPE=REAL

        1         2         3         4         5         6         7         8         9

   0.000000  0.000000  2.000000  0.000000  0.000000  0.000000  0.500000  0.500000  0.500000
   1.000000  0.500000  1.000000  0.000000  0.000000  1.000000  0.000000  0.500000  0.500000
   1.000000  0.500000  1.000000  0.000000  1.000000  0.000000  0.500000  0.000000  0.500000
   1.000000  0.500000  1.000000  0.000000  1.000000  1.000000  0.500000  0.500000  1.000000
   1.000000  0.500000  1.000000  1.000000  0.000000  0.000000  0.500000  0.500000  0.000000
   1.000000  0.500000  1.000000  1.000000  0.000000  1.000000  0.500000  1.000000  0.500000
   1.000000  0.500000  1.000000  1.000000  1.000000  0.000000  1.000000  0.500000  0.500000
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Figure 1: NiO_lat.plb