Silicon (111)

The fragmentation of Silicon (111) is carried out using a unit cell defined by the lattice vectors (Å):

```
a (xyz) = -5.4  0.   0.
b (xyz) =  5.4  5.4  0.
c (xyz) =  5.4  0.  -5.4
```

There are eight atoms in the unit cell with coordinates (fractional coordinates, followed by
Cartesian coordinates in Å):

```
1 Si
   1.000        1.000        1.000
   5.420       -5.420       -5.420
2 Si
   1.000       0.5000       0.5000
  0.0000       -2.710       -2.710
3 Si
   1.000       0.5000        1.000
   2.710       -2.710       -5.420
4 Si
   1.000        1.000       0.5000
   2.710       -5.420       -2.710
5 Si
  0.7500       0.7500       0.7500
   4.065       -4.065       -4.065
6 Si
  0.7500       0.2500       0.2500
  -1.355       -1.355       -1.355
7 Si
  0.7500       0.2500       0.7500
   1.355       -1.355       -4.065
8 Si
  0.7500       0.7500       0.2500
   1.355       -4.065       -1.355
```

These atoms are depicted in Figure 2(b).

LEVEL 2

The bulk crystal structure fragments at Level 2 into 24 fragments. The $F(k_1,k_2,k_3)$ fragments of Eq.(2.10) contain the atoms shown below, where "Atom" designates the number of the atom in the unit cell defined above; the lattice unit cell is defined by adding (k_1,k_2,k_3) to the indicated values below. For the cleaved crystal, (k_1,k_2,k_3) are integers with

$-\infty < k_1 < -1,$

$-\infty < k_2 < \infty$

$-\infty < k_3 < \infty$

Bulk fragments

Fragment Number	f_n	Atom	k_1	k_2	k_3
1	1				
		1	−1	0	0
		5	−1	0	0
		8	−1	0	1
		7	−1	1	0
		6	0	1	1
2	1				
		2	−1	0	0
		6	−1	0	0
		7	−1	0	0
		8	−1	0	0
		5	0	0	0
3	1				
		1	−1	0	0
		3	−2	0	0
		2	−1	0	1
		4	−1	0	1
		8	−1	0	1
4	1				
		3	−1	0	0
		5	−1	0	0
		7	−1	0	0
		6	−1	0	1
		8	0	0	1
5	1				
		2	−1	0	0
		3	−1	0	0
		7	−1	0	0
		4	−2	−1	0
		1	−1	−1	0
6	1				
		4	−1	0	0
		5	−1	0	0
		8	−1	0	0
		6	−1	1	0
		7	0	1	0
7	1				
		1	−1	0	0
		3	−1	0	0
		4	−1	0	0

		5	−1	0	0
		2	−2	0	0
8	1				
		2	−1	0	0
		6	−1	0	0
		1	−2	−1	−1
		4	−1	−1	0
		3	−1	0	−1
9	−1				
		1	−1	0	0
		8	−1	0	1
10	−1				
		3	−1	0	0
		7	−1	0	0
11	−1				
		2	−1	0	0
		7	−1	0	0
12	−1				
		1	−1	0	0
		5	−1	0	0
13	−1				
		4	−1	0	0
		8	−1	0	0
14	−1				
		2	−1	0	0
		6	−1	0	0
15	−1				
		6	0	0	0
		1	−1	−1	−1
16	−1				
		7	−1	0	0
		1	−1	−1	0
17	−1				
		7	0	0	0
		4	−1	−1	0
18	−1				
		8	0	0	0
		3	−1	0	−1
19	−1				
		5	0	0	0

		2	-1	0	0
20	-1				
		6	-1	0	0
		3	-1	0	-1
21	-1				
		6	-1	0	0
		4	-1	-1	0
22	-1				
		2	-1	0	0
		8	-1	0	0
23	-1				
		3	-1	0	0
		5	-1	0	0
24	-1				
		4	-1	0	0
		5	-1	0	0

Surface fragments

There are 20 surface fragments $\{G(k_2,k_3)\}$ of Eq. (2.10) which contain the atoms shown below, where "Atom" designates the number of the atom in the unit cell defined above; the lattice unit cell is defined by adding (k_2,k_3) to the indicated values below. For the cleaved crystal, (k_1,k_2,k_3) are integers with

$-\infty < k_2 < \infty$

$-\infty < k_3 < \infty$

Fragment Number	g_n	Atom	k_1	k_2	k_3
1	1				
		1	-1	0	0
		5	-1	0	0
		8	-1	0	1
		7	-1	1	0
2	1				
		2	-1	0	0
		6	-1	0	0
		7	-1	0	0
		8	-1	0	0
3	1				
		1	-1	0	0
		3	-2	0	0
		2	-1	0	1

		4	−1	0	1
		8	−1	0	1
4	1				
		3	−1	0	0
		5	−1	0	0
		7	−1	0	0
		6	−1	0	1
5	1				
		2	−1	0	0
		3	−1	0	0
		7	−1	0	0
		4	−2	−1	0
		1	−1	−1	0
6	1				
		4	−1	0	0
		5	−1	0	0
		8	−1	0	0
		6	−1	1	0
7	1				
		1	−1	0	0
		3	−1	0	0
		4	−1	0	0
		5	−1	0	0
		2	−2	0	0
8	1				
		2	−1	0	0
		6	−1	0	0
		1	−2	−1	−1
		4	−1	−1	0
		3	−1	0	−1
9	−1				
		1	−1	0	0
		8	−1	0	1
10	−1				
		3	−1	0	0
		7	−1	0	0
11	−1				
		2	−1	0	0
		7	−1	0	0
12	−1				
		1	−1	0	0
		5	−1	0	0

13	-1				
		4	-1	0	0
		8	-1	0	0
14	-1				
		2	-1	0	0
		6	-1	0	0
15	-1				
		7	-1	0	0
		1	-1	-1	0
16	-1				
		6	-1	0	0
		3	-1	0	-1
17	-1				
		6	-1	0	0
		4	-1	-1	0
18	-1				
		2	-1	0	0
		8	-1	0	0
19	-1				
		3	-1	0	0
		5	-1	0	0
20	-1				
		4	-1	0	0
		5	-1	0	0

LEVEL 1

Similarly, at Level 1, we have:

Bulk fragments

Fragment Number	f_n	Atom	k_1	k_2	k_3
1	1				
		1	-1	0	0
		5	-1	0	0
2	1				
		2	-1	0	0
		6	-1	0	0
3	1				
		3	-1	0	0

		5	−1	0	0
4	1				
		4	−1	0	0
		5	−1	0	0
5	1				
		2	−1	0	0
		7	−1	0	0
6	1				
		2	−1	0	0
		8	−1	0	0
7	1				
		6	0	0	0
		1	−1	−1	−1
8	1				
		7	0	0	0
		4	−1	−1	0
9	1				
		8	0	0	0
		3	−1	0	−1
10	1				
		5	0	0	0
		2	−1	0	0
11	1				
		7	−1	0	0
		1	−1	−1	0
12	1				
		6	−1	0	0
		4	−1	−1	0
13	1				
		8	−1	0	0
		1	−1	0	−1
14	1				
		6	−1	0	0
		3	−1	0	−1
15	1				
		3	−1	0	0
		7	−1	0	0
16	1				
		4	−1	0	0

		8	-1	0	0
17	-3				
		5	0	0	0
18	-3				
		6	0	0	0
19	-3				
		2	-1	0	0
20	-3				
		3	-1	0	0
21	-3				
		7	0	0	0
22	-3				
		4	-1	0	0
23	-3				
		8	0	0	0
24	-3				
		1	-1	0	0

Surface fragments

There are 16 surface fragments at Level 1:

Fragment Number	g_n	Atom	k_1	k_2	k_3
1	-2				
		1	-1	-1	-1
2	-2				
		4	-1	-1	0
3	-2				
		3	-1	0	-1
4	-2				
		2	-1	0	0
5	1				
		1	-1	0	0
		5	-1	0	0
6	1				
		2	-1	0	0
		6	-1	0	0

```
 7            1
                      3     -1     0     0
                      5     -1     0     0

 8            1
                      4     -1     0     0
                      5     -1     0     0

 9            1
                      2     -1     0     0
                      7     -1     0     0

10            1
                      2     -1     0     0
                      8     -1     0     0

11            1
                      7     -1     0     0
                      1     -1    -1     0

12            1
                      6     -1     0     0
                      4     -1    -1     0

13            1
                      8     -1     0     0
                      1     -1     0    -1

14            1
                      6     -1     0     0
                      3     -1     0    -1

15            1
                      3     -1     0     0
                      7     -1     0     0

16            1
                      4     -1     0     0
                      8     -1     0     0
```

Silicon (100)

The fragmentation of Silicon (111) is carried out using a unit cell defined by the lattice vectors (Å):

```
a (xyz) = -5.4  0.   0.
b (xyz) =  0.   5.4  0.
c (xyz) =  0.   0.   5.4
```

There are eight atoms in the unit cell with coordinates (fractional coordinates, followed by Cartesian coordinates):

```
1 Si
   1.000        1.000        1.000
  -5.420        5.420        5.420
2 Si
   1.000       0.5000       0.5000
  -5.420        2.710        2.710
3 Si
  0.5000       0.5000        1.000
  -2.710        2.710        5.420
4 Si
  0.5000        1.000       0.5000
  -2.710        5.420        2.710
5 Si
  0.2500       0.2500       0.2500
  -1.355        1.355        1.355
6 Si
  0.2500       0.7500       0.7500
  -1.355        4.065        4.065
7 Si
  0.7500       0.7500       0.2500
  -4.065        4.065        1.355
8 Si
  0.7500       0.2500       0.7500
  -4.065        1.355        4.065
```

These atoms are depicted in Figure 2(a).

LEVEL 2

Bulk fragments

Fragment Number	f_n	Atom	k_1	k_2	k_3
1	1				
		1	-1	0	0
		7	-1	0	1
		8	-1	1	0
		6	0	0	0
		5	0	1	1
2	1				
		2	-1	0	0
		7	-1	0	0
		8	-1	0	0
		5	0	0	0
		6	0	0	0
3	1				
		1	-1	0	0

		4	−1	0	0
		2	−1	1	0
		3	−1	1	0
		8	−1	1	0
4	1				
		3	0	0	0
		6	0	0	0
		8	0	0	0
		5	0	0	1
		7	0	0	1
5	1				
		4	0	0	0
		6	0	0	0
		7	0	0	0
		5	0	1	0
		8	0	1	0
6	1				
		5	0	0	0
		1	−1	−1	−1
		2	−1	0	0
		4	0	−1	0
		3	0	0	−1
7	1				
		3	0	0	0
		4	0	0	0
		6	0	0	0
		1	−1	0	0
		2	−1	0	0
8	1				
		2	−1	0	0
		4	−1	0	0
		7	−1	0	0
		1	−1	0	−1
		3	−1	0	−1
9	−1				
		1	−1	0	0
		8	−1	1	0
10	−1				
		3	0	0	0
		8	0	0	0
11	−1				
		2	−1	0	0
		8	−1	0	0

```
12          -1
                    4       0     0     0
                    8       0     1     0

13          -1
                    3       0     0     0
                    6       0     0     0

14          -1
                    5       0     0     0
                    2      -1     0     0

15          -1
                    2      -1     0     0
                    7      -1     0     0

16          -1
                    5       0     0     0
                    1      -1    -1    -1

17          -1
                    6       0     0     0
                    1      -1     0     0

18          -1
                    5       0     0     0
                    4       0    -1     0

19          -1
                    7      -1     0     0
                    1      -1     0    -1

20          -1
                    5       0     0     0
                    3       0     0    -1

21          -1
                    3       0     0     0
                    7       0     0     1

22          -1
                    2      -1     0     0
                    6       0     0     0

23          -1
                    4       0     0     0
                    6       0     0     0

24          -1
                    4       0     0     0
                    7       0     0     0
```

There are 8 surface fragments:

Surface fragments

Fragment Number	g_n	Atom	k_1	k_2	k_3
1	1				
		1	-1	0	0
		7	-1	0	1
		8	-1	1	0
2	1				
		2	-1	0	0
		7	-1	0	0
		8	-1	0	0
3	1				
		1	-1	0	0
		4	-1	0	0
		2	-1	1	0
		3	-1	1	0
		8	-1	1	0
4	1				
		2	-1	0	0
		4	-1	0	0
		7	-1	0	0
		1	-1	0	-1
		3	-1	0	-1
5	-1				
		1	-1	0	0
		8	-1	1	0
6	-1				
		2	-1	0	0
		8	-1	0	0
7	-1				
		2	-1	0	0
		7	-1	0	0
8	-1				
		7	-1	0	0
		1	-1	0	-1

LEVEL 1

Bulk fragments

Fragment Number	f_n	Atom	k_1	k_2	k_3
1	1				
		1	-1	0	0
		7	-1	0	1
2	1				
		2	-1	0	0
		7	-1	0	0
3	1				
		3	0	0	0
		7	0	0	1
4	1				
		4	0	0	0
		7	0	0	0
5	1				
		5	0	0	0
		1	-1	-1	-1
6	1				
		3	0	0	0
		6	0	0	0
7	1				
		3	0	0	0
		8	0	0	0
8	1				
		6	0	0	0
		1	-1	0	0
9	1				
		6	0	0	0
		2	-1	0	0
10	1				
		8	-1	0	0
		1	-1	-1	0
11	1				
		8	0	0	0
		4	0	-1	0
12	1				
		3	0	0	0
		5	0	0	1

13	1				
		2	-1	0	0
		8	-1	0	0
14	1				
		4	0	0	0
		6	0	0	0
15	1				
		5	0	0	0
		2	-1	0	0
16	1				
		5	0	0	0
		4	0	-1	0
17	-3				
		7	0	0	0
18	-3				
		3	0	0	0
19	-3				
		8	0	0	0
20	-3				
		6	0	0	0
21	-3				
		5	0	0	0
22	-3				
		4	0	0	0
23	-3				
		1	-1	0	0
24	-3				
		2	-1	0	0

There are 6 surface fragments:

Surface fragments

Fragment Number	g_n	Atom	k_1	k_2	k_3
1	-1				
		1	-1	-1	-1
2	-1				

		2	−1	0	0
3	1				
		1	−1	0	0
		7	−1	0	1
4	1				
		2	−1	0	0
		7	−1	0	0
5	1				
		8	−1	0	0
		1	−1	−1	0
6	1				
		2	−1	0	0
		8	−1	0	0