

SrTiO₃(100)衬底

氧化物

SrTiO₃ substrate, lattice constant: $a = 3.905\text{\AA}$, mass density: $\rho = 5.122\text{g/cm}^3$,

Bragg formula:

$$2d \sin \theta = n\lambda$$

X-ray Cu K- α line, wave length: $\lambda = 1.5405952\text{\AA}$ (8.04 kV)

$$\theta = \sin^{-1} \frac{\lambda}{2d}$$

$$\frac{\pi}{180^\circ} = \frac{\Delta}{\theta}, \theta = \frac{180 \times \Delta}{\pi}$$

```
1.  #!/usr/bin/python
2.  import math
3.
4.  L = 1.5406
5.  d = 3.905
6.
7.  delta = math.asin (L/(2*d))
8.
9.  print ("Angle (100) direction in arc : ", delta)
10.
11.  theta = 180*delta/math.pi
12.
13.  print ("Theta : ", theta)
14.
15.  print ("2Theta : ", 2*theta)
16.
```

```
Angle (100) direction in arc :  0.1985621357086395
Theta :  11.37677234720894
2Theta :  22.75354469441788
```

Separation between Lattice Planes in a cubic Crystal, (h, k, l) direction

$$d_{h,k,l}^2 = \frac{a^2}{h^2 + k^2 + l^2}$$

$$d_{h,k,l} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Separation between (200) planes,

$$d = \frac{a}{2}$$

```
1. L = 1.5406
2. d = 3.905/2
3.
4. delta = math.asin (L/(2*d))
5.
6. print ("Angle (200) direction in arc : ", delta)
7.
8. theta = 180*delta/math.pi
9.
10. print ("Theta : ", theta)
11.
12. print ("2Theta : ", 2*theta)
```

```
Angle (200) direction in arc : 0.40554525434572886
Theta : 23.23603147556977
2Theta : 46.47206295113954
```

一般实验，对STO(100)取向的衬底，取(set)2Theta为46.48，Theta为23.24。

对比Materials project，SrTiO3 (ID: mp-5229), $a = 3.945\text{\AA}$

```
1. L = 1.5406
2. d = 3.945/2
3.
4. delta = math.asin (L/(2*d))
5.
6. print ("Angle (200) direction in arc : ", delta)
7.
8. theta = 180*delta/math.pi
```

```

9.
10. print ("Theta : ", theta)
11.
12. print ("2Theta : ", 2*theta)

```

```

Angle (200) direction in arc : 0.4011959920058513
Theta : 22.986837099499596
2Theta : 45.97367419899919

```

考虑STO(111)方向, $d_{111} = \frac{a}{\sqrt{3}}$

```

1. a = 3.945
2.
3. d = a/math.sqrt(3)
4.
5. print ("Separation between (111) planes:", d)
6. print ("\n\n")
7.
8. L = 1.5406
9.
10. delta = math.asin (L/(2*d))
11.
12. print ("Angle (111) direction in arc : ", delta)
13.
14. theta = 180*delta/math.pi
15.
16. print ("Theta : ", theta)
17.
18. print ("2Theta : ", 2*theta)

```

```

Separation between (111) planes: 2.2776468119530735

```

```

Angle (111) direction in arc : 0.34500345998334037
Theta : 19.76724217445599
2Theta : 39.53448434891198

```

考虑STO(110)取向, $d_{110} = \frac{a}{\sqrt{2}}$

```

1. a = 3.945
2.

```

```

3.  d = a/math.sqrt(2)
4.
5.  print ("Separation between (110) planes:", d)
6.  print ("\n\n")
7.
8.  L = 1.5406
9.
10. delta = math.asin (L/(2*d))
11.
12. print ("Angle (110) direction in arc : ", delta)
13.
14. theta = 180*delta/math.pi
15.
16. print ("Theta : ", theta)
17.
18. print ("2Theta : ", 2*theta)

```

Separation between (110) planes: 2.78953625178093

Angle (110) direction in arc : 0.2797746724169339
 Theta : 16.029907944145478
 2Theta : 32.059815888290956

EOF