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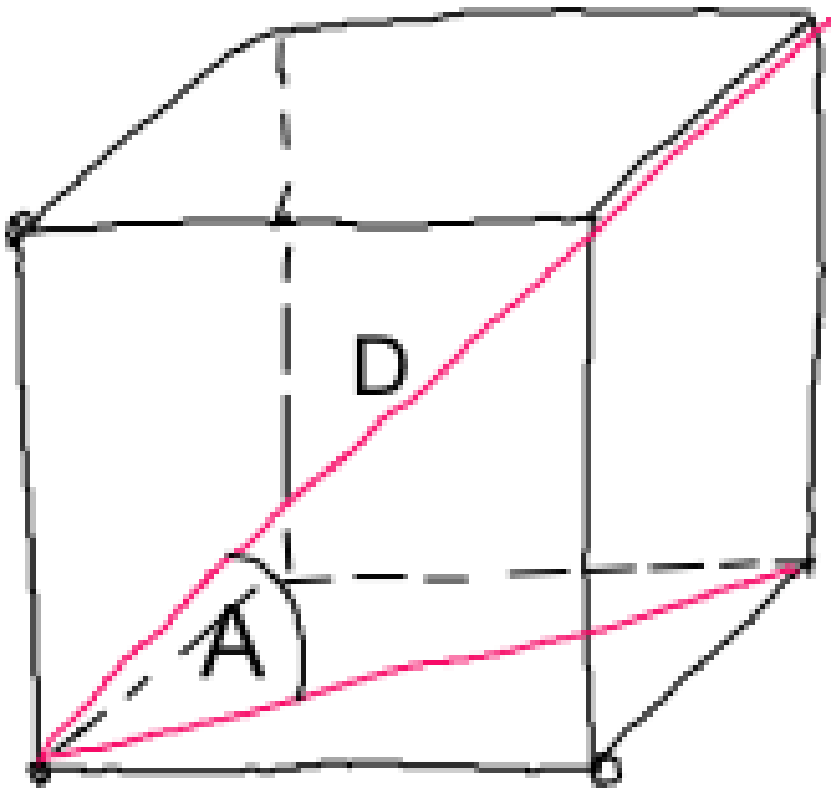
Contents

1 Compute the distance between the (111) planes of Ag.

Use the experimental lattice constant of Ag.

2 Angles and distances

Compute the length of the vector indicated by D, and the angle indicated by A. You can assume the unit cell is a cube with length of 3.6 nm on each side.



3 Coordinate system transformations

The unit cell of a material is given by:

4.2266540199664249	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.2266540199664249	0.0000000000000000
0.0000000000000000	0.0000000000000000	2.6888359272289208

The coordinates of the atoms in the unit cell are given in fractional coordinates as:

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.3067891334429594	0.3067891334429594	0.0000000000000000
0.6932108665570406	0.6932108665570406	0.0000000000000000
0.1932108665570406	0.8067891334429594	0.5000000000000000
0.8067891334429594	0.1932108665570406	0.5000000000000000

Compute the Cartesian coordinates of each atom.

4 Computing unit cell parameters

For the following unit cell (in rows), compute the length of each vector, and the angle between the vectors, e.g. the "a b c α β γ" representation.

```
3.817   -0.011  -0.243
-0.011  3.817   -0.243
-1.519  -1.519  4.986
```

5 Computing fractional coordinates

Given this unit cell (in rows)

```
3.817   -0.011  -0.243
-0.011  3.817   -0.243
-1.519  -1.519  4.986
```

And atoms at these cartesian coordinates:

```
[[ 1.23141,   0.239958,  3.102345]
 [ 1.05559,   2.047042,  1.397655]
 [-0.626458,  2.21009,   3.890655]
 [ 2.913458,  0.07691,   0.609345]
 [ 1.004314,  0.139186,  1.125   ]
 [ 1.282686,  2.147814,  3.375   ]]
```

Compute the fractional coordinates of each atom in the unit cell.