two-dimensional Example

In selecting our real space translation vectors, we began with the two-dimensional graphite lattice (Figure 1) and its unit cell, defined by the and lattice parameters. In this example, we chose the real space translation vectors and depicted in Figure 2. The crystal coordinates are also provided in Figure 2. For example, point (1,1) represents translating one unit in the x-direction of the unit cell and one unit in the y-direction of the unit cell.

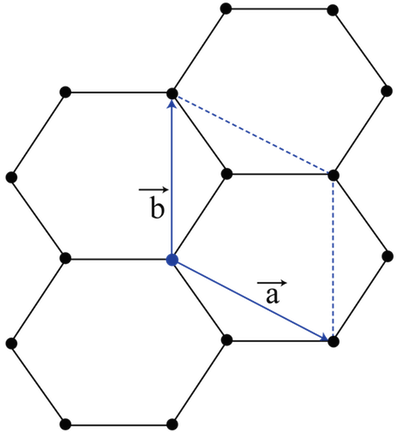


Figure 1. Two-dimensional representation of the graphite lattice with the hexagonal unit cell depicted in blue. The and lattice parameters define the unit cell. This image was prepared using Adobe Illustrator.

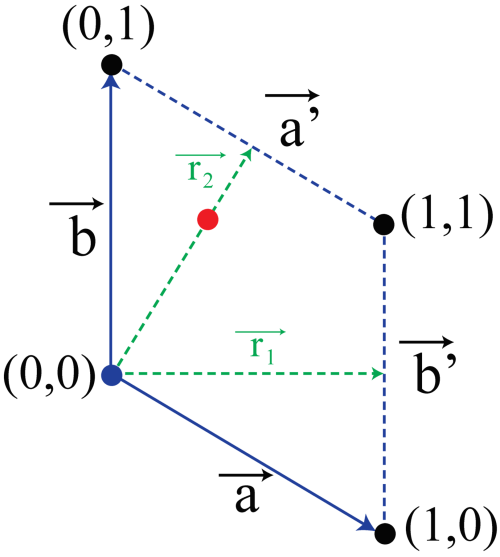


Figure 2. The hexagonal unit cell of graphite with the real space translation vectors and , which were selected for conversion to reciprocal space vectors. This image was prepared using Adobe Illustrator.

The coordinates, determined from the dimensions of a 30-60-90 right triangle (Figure 3), of the real space translation vectors are provided in Equation 1. There are many other real space translation vectors that could be selected, but those provided in Equation 1 were selected because of their similarity to the vectors used in Pisanty’s paper.

(1)

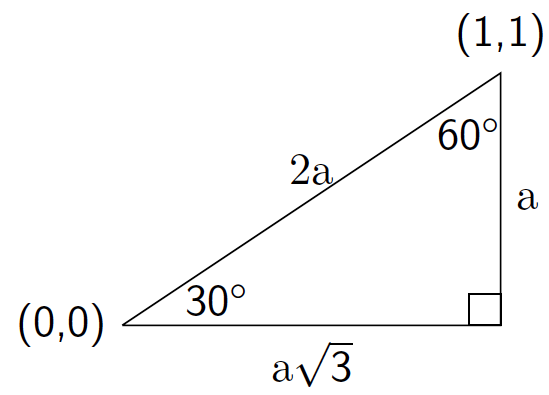


Figure 3. The conventional 30-60-90 right triangle with the corresponding crystal coordinates from the graphite unit cell included at the 30 and 60 degree angles. Visual inspection of the hexagonal unit cell of graphite indicates that it is composed of four 30-60-90 right triangles and these are utilized to determine the coordinates of the real space translation vectors and . This image was prepared using pstricks of LaTeX.

Upon selecting the and real space translation vectors, these were converted to reciprocal space vectors using the formulas provided in Equation 2 for a two-dimensional system,

(2)

where γ is a 90° clockwise rotational matrix (Equation 3) and superscript “*T* ” indicates the transpose of the matrix.

(3)

Next, we evaluated the **k**1 and **k**2 expressions from Equation 2. We first evaluated the denominator of **k**1 in Equation 2, which is shown in Equation 4.

(4)

Evaluating the product of the last two matrices in Equation 4 gives rise to Equation 5,

(5)

which is further simplified to Equation 6.

(6)

Finally, the product of the two matrices remaining in Equation 6 was evaluated and simplified to give the final denominator expression for **k**1 of Equation 2. This is shown below in Equation 7.

(7)

With the denominator expression determined, we evaluated the full **k**1 expression as shown in Equation 8.

(8)

Next, we combined the denominator with the 2π coefficient and evaluated the product of the two matrices in the numerator of Equation 8. The resulting expression is provided in Equation 9,

(9)

which was then simplified to give the resulting coordinates of the **k**1 reciprocal space vector (Equation 10).

(10)

In comparing the **k**1 and **k**2 expressions from Equation 2, it is apparent that the denominators are equivalent, which allowed us to evaluate the **k**2 reciprocal space vector in a similar fashion as above (Equation 11).

(11)

Again, we combined the denominator of Equation 11 with the 2π coefficient in the numerator and evaluated the product of the two remaining matrices. The resulting expression is provided in Equation 12.

(12)

Equation 12 was then simplified to give the resulting coordinates of the **k**2 reciprocal space vector, which is given in Equation 13.

(13)

Finally, we validated the correct **k**1 and **k**2 expressions by evaluating the dot products of the real and reciprocal space vectors, which must satisfy the relationships provided in Equation 14.

(14)

The dot product of and **k**1 is evaluated in Equations 15-17.

(15)

(16)

(17)

The dot product of and **k**2 is evaluated in Equations 18-20.

(18)

 (19)

(20)

The dot product of and **k**2 is evaluated in Equations 21-23.

(21)

(22)

(23)

The dot product of and **k**1 is evaluated in Equations 24-26.

(24)

 (25)

(26)