Davisson and Germer experiment

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Here we discuss the detail of the Davisson-Germer experiment. This experiment (Davisson-Germer experiment) is very important one to the duality of wave and particle nature in quantum mechanics. It demonstrates the validity of de Broglie's postulate because it can only be explained as a constructive interference of waves scattered by the periodic arrangement of the atoms of the crystal. Although there are many references on the famous experiments, it is a little difficult for students (in particular for ones taking the course of Modern Physics) to understand the detail of the experiments, since the descriptions of the experiments are different depending on references and are not always specific.

In order to understand what kind of experiments Davisson and Germer have done in their paper of 1927, we will present some concepts on (i) the crystal structure of fcc (face centered cubic) Ni which is used as the target of the electron scattering experiment, (ii) the reciprocal lattice vectors for the fcc Ni, and (iii) Bragg reflections and the Ewald sphere.

In spite of our efforts, I must admit that so far I do not sufficiently understand some of the experimental results which have been reported by Davisson and Germer, including

1. C. Davisson and L.H. Germer, Phys. Rev. **30**, 705 (1927)
2. C. J. Davisson, L. H. Germer, Phys. Rev. **29**,908(1927).
3. C.D. Davisson and L.H. Germer Nature **119**, 558 (1927).
4. C. Davisson, The discovery of electron waves, p.387 (1937). Nobel Prize Lecture

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Clinton Joseph Davisson (October 22, 1881 – February 1, 1958), was an American physicist who won the 1937 Nobel Prize in Physics for his discovery of electron diffraction. Davisson shared the Nobel Prize with George Paget Thomson, who independently discovered electron diffraction at about the same time as Davisson.

http://en.wikipedia.org/wiki/Clinton_Davisson

ABSTRACT:

Here we discuss the detail of the Davisson-Germer experiment. This experiment (Davisson-Germer experiment) is very important one to the duality of wave and particle nature in quantum mechanics . It demonstrates the validity of de Broglie's postulate because it can only be explained as a constructive interference of waves scattered by the periodic arrangement of the atoms of the crystal. Although there are many references on this famous experiments, it is a little difficult for students (in particular for ones taking the course of Modern Physics) to understand the detail of the experiments, since the descriptions of the experiments are different depending on references and are not always specific.

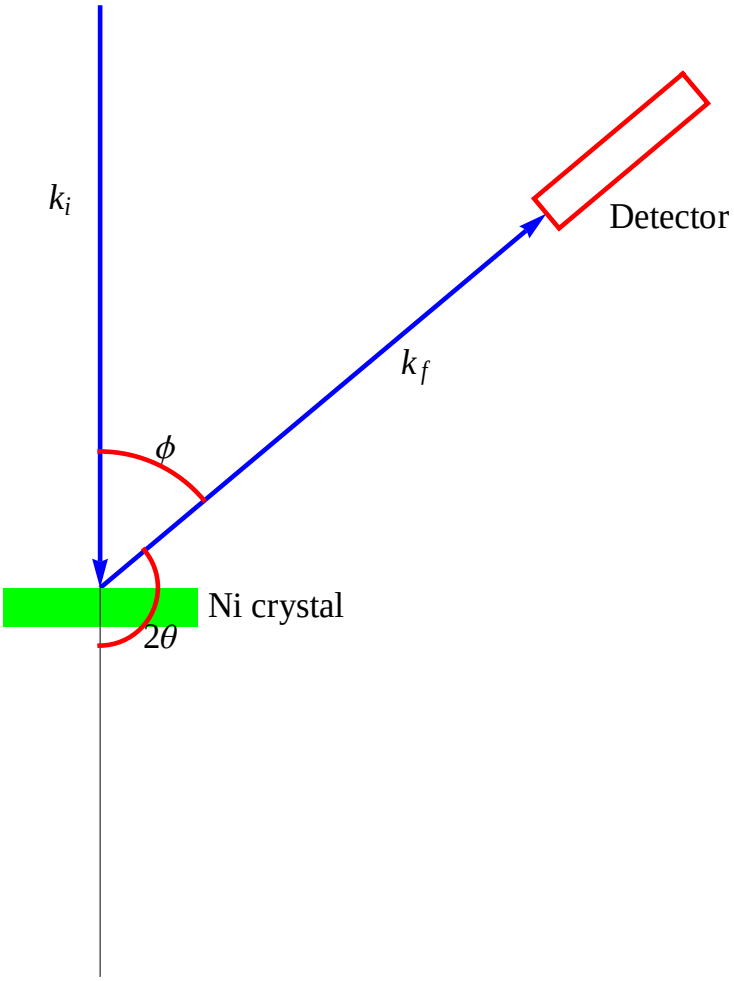
In order to understand what kind of experiments Davisson and Germer have done in their paper of 1927, we will present some concepts on (i) the crystal structure of fcc (face centered cubic) Ni which is used as the target of the electron scattering experiment, (ii) the reciprocal lattice vectors for the fcc Ni, (iii) Bragg reflections and the Ewald sphere.

Here we use the Mathematica, in order to analyze the experimental data of the Davisson and Germer and visualize the undergoing physics. We will discuss what kind of experiments Davisson and Germer have done.

1. Introduction

In 1925, Clinton Davisson and Lester .H. Germer investigated the properties of Ni metallic surfaces by scattering electrons. Their experiments (Davisson-Germer experiment) demonstrates the validity of de Broglie's postulate because it can only be explained as a constructive interference of waves scattered by the periodic arrangement of the atoms of the

crystal. The Bragg law for the diffraction had been applied to the x-ray diffraction, but this was first application to the electron waves.



This figure shows schematically the apparatus of Davisson and Germer. Electrons from a heated filament are accelerated through a potential difference V and emerges from the electron gun with kinetic energy eV. The electron beam falls at normal incidence on a single crystal of nickel. The detector D is set at a particular angle ϕ. The intensity of the reflected beams is measured as a function of f at various values of the accelerating potential V. Davisson and Germer detected a strong beam at $\phi = 50°$ and $V = 54$ V. All such strong reflected beams can be explained by assuming that the electrons have a wavelength given by a de Broglie wavelength,

$$\lambda = \frac{h}{p},$$

and that Bragg reflections occur from certain families of atomic planes precisely as described for x-rays.

2. de Broglie length of electron

Here we calculate the de Broglie wave length as follows. The de Broglie relation is given by

$$p = \frac{h}{\lambda}.$$

The energy dispersion relation of electron is

$$E = \frac{1}{2m} p^2 \qquad\qquad p = \sqrt{2mE}$$

where E is the kinetic energy and p is the linear momentum. Then we get the relation

$$\lambda = \frac{h}{\sqrt{2mE}}$$

or

$$\lambda = \frac{12.2643}{\sqrt{V}}, \qquad \text{(in the units of Å).}$$

where E = eV, -e is the charge of electron$V$ is in the units of V (voltage). When V = 54 V, the wavelenght is calculated as 1.669 Å.

((**Example**)) Ewald's sphere

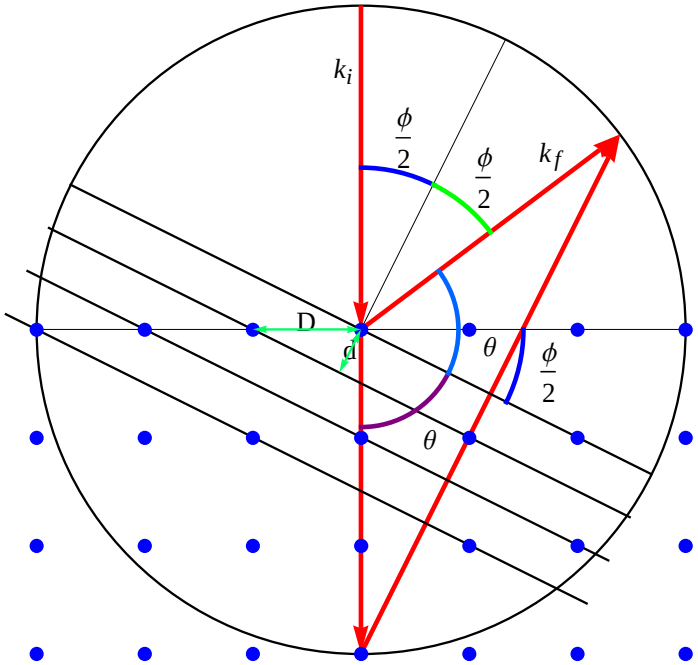


Fig. Davisson-Germer experiment. $k_i = k_f = \frac{2\pi}{\lambda}$. 2θ is the scattering angle.

$2\theta + \phi = \pi$. $D \sin\frac{\phi}{2} = d$.

For γ-ray

$$E = \frac{hc}{\lambda}$$

or

$$\lambda = \frac{hc}{E}$$

Bragg condition:

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

where

$$d = D\sin\frac{\phi}{2}$$

$$\lambda = 2d\sin\theta = 2D\sin(\frac{\pi}{2} - \frac{\phi}{2})\sin\frac{\phi}{2} = 2D\sin\frac{\phi}{2}\cos\frac{\phi}{2} = D\sin\phi$$

where

$$\theta = \frac{\pi}{2} - \frac{\phi}{2}$$

Then we get

$$\phi = \sin^{-1}(\frac{\lambda}{D}) = \sin^{-1}(\frac{hc}{ED}).$$

When D = 2.15 Å and ϕ = 50°,

$$d = D\sin\frac{\phi}{2} = 2.15\sin(25°) = 0.9086 \text{ Å}.$$

$$\lambda = D\sin\phi = 2.15\sin(50°) = 1.647 \text{ Å}$$

This value of l is very close to that derived from the corresponding de Broglie wavelength (1.669 Å).

((**Note**))

fcc Ni lattice constant: a = 3.520 Å.

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3. Reciprocal lattice of fcc Ni

(a) Primitive unit cell

In the experiment of Davisson-Germer, they use a fcc Ni as a target. Here we discuss the crystal structure and the reciprocal lattice vectors. The primitive translation vectors of the fcc lattice are expressed by

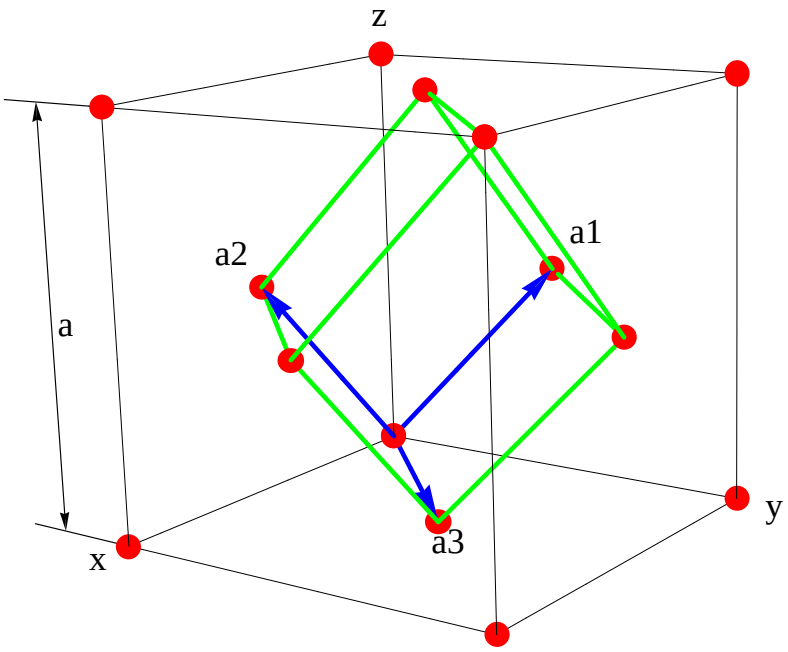
$$\mathbf{a}_1 = \frac{1}{2}a(0,1,1), \qquad \mathbf{a}_2 = \frac{1}{2}a(1,0,1), \qquad \mathbf{a}_3 = \frac{1}{2}a(1,1,0)$$

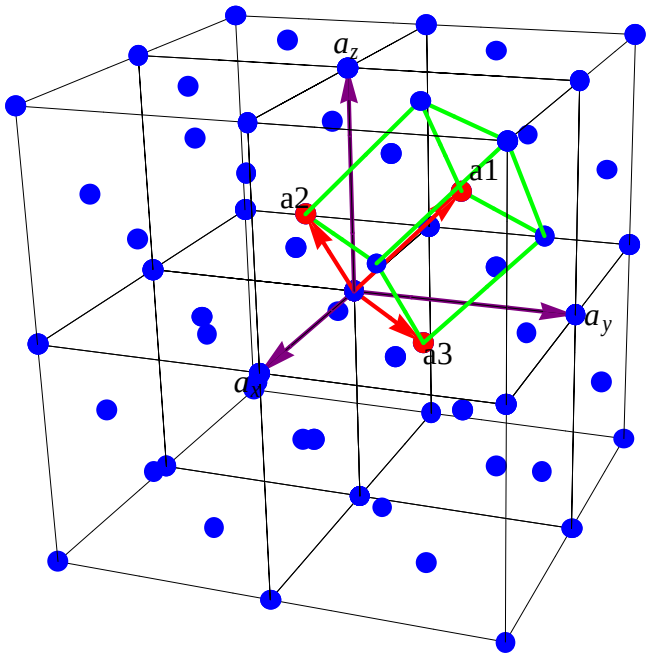
where there is one atom per this primitive cell. We can generate all the points of the fcc lattice is described by

$$\mathbf{l} = l_1\mathbf{a}_1 + l_2\mathbf{a}_2 + l_3\mathbf{a}_3$$

with l_1, l_2, and l_3 integers. The volume of the primitive cell is

$$\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a^3}{4}$$





The corresponding reciprocal lattice vectors are given by

$$\mathbf{b}_1 = \frac{2\pi(\mathbf{a}_2 \times \mathbf{a}_3)}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = \frac{2\pi}{a}(-1,1,1)$$

$$\mathbf{b}_2 = \frac{2\pi(\mathbf{a}_3 \times \mathbf{a}_1)}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = \frac{2\pi}{a}(1,-1,1)$$

$$\mathbf{b}_3 = \frac{2\pi(\mathbf{a}_1 \times \mathbf{a}_2)}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = \frac{2\pi}{a}(1,1,-1)$$

The reciprocal lattice vector is described by

$$\mathbf{G} = g_1\mathbf{b}_1 + g_2\mathbf{b}_2 + g_3\mathbf{b}_3 = \frac{2\pi}{a}(-g_1 + g_2 + g_3, g_1 - g_2 + g_3, g_1 + g_2 - g_3)$$

where g_1, g_2, and g_3 are integers.

(b) Conventional cubic unit cell

The translation vectors of the conventional unit cell (cubic) are expressed by

$$\mathbf{a}_x = a(1,0,0), \qquad \mathbf{a}_y = a(0,1,0), \qquad \mathbf{a}_z = a(0,0,1),$$

where there are two atoms per this conventional unit cell. The volume of the cubic cell is

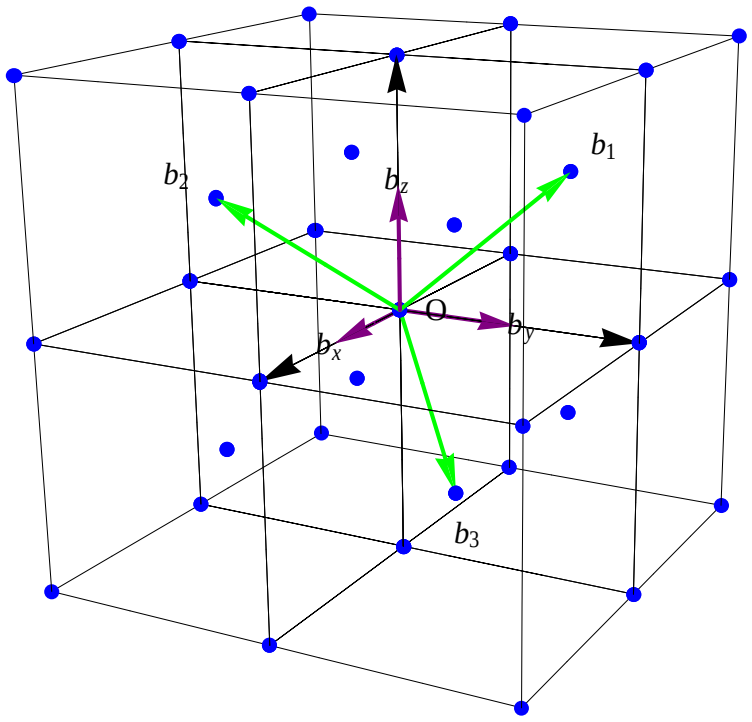
$$\mathbf{a}_x \cdot (\mathbf{a}_y \times \mathbf{a}_z) = a^3 .$$

The reciprocal lattice vectors are defined by

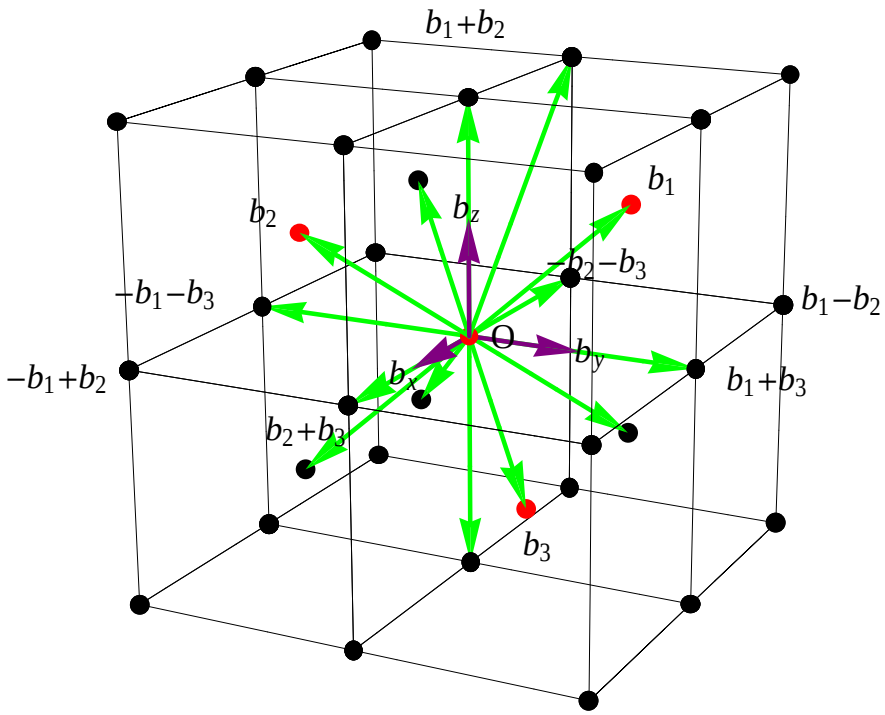
$$\mathbf{b}_x = \frac{2\pi(\mathbf{a}_y \times \mathbf{a}_z)}{\mathbf{a}_x \cdot (\mathbf{a}_y \times \mathbf{a}_z)} = \frac{2\pi}{a}(1,0,0)$$

$$\mathbf{b}_y = \frac{2\pi(\mathbf{a}_z \times \mathbf{a}_x)}{\mathbf{a}_x \cdot (\mathbf{a}_y \times \mathbf{a}_z)} = \frac{2\pi}{a}(0,1,0)$$

$$\mathbf{b}_z = \frac{2\pi(\mathbf{a}_x \times \mathbf{a}_y)}{\mathbf{a}_x \cdot (\mathbf{a}_y \times \mathbf{a}_z)} = \frac{2\pi}{a}(0,1,0)$$



The reciprocal lattice vectors, $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, and $\boldsymbol{b}_3$ for the primitive cell and $\boldsymbol{b}_x$, $\boldsymbol{b}_y$, and $\boldsymbol{b}_z$ for the cubic cell (conventional cell) for the fcc lattice. The reciprocal lattice points (denoted by solid blue circles) are located on a bcc lattice.



Reciprocal lattice vectors

In general, the reciprocal lattice vector is given by

$$\mathbf{G} = g_x\mathbf{b}_x + g_y\mathbf{b}_y + g_z\mathbf{b}_x = \frac{2\pi}{a}(g_x, g_y, g_z)$$

with

$$g_x = -g_1 + g_2 + g_3$$
$$g_y = g_1 - g_2 + g_3$$
$$g_z = g_1 + g_2 - g_3$$

There are relations between (g_x, g_y, g_z) and (g_1, g_2, g_3). Note that all indices of (g_x, g_y, g_z) are odd or even. There is a selection rule for the indices (g_x, g_y, g_z).

g_x	g_y	g_z	g_1	g_2	g_3
1	1	1	1	1	1
2	0	0	0	1	1
2	2	0	1	1	2
3	1	1	1	2	2
2	2	2	2	2	2
4	0	0	0	2	2
3	3	1	2	2	3
4	2	0	1	2	3
4	2	2	2	3	3
5	1	1	1	3	3

The Selection rule for the indices (g_1, g_2, g_3) for fcc, which arises from the fact that the volume of the conventional cubic cell is four times larger than that of the primitive unit cell.

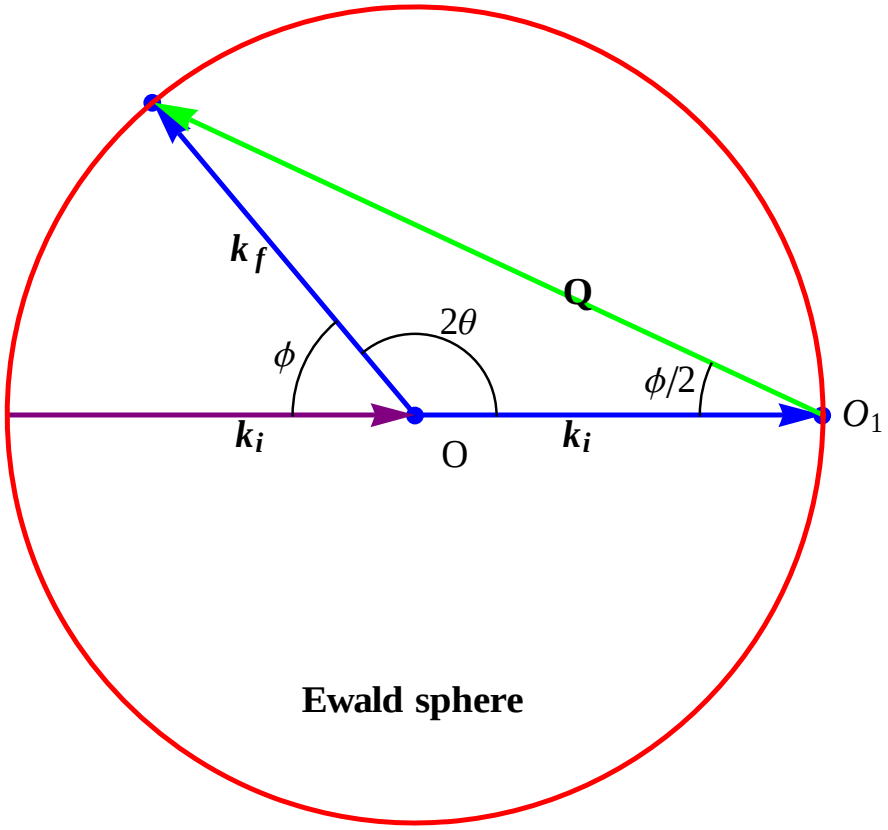
4. Bragg condition and Ewald sphere

Using the Ewald sphere, the Bragg condition is represented by

$$\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i = \mathbf{G}$$

where $\boldsymbol{k}_i$ is the wavevector of incident wave and $\boldsymbol{k}_f$ is the wavevector of the outgoing wave. The angle ϕ is related to the scattering 2θ by

$$\phi + 2\theta = \pi$$



Since

$$|\mathbf{k}_i| = |\mathbf{k}_f| = k = \frac{2\pi}{\lambda}$$

the magnitude of the scattering wave vector **Q** is given by

$$Q = |\mathbf{Q}| = 2k\sin\theta = \frac{4\pi}{\lambda}\sin\theta = |\mathbf{G}|$$

where

$$\mathbf{G} = g_x b_x + g_y b_y + g_z b_z = \frac{2\pi}{a}(g_x, g_y, g_z)$$

is the reciprocal lattice vector of fcc Ni and *a* is the lattice constant (a = 3.52 Å). Then we have the relation

$$G^2 = (\frac{4\pi}{\lambda})^2 \sin^2\theta = \frac{4\pi^2}{a^2}(g_x{}^2 + g_y{}^2 + g_z{}^2)$$

where

$$g_x = -g_1 + g_2 + g_3$$
$$g_y = g_1 - g_2 + g_3$$
$$g_z = g_1 + g_2 - g_3$$

and g_1, g_2, and g_3 are integers.

For fcc structure, it is required that

$$g_x{}^2 + g_y{}^2 + g_z{}^2 = 3, 4, 8, 11, 12, 16, 19, 20, 24, 27, 32, 35, 40, 36, 43, 44, 48$$

(see the Appendix for the derivation).

5. Interpretation of the experimental results reported by Davisson and Germer

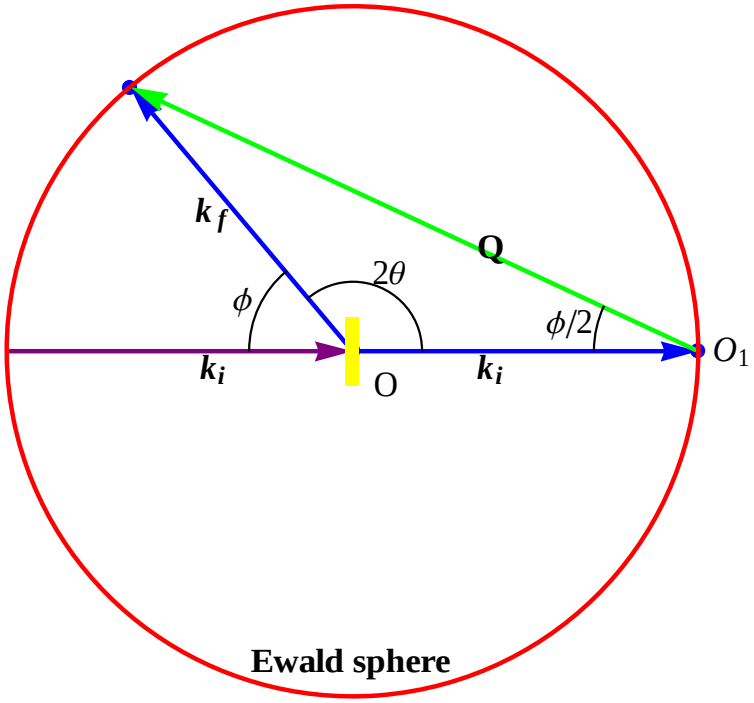


Fig. Ni single crystal on the sample table. O1 is the origin of the reciprocal lattice vector.

In the Davisson and Germer experiment, it is reported that

V = 54 V. λ = 1.66895 Å from the de Broglie relation (we assume this),
$\phi = 50°$
$2\theta = 180° - 50° = 130°$

which leads to the value of

$$G = \frac{4\pi}{\lambda}\sin\theta = 6.8240\ \text{Å}^{-1},$$

Using the lattice constant a = 3.520 Å for Ni (a = 3.62 Å was used in the Davisson-Germer experiment), we have

$$G^2\frac{a^2}{4\pi^2} = (g_x{}^2 + g_y{}^2 + g_z{}^2) = 14.615$$

which is close to 16 for fcc structure. The possible values of $\{g_x, g_y, g_z\}$ and $\{g_1, g_2, g_3\}$ are given by

g_1	g_2	g_3	g_x	g_y	g_z
-2	-2	0	0	0	-4
-2	0	-2	0	-4	0
0	-2	-2	-4	0	0
0	2	2	4	0	0
2	0	2	0	4	0
2	2	0	0	0	4

where

$$(g_x^{\,2} + g_y^{\,2} + g_z^{\,2} = 14.615$$

For simplicity, we choose

g_1=2, g_2 = 2, g_3 = 0 or g_x = 0, g_y = 0, g_z = 4.

or

$$\mathbf{G} = \frac{2\pi}{a}(0,0,4) = 4b_z$$

If we assume that

$$G = \frac{8\pi}{a} = \frac{2\pi}{d}$$

then the *d*-spacing for the (004) cubic plane is estimated as

$$d = \frac{a}{4} = 0.88 \text{ Å}.$$