Formation of Standing Waves Within Crystal Unitcell

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Formation of Standing waves within Crystal Unitcell.

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Abstract.

We show that the historic Davisson-Germer experiment demonstrates formation of standing waves within nickel crystal unitcell. Cartesian Fourier transform cannot offer description in terms of standing waves because Cartesian Fourier theory cannot accommodate π in place of 2π. Thus, formation of standing waves within unitcell in Davisson-Germer experiment necessarily requires spherical polar coordinate description of crystal diffraction. Description in spherical polar coordinates permits to incorporate precision angles from the experiment for better convergence in structure determination calculations.

1 Introduction.

Currently existing Cartesian description of crystal diffraction, including in text books, has no mention of formation of standing waves within the unitcell. In this article, we introduce standing waves within the unitcell with experimental proof from the historic Davisson-Germer experiment.

Davisson-Germer experiment[1] demonstrated de Broglie hypothesis[2,3,4] and wave-particle duality of electrons[6,7,8].

Davisson and Germer reported failure of the data to satisfy Bragg's law[1,5,7,10] in explaining all the Davisson-Germer peaks recorded in the experiment. We now show that the reported failure has nothing to do with Bragg's law and that the actual reason for the reported failure of data to satisfy Bragg's law is the formation of standing waves within the nickel crystal unitcell.

2 Davisson-Germer experiment as experimental proof for the formation of standing waves within unitcell.

We now show that formation of standing wave radiation field within nickel crystal unitcell alone can successfully explain all the six Davisson-Germer peaks recorded in the experiment as shown in figure 1[1,7,10].

Davisson-Germer experiment. In Davisson-Germer experiment with incident electrons at an accelerating voltage of 54 $volts$ directed onto atomic surface of crystalline nickel, highest intensity for diffracted electrons was observed at a colatitude angle of 50° which corresponds to a diffraction angle of 130° relative to primary beam direction and an incident angle of 25° relative to the normal to the crystal planes parallel to the surface of the crystal. An incident angle of 25° corresponds to a Bragg angle of 65°. An accelerating voltage of 54 $volts$ accelerates electrons to 54 eV kinetic energy[9]. According to de Broglie relation, an electron with kinetic energy T of 54 eV(i.e., $T = 54 \times 1.6 \times 10^{-19}\ joules$) has a momentum p and wavelength λ given by,

$$p = \sqrt{2mT} = 4.0 \times 10^{-24} \text{ kg-m/s}^2 \tag{1}$$

$$\lambda = \frac{h}{p} = 1.67 \text{ Å} \tag{2}$$

where m is mass of electron and h is Planck constant.

From the interplanar spacing $d = 0.91$ Å in nickel crystal determined earlier from x-ray diffraction experiments[9], Bragg's law with the Bragg angle of 65° used in the measurement in Davisson-Germer experiment gives the wavelength as,

$$\lambda = 2d \sin\theta_{65^\circ} = 1.65 \text{ Å} \tag{3}$$

The excellent agreement between wavelengths obtained from two ways, the first from de Broglie relation and the second from Bragg's law, is the success point in Davisson-Germer experiment that confirmed the wave-particle duality of electrons.

The x-ray diffraction experiment on nickel crystal prior to Davisson-Germer experiment may have mostly been conducted with $Cu\ K_\alpha$ radiation. With $Cu\ K_\alpha$ incident x-rays at $\lambda = 1.5406$Å diffraction intensity corresponding to $d = 0.91$Å occurs at $\theta_{\text{Bragg}} = \sin^{-1}(1.54/2 * 0.91) = 57.8^\circ$ such that $d = 1.54/(2 * \sin 57.8^\circ) = 0.92$Å. The $Cu\ K_\alpha\ \lambda = 1.54$Å corresponds to an incident accelerating voltage of $V = 64\ volts(\sqrt{V} = 8.0)$. Hence, the peak at $\sqrt{V} = 8.0$ Davisson & Germer measured measured later on[7] is indicative that Davisson-Germer were closely following x-ray diffraction experiment for the proof for wave-particle duality.

But the peak measured at $\sqrt{V} = 8.0$[7] was from $\{111\}$ Bragg planes with interplanar spacing of $d_{\{111\}} = 2.03$Å at 20° colatitude, which is 10° angle of incident such that $\theta_{\text{Bragg}} = 80^\circ$. The corresponding λ becomes $\lambda = 2 * 2.03 * \sin 80^\circ = 4.0$Å which corresponds to $\sqrt{=}3.1$, i.e., at an accelerating voltage of $V = 9.4\ volts$. Davisson & Germer could not handle such low voltage

in the experiment and thus could not obtain equivalence in wavelengths as proof to wave-particle duality at $\lambda = 4.0$Åwith $d_{\{111\}} = 2.03$Å and $\theta_{\text{Bragg}} = 80^\circ$ in the experiment.

Hence, the set of $\{111\}$ Bragg planes with $d_{\{111\}} = 2.03$Å from which planes the peaks were measured in varying angles of incidence and Davisson & Germer discuss about in their articles[1,7,10] have nothing to do with the x-ray diffraction experiment determined interplanar spacing value $d = 0.91$Å in nickel crystal. The 50° colatitude, which is $\theta_{\text{Bragg}} = 65^\circ$ indicates that Davisson & Germer closely followed θ_{Bragg} for $d = 0.91$Å from earlier x-ray diffraction experiments in measuring intensities of diffracted electrons in the experiment. The six historic Davisson-Germer peaks, measured from planes with $d = 0.91$Å at $\theta_{\text{Bragg}} = 65^\circ$, published in the plot in Davisson & Germer, Journal of Franklin Institute in 1928 are located approximately at,

$$\sqrt{V} = 7.5, \quad 11.5, \quad 14.5, \quad 18.5, \quad 21.5, \quad 24.0 \tag{4}$$

in the $\sqrt{V} - Intensity$ plot shown[10] in figure 1. We note that the relative orientations of incident beam, reflected beam and the surface of nickel crystal remain invariant in measuring all the above six peaks.

We now investigate whether it is the running wave description or the standing wave description that can explain all the six Davisson-Germer peaks recorded in the experiment.

Running wave description. Following de Broglie relation, kinetic energy T contained in one wavelength of a running wave is given by,

$$T = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} \tag{5}$$

in units of eV or $joules$. In a crystal diffraction condition, integer multiplier n to λ can also be viewed as multiplier to inter-planar spacing. Hence, eq. (5) can also be written with n^2 in the numerator as,

$$T = \frac{p^2}{2m} = \frac{n^2 h^2}{2m\lambda^2} \tag{6}$$

From eq. (6), kinetic energy T in eV is equal to accelerating potential V in volts given by,

$$V = 151 \left(\frac{n^2}{(\lambda \text{ in Å})^2} \right) \quad ; \quad \sqrt{V} = 12.3 \left(\frac{n}{\lambda \text{ in Å}} \right) \tag{7}$$

For $\lambda = 1.67$ Å and for $n = 1, 2, 3, \cdots$, eq. (7) gives calculated peaks for $\sqrt{V}$ at,

$$\sqrt{V} = 7.4, \quad 14.8, \quad 22.2, \quad 29.6, \quad 37.0 \quad \text{etc.} \tag{8}$$

which peaks obviously do not correspond to all the six Davisson-Germer peaks from the experiment shown in figure 1 and listed in eq. (4). Because λ in the denominator in eq. (7) can substitute for Bragg's law, Davisson and Germer reported the reason as the failure of data to satisfy Bragg's law[7,10] in explaining $\sqrt{V}$ values for all the six peaks measured in the experiment. Therefore, running wave description and hence Bragg's law could explain only first, third, fifth peaks recorded in the experiment.

We now show that formation of standing wave radiation field within unitcell in Nickel crystal successfully explains all the six Davisson-Gemer peaks and thus confirms existence of standing waves within the unitcell in crystal diffraction.

Standing wave description. A standing wave does not transport energy, but stores kinetic energy in its anti-nodes. Because two opposite traveling waves of equal wavelength constitute a stand-

ing wave, kinetic energy stored in one wavelength of a standing wave is equal to kinetic energy contained in two wavelengths of the constituent running waves. Thus, with 2λ in place of λ in the denominator in eq. (6) and with n^2 in the numerator, kinetic energy T in one wavelength of a standing wave is given by,

$$T = \frac{p^2}{2m} = \frac{n^2h^2}{2m(2\lambda)^2} = \left(\frac{n^2h^2}{8m\lambda^2}\right) \tag{9}$$

in units of eV or $joules$. From eq. (9), the kinetic energy T in eV is equal to the accelerating potential V in volts given by,

$$V = 37.7\left(\frac{n^2}{(\lambda \text{ in Å})^2}\right) \quad ; \quad \sqrt{V} = 6.14\left(\frac{n}{\lambda \text{ in Å}}\right) \tag{10}$$

For $\lambda = 1.67$ Å and for $n = 1, 2, 3, \cdots$, eq. (10) gives calculated peaks for $\sqrt{V}$ at,

$$\sqrt{V} = 7.4, \quad 11.2, \quad 14.8, \quad 18.5, \quad 22.2, \quad 25.9 \text{ etc.} \tag{11}$$

The peaks in eq. (11), calculated from standing wave description, are in perfect agreement with all the six Davisson-Germer peaks in eq. (4) recorded in the experiment, except a little aberration in calculated $\sqrt{V}$ only for the last peak. Higher accelerating potentials correspond to higher energy electrons and hence the aberration may be due to onset of Comptom effect[12].

The excellent agreement between theoretical and experimental values of $\sqrt{V}$ for all the six historic Davisson-Germer peaks shown in figure 1 confirms the formation of standing wave radiation field within Nickel crystal unitcell. Thus, standing wave description alone can explain all the six peaks recorded in Davisson-Germer experiment.

We note that whether it is λ or 2λ in the denominator in the expression for kinetic energy, not

Bragg's law or the pair of parameters contained in Bragg's law, that determines the formation of standing waves within the unitcell. Hence, the failure of data to satisfy Bragg's law as reported by Davisson and Germer in explaining all the six Davisson-Germer peaks is because of the formation of standing waves within nickel crystal unitcell, not Bragg's law.

Thus, Davisson-Germer experiment becomes direct experimental proof for the formation of standing wave radiation field within unitcell in crystal diffraction.

Incident beam in Davisson-Germer experiment is electron beam, which is particle radiation beam. Applicability of Karle-Hauptman triple phase tangent formula based probabilistic direct methods[13] for both x-ray crystal diffraction and neutron crystal diffraction demonstrates that the phenomenon of diffraction in both is the same. Hence, presence of standing waves in one and absence of standing waves in the other is not possible. Thus, formation of standing waves within nickel crystal unitcell in electron diffraction in Davisson-Germer experiment implies formation of standing waves in x-ray crystal diffraction also. The standing wave anti-nodes within unitcell act as secondary sources and re-radiate incident energy.

3 Multiples of π and spherical coordinate description.

In running wave, a full wavelength is equivalent to a phase difference of 2π radians. In Cartesian FT description, Miller indices defined harmonic waves are running waves and hence we count integer multiple of 2π radians along each axial dimension of the unitcell. With standing waves within unitcell, we count number of antinodes along each axial dimension. Each antinode can only

correspond to π radians because the length of an antinode is equivalent to a phase difference of π radians. Hence in standing wave description, we count integer multiples of π along each axial dimension of the unitcell. Therefore in the integral transform kernel, 2π becomes characteristic of running waves and π becomes characteristic of standing waves in the description.

Likewise, Miller indices defined interplanar spacing too corresponds to 2π radians in running wave description and to π radians in standing wave description. It is this interplanar spacing as π radians that requires description in spherical polar coordinates.

Cartesian Fourier theory cannot accommodate π in place of 2π for description in terms of standing waves. Thus, Cartesian Fourier transform can offer description only in terms of running waves. We note that such restriction does not exist in spherical coordinate description, which means spherical coordinates can offer description in terms of standing waves. Hence, the next best choice becomes the spherical polar coordinate description[11], where the orthogonal set of basis functions can accommodate π in place of 2π in series expansion.

Therefore, formation of standing waves within unitcell in Davisson-Germer experiment demonstrates the necessity for spherical polar coordinate description of crystal diffraction.

4 Conclusions.

Successful explanation for all the six peaks in the historic Davisson-Germer experiment for the first time in almost a century demonstrates formation of standing wave radiation field within Nickel

crystal unitcell. Hence, Davisson-Germer experiment necessitates description of crystal diffraction in terms of standing waves within the unitcell.

Cartesian Fourier transform cannot offer description in terms of standing waves and description in terms spherical coordinates has no such restriction. Hence, description in terms of standing waves implies description in terms of spherical polar coordinates. We note that description of crystal diffraction in spherical polar coordinates permits to incorporate the precision angles as additional diffraction data from the experiment for better convergence in structure determination calculations.

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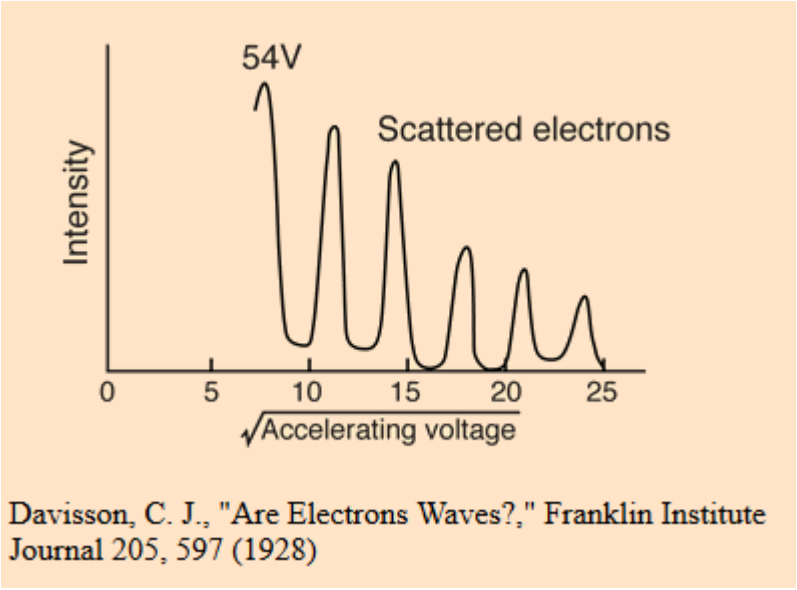

Figure 1. **Historic Davisson-Germer peaks.** Reproduced with citation of reference[10] and with courtesy of Franklin Institute Journal.

Figures

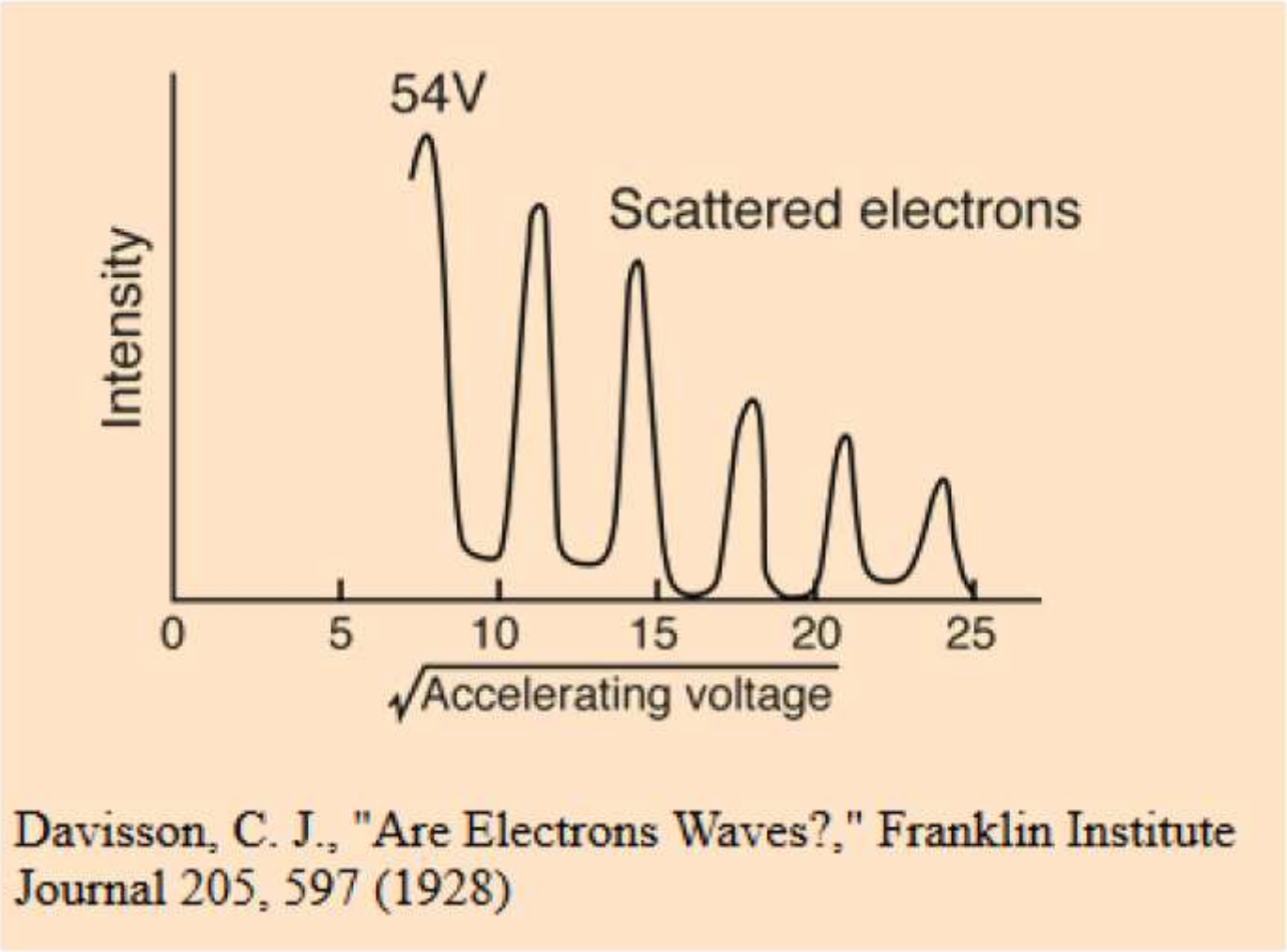

Figure 1

Historic Davisson-Germer peaks. Reproduced with citation of reference10 and with courtesy of Franklin Institute Journal.