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X-ray Version of Davisson-Germer Experiment.

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Abstract.

Application of unitcell defined boundary conditions leads to the question on the formation of standing waves within unitcell. We design and propose X-ray version of Davisson-Germer experiment as the answer. In the proposed experiment, a tunable synchrotron beam replaces the variable de Broglie wavelength of incident electron beam. Among the two series of Davisson-Germer peaks from original experiments available in literature, first series demonstrates standing wave description and the second series demonstrates running wave description. Both running waves and standing waves cannot simultaneously exist within the unitcell and the proposed experiment alone can resolve between the two. The experiment can be conducted on a macromolecular crystal also.

1 Introduction.

Currently existing Cartesian description of crystal diffraction, including in text books, has no mention of standing waves within the unitcell. On a stretched string, the fixed end points as boundaries give rise to formation of standing waves. Likewise, the fixed boundary planes of the unitcell presents possibility for the formation of standing waves. To investigate the possibility, we take recourse to the X-ray version of the historic Davisson-Germer(*DG* henceforth) experiment. *DG*

experiment¹ demonstrated de Broglie hypothesis^{2,3,4} and wave-particle duality of electrons^{7,8,9}.

The objective of the X-ray version of *DG* experiment being proposed in this article is to discover whether or not standing waves exist within the unitcell in crystal diffraction.

2 Bragg planes and *DG* planes.

A series of *DG* peaks can be measured from any *hkl* set of Bragg planes. A given *hkl* set of Bragg planes defines a superset of *DG* planes for which the interplanar spacings are given by,

$$d_{hkl-n} = d_{nh,nk,nl} = \frac{d_{hkl}}{n} \quad (1)$$

where $nh = n * h$, $nk = n * k$, $nl = n * l$ and n is the order of the *DG* peak counted from left to right on the $\sqrt{V} - I$ plot, where I is diffraction intensity. The Bragg angle at which the six *DG* peaks are measured is given by,

$$\theta_{hkl-\text{Bragg}} = \sin^{-1} \left(\frac{\lambda}{2d_{hkl}} \right) \quad (2)$$

We note that the Bragg angle remains invariant for all the six *DG* peaks while the incident λ varies from peak to peak.

3 The historic *DG* experiment.

We need a series of six *DG* peaks to investigate the formation of standing waves within crystal unitcell. We have two such series from the original experiments by Davisson and Germer(*D&G* henceforth), which we designate as first series⁶ reproduced as figure 1 and second series⁷ reproduced as figure 2 for our reference in this article. Both series have six peaks each. The running

wave description could predict only the first, third and fifth DG peaks, but not all six peaks and $D\&G$ reported the reason to be experimental errors. Subsequently, $D\&G$ measured a second series of DG peaks from a different set of hkl planes with different experimental parameters. And $D\&G$ claimed that the second series obeys running wave description.

In a DG experiment, electron gun acts as a source of incident beam tunable in a range of continuous wavelengths defined by the operable accelerating voltage. If the incident beam of de Broglie(dB) wavelength λ_{dB} from electron gun encounters a crystal in its way with inter-planar distance such that Bragg's law $\lambda_{dB} = 2d_{hkl} \sin \theta_{hkl-\text{Bragg}}$ is satisfied, diffraction occurs giving rise to a DG peak. By changing accelerating voltage, i.e., by changing λ_{dB} , $D\&G$ measured peaks while keeping the Bragg angle $\theta_{hkl-\text{Bragg}}$ invariant within a given series of six peaks. In a typical experiment, $D\&G$ measured six peaks in a series within the operable range of accelerating potential. We note that every measurable hkl diffraction from a crystal can in principle be used for measuring a series of DG peaks. The first series of six DG peaks shown in figure 1 published in the graph by Davisson⁶ are located approximately at,

$$\sqrt{V} = 7.5, \quad 11.5, \quad 14.5, \quad 18.5, \quad 21.5, \quad 24.0 \quad (3)$$

in the $\sqrt{V} - I$ plot, where V is accelerating voltage and I is intensity, shown⁶ in figure 1.

We now investigate whether it is the running wave description or the standing wave description that can explain all the six DG 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,

$$T = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} \quad (4)$$

in units of eV or *joules*, where m is mass of electron and h is Planck constant. In a crystal diffraction condition, integer multiplier n to λ can also be viewed as multiplier to inter-planar spacing. Hence, eq. (4) can also be written with n^2 in the numerator as,

$$T = \frac{p^2}{2m} = \frac{n^2 h^2}{2m\lambda^2} \quad (5)$$

From eq. (5), kinetic energy T in eV is equal to accelerating potential V in volts given by,

$$V = 151 \left(\frac{n^2}{(\lambda \text{ in } \text{\AA})^2} \right) \quad ; \quad \sqrt{V} = 12.3 \left(\frac{n}{\lambda \text{ in } \text{\AA}} \right) \quad (6)$$

We call eq. (6) as running wave kinetic energy relation or simply running wave relation. From Bragg's law given $\lambda = 1.65 \text{ \AA}$ and eq. (6), the calculated $\sqrt{V}$ peaks for $n = 1, 2, 3, \dots$ are given by,

$$\sqrt{V_n} = 7.5, \quad 14.9, \quad 22.3, \quad 29.8, \quad 37.2 \quad \text{etc.} \quad (7)$$

which peaks are not equal to the six DG peaks shown in figure 1 and listed in eq. (3). Thus, running wave description and hence Bragg's law could explain only first, third, fifth peaks. Because λ in the denominator in eq. (6) can substitute for Bragg's law, $D\&G$ reported the reason as the failure of data to satisfy Bragg's law^{7,6} in explaining $\sqrt{V}$ values for all the six peaks measured in the experiment.

We now show that formation of standing wave radiation field within unitcell successfully explains all the six Davisson-Gemer peaks and thus demonstrates 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 standing 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. (5), kinetic energy T in one wavelength of a standing wave is given by,

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

in units of eV or *joules*. From eq. (8), the kinetic energy T in eV is equal to the accelerating potential V in volts given by,

$$V = 37.7 \left(\frac{n^2}{(\lambda \text{ in } \text{\AA})^2} \right) \quad ; \quad \sqrt{V} = 6.14 \left(\frac{n}{\lambda \text{ in } \text{\AA}} \right) \quad (9)$$

We call eq. (9) as standing wave kinetic energy relation or simply standing wave relation. From Bragg's law given $\lambda = 1.65 \text{ \AA}$ and eq. (6), the calculated $\sqrt{V}$ peaks for $n = 2, 3, 4, \dots$ are given by,

$$\sqrt{V} = 7.5, \quad 11.2, \quad 14.9, \quad 18.6, \quad 22.3, \quad 26.1 \text{ etc.} \quad (10)$$

The peaks in eq. (10), calculated from standing wave description, are in perfect agreement with all the six DG peaks listed in eq. (3) 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 Compton effect¹².

The excellent agreement between theoretical and experimental values of $\sqrt{V}$ for all the six historic *DG* peaks shown in figure 1 demonstrates the formation of standing wave radiation field within Nickel crystal unitcell. Thus, standing wave description alone can explain all the six peaks recorded in *DG* experiment. Thus, *DG* experiment becomes direct experimental proof for the formation of standing wave radiation field within unitcell in crystal diffraction.

Incident beam in *DG* experiment is an electron beam, which is particle radiation beam¹. Applicability of Karle-Hauptman triple phase tangent formula based probabilistic direct methods¹³ to 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 *DG* experiment implies formation of standing waves in the unitcell in X-ray crystal diffraction also. The harmonic standing wave anti-nodes within unitcell act as secondary sources and re-radiate incident energy into the diffraction intensities.

4 Prediction of all the six peaks in a *DG* peak series.

In section 3, we have seen that eq. (6) predicts only first, third and fifth peaks and eq. (9) predicts all six peaks from the Bragg's law derived λ from $d_{hkl} = 0.91\text{\AA}$ and $\theta_{hkl-\text{Bragg}} = 65^\circ$. The operable accelerating voltage range in a *DG* experiment defines allowed range for other parameters in the experiment. We note that the parameters $d_{hkl} = 0.91\text{\AA}$ of $\{hkl\}$ Bragg planes and $\theta_{hkl-\text{Bragg}} = 65^\circ$ used in the *DG* experiment are within the allowed range in measuring the first series of *DG* peaks.

Only when the parameters are within allowed range, Bragg's law derived $\lambda = 1.65\text{\AA}$ agrees with the $\lambda_{dB} = 1.67\text{\AA}$ of the first DG peak and the agreement between the two values becomes the proof for wave-particle duality.

The allowed range of parameters in a DG experiment. The operable range of accelerating voltage ($V \sim 50 - 600 \text{ volts}$) in a DG experiment produces an allowed range ($\sim 1.75 - 0.5 \text{\AA}$) of de Broglie wavelengths λ_{dB} for electrons. For the first series of DG peaks, we have $V = 54 - 576$ in volts , $\sqrt{V} = 7.4 - 24.0$ in units of $\sqrt{\text{volts}}$ and $\lambda_{dB} = 1.67 - 0.51 \text{\AA}$. Even for second series of peaks, we note that the range of V is $\sqrt{V} = 8.0 - 24.5$, which is $\sim 64 - 600 \text{ volts}$, which is within the operable range of V . To measure a series of DG peaks from a chosen series of hkl planes with interplanar distance d_{hkl} , the operable range of V and thus the allowed range of λ defines,

$$(\theta_{hkl-\text{Bragg}})_{\min} = \sin^{-1} \left(\frac{0.5}{2 * d_{hkl}} \right) \quad ; \quad (\theta_{hkl-\text{Bragg}})_{\max} = \sin^{-1} \left(\frac{1.75}{2 * d_{hkl}} \right) \quad (11)$$

as an allowed range for $\theta_{hkl-\text{Bragg}}$ in the experiment. For all DG peaks measured from $\{hkl\}$ planes in a given crystal, the Bragg angle $\sin \theta_{hkl-\text{Bragg}}$ remains invariant at a value within allowed range and only accelerating V varies from peak to peak.

Validity of $d = 0.91 \text{\AA}$ in the proof for wave-particle duality. For a given crystal, X-ray diffraction experiment measures Bragg angle for a diffracted beam and Bragg's law gives $d = \lambda / (2 * \sin \theta_{\text{Bragg}})$ as the interplanar spacing of Bragg planes for the diffracted beam. We note that we have no need to know even the unitcell dimensions of the crystal in determining the interplanar spacing.

Among the three parameters in Bragg's law, incident λ is known and cannot be doubted. Bragg angle is measured in the experiment. With Bragg angle and λ , Bragg's law determines d value. Hence, we have no parameter among the three parameters that can be doubted. If we doubt the validity of d value, the only thing we have to doubt is the validity of Bragg's law itself. Therefore, the validity of d from an X-ray diffraction experiment cannot be doubted or disputed. For nickel crystal, X-ray diffraction experiments established that $d = 0.91\text{\AA}$ is an interplanar distance for some Bragg planes within the crystal¹⁰. *D&G* used $d = 0.91\text{\AA}$ as an interplanar spacing within nickel crystal and Bragg angle from *DG* experiment in calculating the λ for the first *DG* peak. We specifically note that it is the value $d = 0.91\text{\AA}$ from X-ray diffraction experiments that provided the proof for wave particle duality.

The X-ray diffraction experiment on nickel crystal prior to *DG* experiment may have been conducted with *Cu K α* radiation. With *Cu K α* incident X-rays at $\lambda = 1.5406\text{\AA}$ diffraction intensity corresponding to $d = 0.91\text{\AA}$ occurs at $\theta_{\text{Bragg}} = \sin^{-1}(1.5406/2 * 0.91) = 57.8^\circ$ such that $d = 1.5406/(2 * \sin 57.8^\circ) = 0.91\text{ \AA}$. Bragg angle of 65° used for measuring the first series of *DG* peaks shows that *D&G* may have closely followed the Bragg angle and orientation of the crystal in X-ray diffraction experiment with nickel crystal.

For the first series of peaks with $d = 0.91\text{\AA}$, the allowed range of $\theta_{hkl-\text{Bragg}}$ from eq. (11) is $16.0^\circ - 74.1^\circ$. Hence, $\theta_{hkl-\text{Bragg}} = 65^\circ$ and $\lambda = 2 * 0.91 \sin 65^\circ = 1.65\text{ \AA}$ are well within the allowed range in the *DG* experiment. Therefore, first series of peaks exhibits excellent agreement between calculated and experimental peaks for all six peaks in standing wave description.

We note that the second series of DG peaks were measured from $\{111\}$ Bragg planes of nickel crystal⁷. The parameter $d_{111} = 2.03\text{\AA}$ used in the second series of DG peaks is calculated⁷ from the unitcell dimension a of nickel crystal $a = 3.524\text{\AA}$ using $1/d^2$ formula. Hence, $d = 0.91\text{\AA}$ which is straight from the experiment as an interplanar distance is more reliable than $d_{111} = 2.03\text{\AA}$ calculated from unitcell dimension.

5 The second series of DG peaks.

$D\&G$ recorded first series of peaks even before knowing that the running wave description and thus Bragg's law did not explain all the six peaks in the first series. Later on, the experiment was repeated and the second series of peaks⁷ were recorded. The second series of six DG peaks published⁷ are listed as,

$$\sqrt{V} = 8.0, 11.4, 14.7, 18.1, 21.2, 24.2 \quad (12)$$

Again, the first measured peak at $\sqrt{V} = 8.0$ that corresponds to de Broglie $\lambda = 1.54\text{\AA}$ is indicative that $D\&G$ were trying to closely follow X-ray diffraction experiment on nickel crystal with X-rays of λ from $Cu K_\alpha$ source. The second series of peaks were reported to have been measured from $\{111\}$ Bragg planes within nickel crystal with $d_{111} = 2.03\text{\AA}$ and at $\theta_{\text{Bragg}} = 80^\circ$ ⁷. The Bragg's law calculated wavelength for the first DG peak is $\lambda = 2 * 2.03 * \sin 80^\circ = 4.0\text{\AA}$.

The second series of DG peaks is less reliable due to following reasons.

1). For $d_{111} = 2.03 \text{ \AA}$ in nickel crystal⁷, the allowed range of $\theta_{hkl-\text{Bragg}}$ from eq. (11) is $7.1^\circ - 25.5^\circ$. We note that the Bragg angle of 80° used in measuring the DG peaks is not within the allowed range defined by the operable V in a DG experiment. Only when all the parameters in the experiment are within allowed range, the de Broglie λ for the first measurable DG peak and Bragg's law derived λ become equal in obtaining the proof for wave-particle duality of electron. Bragg's law derived $\lambda = 4.0 \text{ \AA}$ is outside the allowed range of λ_{dB} in measuring the second series of DG peaks.

2). $D\&G$ claimed that the first peak with Bragg's law derived $\lambda = 4.0 \text{ \AA}$ corresponds to $\sqrt{V} = 3.1$ which is too low and hence is not measurable. If a DG experiment cannot measure the largest d_{111} peak as the first peak, it is like an X-ray diffraction experiment that cannot measure the $\{111\}$ or similar lower order intensities and can measure only the higher order intensities. Any given crystal has innumerably many sets of hkl planes, in principle, and we can choose any set of planes for all the parameters are within allowed range in the DG experiment. If $D\&G$ had simply chosen a d_{hkl} in nickel crystal such that the Bragg's law calculated λ becomes $\lambda = 1.54$ corresponding to de Broglie λ of the first experimental $\sqrt{V} = 8.0$ peak, the predicted values from eq. (9) would have been correct without uncertainty for $\sqrt{V} = 8$ peak between third and second experimental peaks reported by $D\&G$ ⁷. When a peak is not measurable, it is not a valid DG peak. Hence, counting $\sqrt{V} = 3.1$ as the first DG peak led to the uncertainty to $D\&G$ in identifying the first experimentally measured peak for $\sqrt{V} = 8.0$ ⁷ either as third peak or as second peak⁷.

3). In the expression for kinetic energy in a DG experiment, it is whether 2λ or λ in the

denominator that respectively determines whether it is standing waves or running waves within the unitcell. This feature of the expression for kinetic energy cannot be changed by changing the remaining two parameters in Bragg's law. At an accelerating V defined incident λ_{dB} in the experiment, d_{hkl} and $\theta_{hkl-\text{Bragg}}$ determine each other for diffraction to occur. *D&G* claimed⁷ that the running wave description itself could explain all the six peaks by merely changing d_{hkl} and $\theta_{hkl-\text{Bragg}}$ in the experiment. Our analysis contends that such a reasoning is not acceptable. Hence, the second series of *DG* peaks is less reliable.

4). *D&G* claimed that running wave relation eq. (6) itself with Bragg's law derived $\lambda = 4.0$ Å from $d_{111} = 2.03$ Å predicts all the six peaks⁷. Both running wave and standing wave descriptions are not simultaneously acceptable for the second series of peaks because both running waves and standing waves cannot simultaneously exist within the unitcell. At the same time, we cannot accept standing wave description for the first series and running wave description for the second series. Only either one of the descriptions is possible for both first and second series. Which means only either one of the two series of *DG* peaks is acceptable as valid data from the experiment.

Because of the above five reasons, we need to perform the x-ray version of the *DG* experiment to discover which one of the two peaks is experimentally correct.

6 The X-ray version of *DG* experiment.

The historic *DG* experiment with incident electron beam demonstrated wave-particle duality of electrons. Likewise, the objective of X-ray version of *DG* experiment is to demonstrate the proof

for formation of standing waves within crystal unitcell.

D&G reported that the running wave description could not predict all six peaks in the first series⁶ because of the experimental errors in measuring the peaks⁷. The X-ray version of *DG* experiment does not involve vacuum tube and voltage monitoring electronics and thus avoids experimental errors. Hence measurement from X-ray version of *DG* experiment is extremely precise and reliable. Our question now is not the proof of wave-particle duality. Our question now is whether or not standing waves exist within crystal unitcell. To address our question, we need to know which one of the two series of *DG* peaks in the manuscript is reliable and acceptable. One way is to repeat the experiment with nickel crystal. But nickel crystal gives only back scattered beams from surface scattering and hence may not be effective for the objective of our experiment.

From the kinetic energy relation between λ and $\sqrt{V}$, we can represent *DG* peaks either on $\sqrt{V} - I$ plot or on $\lambda - I$ plot. Because of inverse proportionality between $\sqrt{V}$ and λ , the first *DG* peak on $\sqrt{V} - I$ plot becomes the last *DG* peak on the $\lambda - I$ plot.

The $\sqrt{V} - I$ plot of electron version of *DG* experiment becomes $E - I$ or $\lambda - I$ plot in the X-ray version of *DG* experiment. Similarly as in eq. (6) and eq. (9), running wave description implies λ in the denominator and 2λ in the denominator implies standing wave description. In running wave description,

$$E = \frac{hc}{\lambda} \quad (13)$$

$$E(\text{in } keV) = \frac{3.0 * 10^8 * 6.63 * 10^{-34}}{10^3 * 1.6 * 10^{-19} * \lambda(\text{in } \text{\AA})} = \frac{12.4}{\lambda(\text{in } \text{\AA})} \quad (14)$$

and in standing wave description,

$$E = \frac{hc}{2\lambda} \quad (15)$$

$$E(\text{in } keV) = \frac{6.2}{\lambda(\text{in } \text{\AA})} \quad (16)$$

The striking agreement between the digits in eq. (6), eq. (9) and eq. (14), eq. (16) demonstrates that we can reach conclusive on the objective. We note that the X-ray version of *DG* experiment is devoid of the uncertainties and experimental errors involved in vacuum tube, surface diffraction, LEED experiments. We note that the objective of the experiment is to confirm whether the experiment locates all six peaks or only odd integer count peaks only and therefore we are not concerned about the accuracy in the intensities of the peaks. Hence, we do not need explanation from dynamical theory of crystal diffraction.

The choice of d_{hkl} to measure the *DG* peaks from is arbitrary and hence we can choose a strong reflection in the more reliable mid-angle region of the diffraction space. Only precaution we must exercise is that the predicted and experimental λ values must be in agreement for the first measurable *DG* peaks for the measured series of *DG* peaks to be valid and acceptable. We can conduct the experiment on a protein crystal also.

If eq. (14) predicts all six peaks, we do not have standing waves within unitcell. If eq. (16) predicts all six peaks, we have the proof for the formation of standing waves within unitcell.

7 Conclusions.

We propose the X-ray version of *DG* experiment to avoid the experimental errors reported by Davisson and Germer in measuring the first series. A strong Bragg reflection implies stronger Davisson-Germer peaks. We can measure a series of six Davisson-Germer peaks from any set of Bragg planes. Thus, X-ray version of Davisson-Germer experiment with tunable incident beam from a synchrotron resolves the question on the formation of standing waves within the unitcell.

The experiment is very important in that the discovery of the presence of standing waves will have transformational consequences in the description of crystal diffraction. Hence, the experiment is as important to quantum crystallography as the photoelectric effect is to quantum mechanics.

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Figure 1. **Historic DG peaks measured at $\theta_{hkl-\text{Bragg}} = 65^\circ$ fro unknown hkl planes.** Reproduced with citation of reference⁶ and with courtesy of Franklin Institute Journal.

FIGURE 3

Variation of the intensity of the regularly reflected electron beam with bombarding potential, for 10° incidence—Intensity vs. $V^{1/2}$.

Figure 2. **Historic DG peaks measured at $\theta_{111-\text{Bragg}} = 80^\circ$ from $\{111\}$ planes.** Reproduced with citation of reference⁷.