Chapter 2: Experimental Methods

Scanning Probe Methods

Volume / Surface Averaging Techniques

Scanning Probe Microscopy







Atomic Force Microscopy (AFM)

Magnetic Force Microscopy (MFM)







Surface Texture

Magnetic Force Image

Scanning Capacitance Microscopy (SCM)





bruker company

NCU, Tw.



Heavily Doped p NO δC/δV Heavily Doped n

Low Doped p

Low Doped n

Scanning Probe Methods:

Strength: excellent real space resolution combined with magnetic, electronics, optical, information

Weakness: slow, no depth information

Wave Diffraction and Reciprocal Lattice 倒晶格 Sir William Lawrence Bragg & William Henry Brag: NP 1915 "For their services in the analysis of crystal structure by means of X-ray"



(Received April 7,-Read April 17, 1913.)

Generation of X-Rays



Spectrum of the X-rays emitted by an X-ray tube with a rhodium target, operated at 60 kV. The smooth, continuous curve is due to bremsstrahlung, and the spikes are characteristic K lines for rhodium atoms.





A Monochromator Set-up



Figure 3 Sketch of a monochromator which by Bragg reflection selects a narrow spectrum of x-ray or neutron wavelengths from a broad spectrum incident beam. The upper part of the figure shows the analysis (obtained by reflection from a second crystal) of the purity of a 1.16 Å beam of neutrons from a calcium fluoride crystal monochromator. (After G. Bacon.)

X-ray Powder diffraction pattern of Si

What contributes to the intensities ?



Figure 4 X-ray diffractometer recording of powdered silicon, showing a counter recording of the diffracted beams. (Courtesy of W. Parrish.)

n (x), x element of Basis

Scattering at the Basis (Structure Factor, Atomic Form Factor)

> Scattering at lattice planes (Bragg Reflection)

n(r + T) = n(r)

A crystal is invariant under any translation of the form $T = u_1a_1 + u_2a_2 + u_3a_3$, where u_1 , u_2 , u_3 are integers and a_1 , a_2 , a_3 are the crystal axes

Electron number density n (r) is a periodic function of r: n (r + T) = n (r)



$$n(x + a) = n_0 + \sum [C_p \cos(2\pi px/a + 2\pi p) + S_p \sin(2\pi px/a + 2\pi p)]$$

= $n_0 + \sum [C_p \cos(2\pi px/a) + S_p \sin(2\pi px/a)] = n(x)$ (4)

A lattice point in the Fourier Space

$$n(x) = \sum_{p} n_{p} \exp(i2\pi p x/a)$$
 1D

 n_p now are complex numbers. To ensure that n(x) is a real function

$$n_{-p}^* = n_p$$

3D

The extension of the Fourier analysis to periodic functions $n(\mathbf{r})$ in three dimensions is straightforward. We must find a set of vectors **G** such that

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r})$$
(9)

is invariant under all crystal translations **T** that leave the crystal invariant. It will be shown below that the set of Fourier coefficients $n_{\mathbf{G}}$ determines the x-ray scattering amplitude.

Reciprocal Lattice Vector

To proceed further with the Fourier analysis of the electron concentration we must find the vectors **G** of the Fourier sum $\sum n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r})$ as in (9).

We construct the axis vectors \mathbf{b}_1 , \mathbf{b}_2 , \mathbf{b}_3 of the **reciprocal lattice**: 倒晶格

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} ; \qquad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} ; \qquad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} . \tag{13}$$

If \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 are primitive vectors of the crystal lattice, then \mathbf{b}_1 , \mathbf{b}_2 , \mathbf{b}_3 are **primitive vectors of the reciprocal lattice**. Each vector defined by (13) is orthogonal to two axis vectors of the crystal lattice. Thus \mathbf{b}_1 , \mathbf{b}_2 , \mathbf{b}_3 have the property $\mathbf{b}_1 = 2\pi \delta$.

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} , \qquad (14)$$

where $\delta_{ij} = 1$ if i = j and $\delta_{ij} = 0$ if $i \neq j$.

Points in the reciprocal lattice are mapped by the set of vectors

$$\mathbf{G} = v_1 \mathbf{b}_1 + v_2 \mathbf{b}_2 + v_3 \mathbf{b}_3 \quad , \tag{15}$$

倒晶格向量

where v_1 , v_2 , v_3 are integers. A vector **G** of this form is a **reciprocal lattice** vector.

Reciprocal Lattice 倒晶格

- 2. The reciprocal lattice is a lattice in the Fourier space associated with the crystal.
- 3. A diffraction pattern of crystal is a map of the reciprocal lattice of the crystal.

Bragg angle $\theta = \phi$; $\phi + \phi = 90^{\circ}$; $\sin \theta = \sin \phi = \cos \phi$

 $\mathbf{k} \bullet \mathbf{r} = \mathbf{k}\mathbf{r} \cos \phi = \mathbf{k}\mathbf{r} \sin \phi = \mathbf{k}\mathbf{r} \sin \theta$



Figure 6 The difference in path length of the incident wave **k** at the points O, **r** is $r \sin \varphi$, and the difference in phase angle is $(2\pi r \sin \varphi)/\lambda$, which is equal to $\mathbf{k} \cdot \mathbf{r}$. For the diffracted wave the difference in phase angle is $-\mathbf{k}' \cdot \mathbf{r}$. The total difference in phase angle is $(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}$, and the wave scattered from dV at **r** has the phase factor $\exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}]$ relative to the wave scattered from a volume element at the origin O.



Figure 7 Definition of the scattering vector $\Delta \mathbf{k}$ such that $\mathbf{k} + \Delta \mathbf{k} = \mathbf{k}'$. In elastic scattering the magnitudes satisfy k' = k. Further, in Bragg scattering from a periodic lattice, any allowed $\Delta \mathbf{k}$ must equal some reciprocal lattice vector \mathbf{G} .

Diffraction Conditions

Theorem. The set of reciprocal lattice vectors **G** determines the possible x-ray reflections.

We see in Fig. 6 that the difference in phase factors is $\exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}]$ between beams scattered from volume elements \mathbf{r} apart.

The total amplitude of the scattered wave in the direction of \mathbf{k}' is proportional to the integral over the crystal of $n(\mathbf{r}) d\mathbf{V}$ times the phase factor $\exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}]$.

the quantity F that we call the scattering amplitude:

$$F = \int dV \, n(\mathbf{r}) \, \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}] = \int dV \, n(\mathbf{r}) \, \exp(-i\Delta \mathbf{k} \cdot \mathbf{r}) \quad , \tag{18}$$

where $\mathbf{k} - \mathbf{k}' = -\Delta \mathbf{k}$, or

$$\mathbf{k} + \Delta \mathbf{k} = \mathbf{k}' \quad . \tag{19}$$

Here Δk measures the change in wavevector and is called the scattering vector (Fig. 7).

We introduce into (18) the Fourier components (9) of $n(\mathbf{r})$ to obtain for the scattering amplitude

$$F = \sum_{\mathbf{G}} \int d\mathbf{V} \, n_{\mathbf{G}} \exp[i(\mathbf{G} - \Delta \mathbf{k}) \cdot \mathbf{r}] \quad .$$
 (20)

When the scattering vector $\Delta \mathbf{k}$ is equal to a particular reciprocal lattice vector,

And **F** is ~0 when $\Delta \mathbf{k} \neq \mathbf{G}$

$$\Delta \mathbf{k} = \mathbf{G}$$

(21)

the argument of the exponential vanishes and $F = Vn_G$.

In elastic scattering of a photon its energy $\hbar \omega$ is conserved, Thus the magnitudes k and k' are equal, and $k^2 = k'^2$, a result that holds also for elastic scattering of electron and neutron beams.

 $\mathbf{k} + \mathbf{G} = \mathbf{k}'$, so that the **diffraction condition** is written as $(\mathbf{k} + \mathbf{G})^2 = k^2$, or

$$\mathbf{2k} \cdot \mathbf{G} + \mathbf{G}^2 = \mathbf{0} \tag{22}$$

This is the central result of the theory of elastic scattering of waves in a periodic lattice.

$$2\mathbf{k} \cdot \mathbf{G} = \mathbf{G}^2 \tag{23}$$

This particular expression is often used as the condition for diffraction.

Equation (23) is another statement of the Bragg condition (1). The result of Problem 1 is that the spacing d(hkl) between parallel lattice planes that are normal to the direction $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is $d(hkl) = 2\pi/|\mathbf{G}|$. Thus the result $2\mathbf{k} \cdot \mathbf{G} = G^2$ may be written as

$$2(2\pi/\lambda)\sin\theta = 2\pi/d(hkl)$$
, **G** = $2\pi/d$

or $2d(hkl) \sin \theta = \lambda$. Here θ is the angle between the incident beam and the crystal plane.

The integers hkl that define **G** are not necessarily identical with the indices of an actual crystal plane, because the hkl may contain a common factor n, whereas in the definition of the indices in Chapter 1 the common factor has been eliminated. We thus obtain the Bragg result:

$$2d\sin\theta = n\lambda \quad , \tag{24}$$

where d is the spacing between adjacent parallel planes with indices h/n, k/n, l/n.

Laue Equations

The original result (21) of diffraction theory, namely that $\Delta \mathbf{k} = \mathbf{G}$, may be expressed in another way to give what are called the Laue equations.

Take the scalar product of both $\Delta \mathbf{k}$ and \mathbf{G} successively with \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 . From (14) and (15) we get

$$\mathbf{a}_1 \cdot \Delta \mathbf{k} = 2\pi v_1 \; ; \qquad \mathbf{a}_2 \cdot \Delta \mathbf{k} = 2\pi v_2 \; ; \qquad \mathbf{a}_3 \cdot \Delta \mathbf{k} = 2\pi v_3 \; . \tag{25}$$

These equations have a simple geometrical interpretation. The first equation $\mathbf{a}_1 \cdot \Delta \mathbf{k} = 2\pi v_1$ tells us that $\Delta \mathbf{k}$ lies on a certain cone about the direction of \mathbf{a}_1 . The second equation tells us that $\Delta \mathbf{k}$ lies on a cone about \mathbf{a}_2 as well, and the third equation requires that $\Delta \mathbf{k}$ lies on a cone about \mathbf{a}_3 .

Thus, at a reflection $\Delta \mathbf{k}$ must satisfy all three equations; it must lie at the common line of intersection of *three* cones, which is a severe condition that can be satisfied only by systematic sweeping or searching in wavelength or crystal orientation—or by sheer accident.

Ewald Sphere Construction



Figure 8 The points on the right-hand side are reciprocal-lattice points of the crystal. The vector **k** is drawn in the direction of the incident x-ray beam, and the origin is chosen such that **k** terminates at any reciprocal lattice point. We draw a sphere of radius $k = 2\pi/\lambda$ about the origin of **k**. A diffracted beam will be formed if this sphere intersects any other point in the reciprocal lattice. The sphere as drawn intercepts a point connected with the end of **k** by a reciprocal lattice vector **G**. The diffracted x-ray beam is in the direction $\mathbf{k}' = \mathbf{k} + \mathbf{G}$. The angle θ is the Bragg angle of Fig. 2. This construction is due to P. P. Ewald.

BRILLOUIN ZONES

A Brillouin zone is defined as a Wigner-Seitz primitive cell in the reciprocal lattice.

Take (23) divided by 4 at both sides

$$\mathbf{k} \cdot \left(\frac{1}{2} \,\mathbf{G}\right) = \left(\frac{1}{2} \,G\right)^2 \tag{26}$$

We now work in reciprocal space, the space of the k's and G's. Select a vector **G** from the origin to a reciprocal lattice point. Construct a plane normal to this vector **G** at its midpoint. This plane forms a part of a zone boundary (Fig. 9a). An x-ray beam in the crystal will be diffracted if its wavevector **k** has the magnitude and direction required by (26). The diffracted beam will then be in the direction $\mathbf{k} - \mathbf{G}$, as we see from (19) with $\Delta \mathbf{k} = -\mathbf{G}$. Thus the Brillouin construction exhibits all the wavevectors **k** which can be Bragg-reflected by the crystal.



- **Figure 9a** Reciprocal lattice points near the point O at the origin of the reciprocal lattice. The reciprocal lattice vector \mathbf{G}_C connects points OC; and \mathbf{G}_D connects OD.
- Two planes 1 and 2 are drawn which are the perpendicular bisectors of \mathbf{G}_C and \mathbf{G}_D , respectively. Any vector from the origin to the plane 1, such as \mathbf{k}_1 , will satisfy the diffraction condition $\mathbf{k}_1 \cdot (\frac{1}{2} \mathbf{G}_C) = (\frac{1}{2} \mathbf{G}_C)^2$. Any vector from the origin to the plane 2, such as \mathbf{k}_2 , will satisfy the diffraction condition $\mathbf{k}_2 \cdot (\frac{1}{2} \mathbf{G}_D) = (\frac{1}{2} \mathbf{G}_D)^2$.

The set of planes that are the perpendicular bisectors of the reciprocal lattice vectors is of general importance in the theory of wave propagation in crystals. A wave whose wavevector drawn from the origin terminates on any of these planes will satisfy the condition for diffraction.

These planes divide the Fourier space of the crystal into fragments, as shown in Fig. 9b for a square lattice. The central square is a primitive cell of the reciprocal lattice. It is a **Wigner-Seitz cell** of the reciprocal lattice.



Figure 9b Square reciprocal lattice with reciprocal lattice vectors shown as fine black lines. The lines shown in white are perpendicular bisectors of the reciprocal lattice vectors. The central square is the smallest volume about the origin which is bounded entirely by white lines. The square is the Wigner-Seitz primitive cell of the reciprocal lattice. It is called the first Brillouin zone.

`the first Brillouin zone

The central cell in the reciprocal lattice is of special importance in the theory of solids, and we call it the first Brillouin zone. The first Brillouin zone is the smallest volume entirely enclosed by planes that are the perpendicular bisectors of the reciprocal lattice vectors drawn from the origin.

The first Brillouin zone of an *oblique* lattice in two dimensions is constructed in Fig. 10, and of a *linear* lattice in one dimension in Fig. 11. The zone boundaries of the linear lattice are at $k = \pm \pi/a$, where *a* is the primitive axis of the crystal lattice.

Historically, Brillouin zones are not part of the language of x-ray diffraction analysis of crystal structures, but the zones are an essential part of the analysis of <u>the electronic energy-band structure of crystals</u>.

2-D oblique lattice



First Brillouin zone

Figure 10 Construction of the first Brillouin zone for an oblique lattice in two dimensions. We first draw a number of vectors from O to nearby points in the reciprocal lattice. Next we construct lines perpendicular to these vectors at their midpoints. The smallest enclosed area is the first Brillouin zone.

1-D lattice



Figure 11 Crystal and reciprocal lattices in one dimension. The basis vector in the reciprocal lattice is **b**, of length equal to $2\pi/a$. The shortest reciprocal lattice vectors from the origin are **b** and $-\mathbf{b}$. The perpendicular bisectors of these vectors form the boundaries of the first Brillouin zone. The boundaries are at $k = \pm \pi/a$.

First Brillouin zone

Reciprocal Lattices



Reciprocal Lattice of a bcc Lattice

 $b_1 = (2\pi/a) (y+z)$

(π/a) (±**y** ±**z**)

Real Space Lattice

 $b_2 = (2\pi/a) (x+z)$



Volume:
$$\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3 = \frac{1}{2} a^3$$

$$b_3 = (2\pi/a) (x+y)$$

(π/a) (±**x** ±**y**)

1st Brillouin zone (π/a) (±**x** ±**z**)

 $a_1 = \frac{1}{2} a (-x+y+z)$ $a_2 = \frac{1}{2} a (x-y+z)$ $a_3 = \frac{1}{2} a (+x+y-z)$

cube of volume: $2(2\pi/a)^3$



2π/a

Reciprocal Lattice of a fcc Lattice



2π/a

Fourier Analysis of the Basis

$$F = \sum_{\mathbf{G}} \int d\mathbf{V} \, n_{\mathbf{G}} \exp[i(\mathbf{G} - \Delta \mathbf{k}) \cdot \mathbf{r}] \,. \qquad (20)$$

$$\Delta \mathbf{k} = \mathbf{G}$$

$$F_{\mathbf{G}} = N \int_{cell} d\mathbf{V} \, n(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) = NS_{\mathbf{G}} \,. \qquad (39)$$

$$structure factor$$

$$n(\mathbf{r}) = \sum_{j=1}^{s} n_{j}(\mathbf{r} - \mathbf{r}_{j}) \qquad (40)$$

$$atomic form factor (atomic property)$$

$$f_{j} = \int d\mathbf{V} \, n_{j}(\boldsymbol{\rho}) \exp(-i\mathbf{G} \cdot \boldsymbol{\rho}) \,, \qquad (42)$$

$$S_{\mathbf{G}} = \sum_{j} f_{j} \exp(-i\mathbf{G} \cdot \mathbf{r}_{j}) \,. \qquad (43)$$

bcc unit (cubic) cell For each atom of the unit cell $2:(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ $\mathbf{r}_i = x_i \mathbf{a}_1 + y_i \mathbf{a}_2 + z_i \mathbf{a}_3$ Real Lattice $r_1 = 0; r_2 = \frac{1}{2}a_1 + \frac{1}{2}a_2 + \frac{1}{2}a_3$ $1:(0,0,0)^{-}$ $\mathbf{G} = \mathbf{v}_{ix}\mathbf{b}_1 + \mathbf{v}_{iv}\mathbf{b}_2 + \mathbf{v}_{iz}\mathbf{b}_3$ Reciprocal Lattice $S_{G} = \Sigma f_{i} \exp(-i\mathbf{G} \cdot \mathbf{r}_{i})$ Structure Factor **Atomic Form Factor G** · $\mathbf{r}_{i} = (\mathbf{v}_{i}\mathbf{b}_{1} + \mathbf{v}_{i}\mathbf{b}_{2} + \mathbf{v}_{i}\mathbf{b}_{3}) \cdot (\mathbf{x}_{i}\mathbf{a}_{1} + \mathbf{y}_{i}\mathbf{a}_{2} + \mathbf{z}_{i}\mathbf{a}_{3}) = 2 \pi (\mathbf{v}_{ix}\mathbf{x}_{i} + \mathbf{v}_{iy}\mathbf{y}_{i} + \mathbf{v}_{iz}\mathbf{z}_{i})$ $S_{G} = \sum f_{i} \exp(-i2 \pi (v_{ix}x_{i} + v_{iy}y_{i} + v_{iz}z_{i}))$



the solution is independent of how we choose the unit cell and basis

$$S_{G} = \Sigma f_{j} \exp(-i2 \pi (v_{j}x_{j} + v_{j}y_{j} + v_{j}z_{j}))$$
$$= f (1 + \exp(-i\pi (v_{jx} + v_{jy} + v_{jz}))$$



= 0 if $v_{jx} + v_{jy} + v_{jz}$ = odd integer for example (100), (111),.... = 2f if $v_{jx} + v_{jy} + v_{jz}$ = even integer for example (200), (110), ...



Figure 16 Explanation of the absence of a (100) reflection from a body-centered cubic lattice. The phase difference between successive planes is π , so that the reflected amplitude from two adjacent planes is $1 + e^{-i\pi} = 1 - 1 = 0$.

FCC (conventional unit cell: 4 atoms)



$$S_{G} = \Sigma f_{j} \exp(-i2 \pi (v_{jx}x_{j} + v_{jy}y_{j} + v_{jz}z_{j}))$$

$$= f (1 + \exp(-i\pi (v_{jy}y_j + v_{jy}z_j) + \exp(-i\pi (v_{jx}x_j + v_{jz}z_j) + \exp(-i\pi (v_{jx}x_j + v_{jy}y_{jj}))$$

0 for even – odd (mixed) – (211), (221),

=

4f for only even or only odd – (311), (222),





Looks like sc with a/2 unit cell !

Looks like fcc !

Periodic Table of Elements

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
	1 H Hydrogen 1.00794	Atomic #	C Solid					Metals			Nonmetals							2 ² He Helium 4.002602	к	
:	3 2 Li Lithium 6.941	21 4 22 Be Beryllium 9.012182	Hg Liquid H Gas Rf Unknown			Alkaline earth met Alkali mei		Lanthanoids metals		Poor me	Other nonmetal	Noble ga	5 3 B Boron 10.811	6 2 C Carbon 12.0107	7 25 N Nitrogen 14.0067	8 2 0 0xygen 15.9994	9 ² / ₇ F 18.9984031	10 28 No 1797	CI	
	11 Sodium 22.98976928	² 12 Mg Magnesium 24.3050				tals	tals	Actinoids	_	tals	<u>o</u>	ses	13 28 Al Aluminium 26.9815386	14 28 Silicon 28.0855	15 28 P Phosphorus 30.973762	16 S Sulfur 32.065	17 CI Chlori 35.453	18 28 A Arg 39 8	^٤ K+	
	19 K Potassium 39.0983	2 0 2 8 8 a 2 1 cium .078	21 28 29 2 Scandium 44.955912	22 28 Ti 10 Titanium 47.887	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	² ⁸ ¹³ ² ² ⁸ Fe ¹⁴ ² ¹⁴ ²	27 28 Co 25 Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu _{Copper} 63.546	30 Zn 2inc 65.38	² 31 ² Galium 69.723	32 ² Ge ⁴ ¹⁸ ⁶ ⁶ ^{72.64}	33 28 As Arsenic 74.92160	34 Se ^{Selenium} 78.96	35 Bromine 79.904	6 2 Krypton 83.798	M N	
	37 Rubidium 85.4878	38 28 51 57 8 Strontium 87.62	39 28 Y 92 Yttrium 88.90585	40 28 Zr 10 Zirconium 91.224	41 Niobium 92.90838	42 Mo Molybdenum 95.96	43 Tc Technetium (97.9072)	² ⁸ ¹⁸ ¹⁴ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸	45 28 Rh 18 Rhodium 102.90550	46 Pd Palladium 108.42	47 Ag ^{Silver} 107.8882	48 Cd 112.411	49 28 10 18 10 18 10 18 10 18 114.818	50 28 Sn 18 4 Tin 118.710	51 28 Sb 18 Antimony 121.780	52 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	53 2 18 10 10 10 128.90447	54 28 Xe 18 Xenon 131.293	K M N O	
(55 Cs 1 Caesium 132.9054519	² 56 ² Ba ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸	57–71	72 28 Hf 18 Hafnium 2 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 188.207	² ¹⁸ ¹⁸ ¹⁸ ² ² ¹⁹ ² ¹⁹ ² ¹⁹ ² ¹⁰ ¹⁰ ¹⁰ ¹⁰ ¹⁰ ¹⁰ ¹⁰ ¹⁰	77 28 17 18 17 18 192.217	78 Pt 1 Platinum 195.084	79 Au Gold 196.986589	80 80 Hg 1 Mercury 200.59	81 28 TI 18 204.3833	82 28 Pb 32 Lead 4 207.2	83 28 Bi 18 Bismuth 208.98040	84 Po (208.9824)	85 28 At 32 Astatine 7 (209.9871)	86 28 Rn 32 Radon (222.0178)	K M N P	
7	87 Fr (223)	88 2 Ra 16 Ra 16 22 88 Ra 16 22 18 8 2 22 10 20 20 20 20 20 20 20 20 20 2	89–103	104 28 Rf 322 Rutherfordium 10 (281)	105 Db Dubnium (282)	106 Sg Seaborgium 12 (288)	107 Bh Bohrium (284)	² ⁸ ¹⁸ ¹⁸ ²² ¹³ ¹³ ¹⁴ ¹⁴ ¹⁴ ¹⁵ ¹⁶ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸ ¹⁸	109 28 Mt 322 Meitnerium 12 (288)	110 Ds Damstadium (271)	111 Rg Roentgenium (272)	2 112 Uub 1 Ununbium (285)	2 113 2 8 2 Uut 32 2 Ununtrium 18 (284)	$\begin{array}{c} 114 & {}^2_8 \\ \textbf{Uuq} & {}^{18}_{32} \\ {}^{10}_{\text{Unuquadium}} & {}^{18}_{4} \\ {}^{(289)} \end{array}$	115 Uup Ununpentum (288) 115 18 12 232 18 12 232 18 18 12 232 18 18 18 18 232 18 18 18 18 18 18 18 18 18 18	116 Uuh Ununhexium (292)	117 Uus Unurseptum	118 Uuo Ununoctium (294) 28 18 22 32 22 32 23 23 23 23 23 23	K L M N O P Q	

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.





$$f_j = 4\pi \int dr \, n_j(r) r^2 \quad \frac{\sin Gr}{Gr} \; .$$

(1) if electron density localized at r=0: (sin Gr)/Gr \sim 1

$$f_j = 4\pi \int dr \, n_j(r) r^2 = Z$$
, (51)

(50)

f represents the ration of the radiation amplitude scattered by the actual distribution in an atom to that scattered by one electron localized at a point.

(2) Scattering in forward direction (G = 0)

(3) Most electron scattering centers are not affected by the chemical environment. Therefore, the atomic form factor is not very sensitive to small redistribution of electrons due to bonding (valence electrons)



Figure 18 Absolute experimental atomic scattering factors for metallic aluminum, after Batterman, Chipman, and DeMarco. Each observed reflection is labeled. No reflections occur for indices partly even and partly odd, as predicted for an fcc crystal.