Effect of Temperature on Atomic Scattering Curve

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Abstract

We have calculated the temperature dependence of the atomic scattering curve for the elements Si, C, Pt and Cu. At first we have drawn the general atomic scattering curve for the above elements. A quantity ‘f’, the atomic scattering factor, is said to describe the ‘efficiency’ of scattering of a given atom in a given direction. The actual calculation of ‘f’ involves sin θ, rather than θ, so that the net effect is that ‘f’ decreases as the quantity (sin θ)/λ increases. Secondly, we have considered Debye temperature factor using Debye model. And we observe that for Debye approximation, the curve decreases a little bit.

Keywords: Scattering curve; Scattering factor; Temperature factor; Debye temperature; Debye model, MATLAB software package

Introduction

The atomic scattering factor ‘f’ is defined as the ratio of amplitudes:

\[ f = \frac{\text{amplitude of the wave scattered by one atom}}{\text{amplitude of the wave scattered by one electron}} \]

It is clear that f=Z (atomic number) for any atom scattering in the forward direction [1]. As θ increases, the waves scattered by individual electrons become more and more out of phase and ‘f’ decreases [2]. The atomic scattering factor depends also on the wavelengths of the incident beam [3]. At a fixed value of θ, ‘f’ will be smaller, the shorter the wavelength, leading to greater interference between the scattered beams. Calculated values of ‘f’ for various atoms and various values of (sin θ)/λ are tabulated in the Tables 1-3. We see that the curve begins at the atomic number and decreases to very low values for scattering in the backward direction (θ near 90º) for very short wavelengths [4-8]. Again, we observe that due to temperature factor, the general atomic scattering curve is affected for Debye temperature approximation. From this point of view, we have studied the temperature factor dependence of the atomic scattering curve for Debye temperature approximation [9-11].

Thermal (temperature factor) effects on the atomic scattering curve: (Debye approximation)

So far, a crystal has been considered as a collection of atoms located at fixed points in the lattice [12]. Actually, the atoms undergo thermal vibration about their mean positions even at the absolute zero of temperature, and the amplitude of this vibration increases as the temperature increases [13]. We need any quantitative information about the temperature factor e-M, but it is convenient to describe the calculation here before considering other thermal effects. Formally, this effect is included by defining f as the atomic scattering factor of an atom undergoing thermal vibration, f2 as the same quantity for an atom at rest, and the two is related by [14]

\[ f = f_2 e^{M} \]  

(1)

The quantity f2 is then the scattering factor as usually tabulated. Because the intensity of any line depends on f2 calculated intensities must be multiplied by e-M to allow for thermal vibration [15]. The quantity M depends on both the amplitude u of thermal vibration and the scattering angle 2θ:

\[ M = 2\pi \left( \frac{x}{T} \right) = 8\pi u \left( \frac{\sin \theta}{A} \right) = B \left( \frac{\sin \theta}{A} \right) \]  

(2)

Where, u2 is the mean square displacement of the atom in a direction normal to the diffracting planes. The exact calculation of u2 as a function of temperature is extremely difficult [16], which means that M or B is tough to determine accurately. Peter Debye has given the following expression:

\[ M = \frac{6h^2T}{mk^2} \phi(x) + \frac{x}{4} \left( \frac{\sin \theta}{A} \right)^2 \]  

(Debye approximation)  

(3)

Where, h is the Planck’s constant, T is the absolute temperature, m is the mass of the vibrating atom, k is the Boltzmann’s constant, Θ is the Debye characteristic temperature of the substance in K, Θ = kT/m, and ϕ is a function tabulated [17], along with values of Θ, m=A/N where A=atomic weight and N=Avogadro’s number, the coefficient of the bracketed terms becomes, by inserting the numerical values of the constants in eqn. (3):

\[ \frac{6h^2T}{mk^2} \phi \left( \frac{x}{4} \left( \frac{\sin \theta}{A} \right)^2 \right) = 1.15 \times 10^{-4} \]  

If θ is in radians. In eqn. (3) is approximate and applies only to elements with cubic crystal structure.

So, ultimately in eqn. (3) reduces to,

\[ M = \frac{1.15 \times 10^{-4} T}{\Theta^3} \phi \left( \frac{x}{4} \left( \frac{\sin \theta}{A} \right)^2 \right) \]  

(4)

Again, ϕ can be expressed as:

\[ \phi \left( \frac{x}{4} \right) = 1 + \frac{x^2}{36} - \frac{x^4}{3600} \]

Thus, M can be written as.

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depends on the contributions from individual electrons of the ordering or lack of ordering of the scattering atoms. While it may not be precisely true, assuming that the charge distribution \( \rho = \rho(r) \) of electrons in the atom, and \( f_0 \) the atomic scattering factor is made up of the scattering factors \( f \) in the different "portions" of the atom, and \( f_0 \) the atomic scattering factor is given by

\[
f = f_0 \exp \left( \frac{1.15 \times 10^4 T}{A^2} \left( 1 + \frac{x^2}{36} - \frac{x^4}{3600} \left( \frac{\sin \theta}{\lambda} \right)^2 \right) \right)
\]

Finally, we get,

\[
f = f_0 \exp \left( \frac{1.15 \times 10^4 T}{A^2} \left( 1 + \frac{x^2}{36} - \frac{x^4}{3600} \left( \frac{\sin \theta}{\lambda} \right)^2 \right) \right)
\]

Calculation of general scattering factor

As seen by incident X-ray photons, a sample consists of a spatially inhomogeneous sea of electrons. In fact, quantum mechanics indicates that each electron is itself spread into a diffuse cloud of negative charge.

Using the proper charge distribution \( \rho = \rho(r) \) of electrons in the atom, and \( f_0 \), the atomic scattering factor is made up of the contributions from individual electrons \( f_0 \) given by

\[
f = \int \exp \left( \frac{1.15 \times 10^4 T}{A^2} \left( 1 + \frac{x^2}{36} - \frac{x^4}{3600} \left( \frac{\sin \theta}{\lambda} \right)^2 \right) \right) \rho(r) \, dr
\]

Calculation of the precise values of \( f_0 = \sum(f_i) \) depends on the detailed knowledge of the charge distribution \( \rho \).

Similarly, using the proper charge distribution \( \rho = \rho(r) \) of electrons in the atom of Cu in eqn. (8), we readily obtain the atomic scattering factors for Cu corresponding to sin(\( \theta/\lambda \)), below:

\[
f = f_0 \times \exp \left( \frac{1.15 \times 10^4 T}{A^2} \left( 1 + \frac{x^2}{36} - \frac{x^4}{3600} \left( \frac{\sin \theta}{\lambda} \right)^2 \right) \right) = f_0 \times e^{-\frac{T}{1000}}
\]

For Cu, Atomic weight A=63.546, Debye characteristic Temperature \( \Theta = 343.5 \) K, Absolute Temperature T in Kelvin (100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650).

Using the information obtained in the Tables 1-3, we plot the atomic scattering curve, giving (sin(\( \theta/\lambda \))) in the x-direction and atomic scattering factors \( f_0 \) in the y-direction, we obtain the curve:

C. Calculation of atomic scattering factors for Cu

Similarly, using the proper charge distribution \( \rho = \rho(r) \) of electrons in the atom of Pt in eqn. (8), we readily obtain the atomic scattering factors for Pt corresponding to sin(\( \theta/\lambda \)), below:

D. Calculation for scattered atomic scattering factor (Debye approximation)

Here, the equation:

\[
f = f_0 \times \exp \left( \frac{1.15 \times 10^4 T}{A^2} \left( 1 + \frac{x^2}{36} - \frac{x^4}{3600} \left( \frac{\sin \theta}{\lambda} \right)^2 \right) \right) = f_0 \times e^{-\frac{T}{1000}}
\]

For Pt, Atomic weight A=195.08, Debye characteristic Temperature \( \Theta = 240 \) K, Absolute Temperature T in Kelvin (100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700).

Using the information obtained in the Tables 4-6, we plot the atomic scattering curve, giving (sin(\( \theta/\lambda \))) in the x-direction and atomic scattering factors \( f_0 \) in the y-direction, we obtain the curve.

E. Calculation of atomic scattering factors for Pt

As above, from eqn. (8), we readily obtain the atomic scattering factors for Pt corresponding to sin(\( \theta/\lambda \)), below:

F. Calculation for scattered atomic scattering factor (Debye approximation)

Here, the equation:

\[
f = f_0 \times \exp \left( \frac{1.15 \times 10^4 T}{A^2} \left( 1 + \frac{x^2}{36} - \frac{x^4}{3600} \left( \frac{\sin \theta}{\lambda} \right)^2 \right) \right) = f_0 \times e^{-\frac{T}{1000}}
\]

For Pt, Atomic weight A=195.08, Debye characteristic Temperature \( \Theta = 240 \) K, Absolute Temperature T in Kelvin (100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700).

### Table 1: General Atomic Scattering Factors for Si

| (sinθ)/λ | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 | 1.1 |
|-----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Si (f0)   | 14  | 11.35| 9.4 | 8.2 | 7.15| 6.1 | 5.1 | 4.2 | 3.4 | 2.95| 2.6 | 2.3 |

### Table 2: When the Debye Approximation temperature factor is considered as (e^\( \frac{M}{A^2} \))

| (sinθ)/λ | exp(-M) | exp(-M)×e^\( \frac{M}{A^2} \) |
|-----------|----------|--------------------------|
| 0.0        | 1.00     | 1.00 9958 9901 9744 9484 | 9013 8592 7952 7195 6345 5438 4516 |

### Table 3: Debye approximation temperature factor is considered as (e^\( \frac{M}{A^2} \))

| (sinθ)/λ | exp(-M) | exp(-M)×e^\( \frac{M}{A^2} \) |
|-----------|----------|--------------------------|
| 0.0        | 1.00     | 1.00 9958 9804 9494 8894 | 8287 7383 6324 5176 4025 3957 2039 |
Using the information obtained in the Tables 7-9, we plot the atomic scattering curve for Pt, giving \(\text{sin}\theta/\lambda\) in the x-direction and atomic scattering factors \(f_0\) in the y-direction, we obtain the curve:

### G. Calculation of atomic scattering factors for C

Similarly, in eqn. (8), we readily obtain the atomic scattering factors for C corresponding to \(\text{sin}\theta/\lambda\), below:

#### H. Calculation for scattered atomic scattering factor (Debye approximation)

Here, the equation:

\[
f = f_0 \times \exp \left[ -\frac{1.15 \times 10^4 \mathcal{T}}{24 \mathcal{T}^2} \left( 1 + \frac{\mathcal{T}^2}{36} - \frac{\mathcal{T}^4}{3600} \right) \frac{\text{sin}\theta}{\lambda} \right] = f_0 \times e^{-M}
\]

For C, Atomic weight \(A=12.011\), Debye characteristic Temperature \(\Theta=2230\, \text{K}\), Absolute Temperature \(T\) in Kelvin (100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650).

Using the information obtained in the Tables 10-12 we plot the atomic scattering curve for C, giving \(\text{sin}\theta/\lambda\) in the x-direction and atomic scattering factors \(f_0\) in the y-direction, we obtain the curve

### Results and Discussions

Atomic scattering curve decreases with temperature factor. We have calculated the effect of temperature of the atomic scattering curve.

**Figure 1:** Temperature Dependence of Atomic scattering curve for Si with Debye Approximation.

![Atomic scattering curve for Si](image_url)

**Table 4:** Atomic scattering for Cu.

| \(\text{Sin}\theta/\lambda\) | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 | 1.1 | 1.2 |
|--------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \(\exp(-M)\) Cu (f_0)   | 29  | 25.9| 21.6| 17.9| 15.2| 13.3| 11.7| 10.2| 9.1 | 8.1 | 7.3 | 6.6 | 6.0 |

**Table 5:** Debye approximation temperature factor is \(e^{-M}\).

| \(\exp(-M)\) | 1.0000 | 0.9974 | 0.9948 | 0.9926 | 0.9906 | 0.9886 | 0.9867 | 0.9848 | 0.9832 | 0.9817 | 0.9803 | 0.9792 | 0.9781 |
|---------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| \(f_0\) x \(\exp(-M)\) Cu | 29      | 25.83   | 21.31   | 17.26   | 14.08   | 11.58   | 9.34    | 7.23    | 5.53    | 4.05    | 2.88    | 1.96    | 1.27 |

**Table 6:** Debye approximation temperature factor is \(e^{-2M}\).

| \(\exp(-M)\) | 1.0000 | 0.9994 | 0.9998 | 0.9991 | 0.9984 | 0.9977 | 0.9970 | 0.9963 | 0.9957 | 0.9950 | 0.9943 | 0.9936 | 0.9929 |
|---------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| \(f_0\) x \(\exp(-M)\) Cu | 29      | 25.77   | 21.04   | 16.65   | 13.05   | 10.10   | 7.46    | 5.13    | 3.37    | 2.03    | 1.14    | 0.58    | 0.27 |

**Table 7:** Atomic scattering for Pt.

| \(\text{Sin}\theta/\lambda\) | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 | 1.1 | 1.2 |
|--------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \(\exp(-M)\) Pt (f_0)   | 78  | 72.6| 64.0| 56.2| 48.9| 43.1| 39.2| 35.6| 32.5| 29.5| 27.0| 24.7| 22.7 |

**Table 8:** Debye approximation temperature factor is considered as \(\exp(-M)\).

| \(\exp(-2M)\) | 1.0000 | 0.9967 | 0.9931 | 0.9831 | 0.9593 | 0.9049 | 0.8341 | 0.7425 | 0.6345 | 0.5173 | 0.3998 | 0.2912 | 0.1987 | 0.1262 |
|---------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| \(f_0\) x \(\exp(-2M)\) Pt | 78      | 72.36   | 62.92   | 53.61   | 44.25   | 35.95   | 29.11   | 22.59   | 16.81   | 11.79   | 7.86   | 4.91   | 2.86 |

**Table 9:** Debye approximation temperature factor is considered as \(\exp(-2M)\).

| \(\text{Sin}\theta/\lambda\) | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 | 1.1 | 1.2 |
|--------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \(\exp(-2M)\) C (f_0)   | 6   | 4.6 | 3.0 | 2.2 | 1.9 | 1.7 | 1.6 | 1.4 | 1.3 | 1.1 | 1.0 | 0.9 | 22.7 |

**Table 10:** Atomic scattering for C.

| \(\exp(-M)\) | 1.0000 | 1.0019 | 0.9998 | 0.9981 | 0.9937 | 0.9845 | 0.9723 | 0.9567 | 0.9377 | 0.9150 | 0.8882 | 0.8576 | 0.8227 | 0.3552 |
|---------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| \(f_0\) x \(\exp(-M)\) C | 6        | 4.61    | 3.0     | 2.19    | 1.87    | 1.65    | 1.53    | 1.31    | 1.19    | 1.03    | 0.86    | 0.74    | 0.3552 |

**Table 11:** Debye Approximation temperature factor is considered as \(\exp(-M)\).

| \(\exp(-2M)\) | 1.0000 | 1.0015 | 0.9995 | 0.9875 | 0.9693 | 0.9453 | 0.9154 | 0.8793 | 0.8371 | 0.7890 | 0.7353 | 0.6769 | 0.1262 |
|---------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| \(f_0\) x \(\exp(-2M)\) C | 6        | 4.60    | 2.99    | 2.17    | 1.84    | 1.61    | 1.46    | 1.23    | 1.09    | 0.92    | 0.74    | 0.61    | 2.86 |

**Table 12:** Debye approximation temperature factor is considered as \(\exp(-2M)\).
and observe that the atomic scattering curve decreases a little bit compared with general scattering curve. So, atomic scattering curve is affected by the temperature factor.

References

1. Cullity BD, Stock SR (2014) Elements of X-ray Diffraction. Pearson Education.
2. Mahmud MR, Rahman MO (2010) Temperature dependence of the reflection lines. Jahangirnagar University Journal of Science 3: 23-32.
3. Zachariasen WH (2004) Theory of X-ray Diffraction in Crystals. Courier Corporation.
4. Kittel C (1976) Introduction to solid state physics. New York: Wiley 8.
5. Chang SL, Höche HR (1985) Multiple diffraction of X-rays in crystals. Springer Series in Solid-State Sciences 50.
6. Obaidur RM (2002) Design, fabrication and performance of silicon monolithic monochromators and its application for lattice spacing measurements of Si and GaAs single crystals with synchrotron radiation.
7. Maidul IM (2014) Study of the Dynamical Theory of X-ray Diffraction with Absorption. Jahangirnagar University.
8. Authier A (2004) Dynamical theory of X-ray diffraction. Oxford University Press on Demand 11.
9. Warren BE (1990) X-ray Diffraction. Courier Corporation.
10. Jahirul I (2011) Study of the Dynamical Theory of X-ray Diffraction.
11. Bragg WL (1929) The diffraction of short electromagnetic waves by a crystal.
12. Seeger A (1962) Solid state physics. Zeitschrift für Physikalische Chemie 32: 402-402.
13. Sah CT (1991) Fundamentals of solid state electronics. World Scientific Publishing Company.
14. James R (1948) The Optical Principles of the Diffraction of X-rays (Bell, London).
15. Bragg L (1968) X-ray crystallography. Scientific American 219: 58-74.
16. Reitz JR, Milford FJ, Christy RW (2008) Foundations of electromagnetic theory. Addison-Wesley Publishing Company.
17. Omar MA (1975) Elementary solid state physics: principles and applications. Pearson Education India.