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STUDIES OF EFFECT OF ATOM POSITIONS ON THE NEUTRON DIFFRACTION INTENSITIES

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ABSTRACT

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The occurrence of a diffraction line or particular reflection is determined by diffraction conditions. The present work is a theoretical study in which the condition of reflection for polycrystalline Si with atoms at the various crystal lattice sites in the Fd3m space group have been found out by calculation the structure factors for different reflections. Diffraction patterns have been simulated for the distribution of atoms at different ratio over the sites and the intensities of the Bragg peaks are compared. The effect of atom positions on intensities has thus been found out. This result will be of help to the scientist working in material science at different laboratory in home and abroad.

Key words: *atom position, neutron diffraction intensity, structure factor and reflection condition*

INTRODUCTION

The regular periodic arrangement in crystalline solids is detected by examining the way in which they scatter neutrons. Diffracted beams are built up from the components of scattered neutrons by the individual atoms in the sample. A variety of matters had been studied by this method for precise measurements of lattice parameter and location of different ions into the unit cell of a crystal. The neutron diffraction involves the studies of the spatial ordering of atoms, only the scattering intensities are of interests to us. The regular periodic arrangement in crystalline solids is detected by examining the way in which they scatter neutrons. Diffracted beams are built up from the components of scattered neutrons by the individual atoms in the sample. Neutron diffraction is by now an established technique for revealing the crystallographic structures of condensed matter. In recent years more complicated systems have also been studied by neutron diffraction (Zyumov *et al.* 1970).

The occurrence of a diffraction line or particular reflection is determined by diffraction conditions. The conditions are obtained from the calculation of structure factors. The values of structure factors (Bacon 1975) impose certain limits on various reflections depending on the atom positions in the unit cell. These limits are known as the diffraction conditions. Once a reflection is allowed, its intensity is also dependent on the atom positions. Our present study deals with the calculations of structure factors, to find out the reflection conditions for variable atomic positions and simulation of diffraction pattern with the computer program "FullProf" (Juan 1996) to see the variation of intensities of Bragg diffraction peaks for variable atom positions. The calculations have been done for a standard sample material Si that belongs to the space group Fd3m (Islam *et al.* 2008).

MATERIALS AND METHODS

In the Wyckoff notation (Ralph, 1930) the crystal lattice series are

(8a): $\left(\frac{1}{8}\frac{1}{8}\frac{1}{8}\right), \left(\frac{7}{8}\frac{7}{8}\frac{7}{8}\right)$

(8b): $\left(\frac{3}{8}\frac{3}{8}\frac{3}{8}\right), \left(\frac{5}{8}\frac{5}{8}\frac{5}{8}\right)$

(16c): $(000), \left(0\frac{1}{4}\frac{1}{4}\right), \left(\frac{1}{4}0\frac{1}{4}\right), \left(\frac{1}{4}\frac{1}{4}0\right)$

(16d): $\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right), \left(\frac{1}{2}\frac{1}{4}\frac{1}{4}\right), \left(\frac{1}{4}\frac{1}{2}\frac{1}{4}\right), \left(\frac{1}{4}\frac{1}{4}\frac{1}{2}\right)$

The structure facture F has been calculated from the following equation (Kittel 1976)

$$\text{Structure factor } F = \sum_j n_i b_{si} e^{2\pi i\left(hu_j + kv_j + lw_j\right)} + \text{F.C} \qquad (1)$$

Where, F.C. = Face centering translation, b_{si} = Scattering amplitude factor of Si atom. n_i = Occupation number of Si atom (in this case n_i =1) u_j, v_j and w_j are the atom co-ordinates.

The reflection condition is obtained from the value of structure factor. A popular version of the Rietveld profile refinement program, "FullProf" has been used for the refinement of the neutron diffraction data presented in this dissertation.

This program is based on the code of Young & Wiles program, which in turn is also a major modification of the original Rietveld-Hewat program. The "FullProf" is based on the code DBW3.3s. (Juan 1996). The source is written in standard **FORTRAN 77** language and has been modified in order to be easily adapted to different computers. The author has made the program available in his specific wave site in the internet and it is very widely used in almost all neutron scattering laboratories around the world.

Finally Diffraction patterns have been simulated for the distribution of atoms at different ratio over the sites and the intensities of the Bragg peaks are compared with the computer program "FullProf"(Juan 1996).

RESULTS AND DISCUSSION

For Si with 100% atoms at (8a) position, the structure factor becomes (from eq. 1)

$$\therefore F = b_{si}\left\{1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(l+h)}\right\}\left\{e^{\frac{\pi i}{4}(h+k+l)} + e^{\frac{7\pi i}{4}(h+k+l)}\right\} \quad (2)$$

If the indices are unmixed i.e. all are even or all are odd then, h+k = even, k+l = even and l+h = even, this gives $e^{\pi i(\text{even number})} = 1$, Now equation (2) becomes

$$\therefore F = 4b_{si}\left[e^{\frac{\pi i}{4}(h+k+l)} + e^{\frac{7\pi i}{4}(h+k+l)}\right] \quad (3)$$

If the indices are mixed i.e. even and odd mixed, then there are three possibilities

h+k = even number, k+l = odd number, l+h = odd number, or, h+k = odd number, k+l = even number, l+h = odd number,or, h+k = odd number, k+l = odd number, l+h = even number, this gives $e^{\pi i(\text{odd number})} = -1$, then equation (2) becomes, F = 0

Now to find out the reflection conditions the following calculations are done. At first it is considered that indices are even, then equation (3) becomes

For hkl =111, F = $-5.656\,b_{si}$. For hkl = 311, F = $-5.656\,b_{si}$. For hkl = 331, F = $5.656\,b_{si}$. For hkl = 333, F = $5.656\,b_{si}$. For hkl = 551, F = $-5.656\,b_{si}$. For hkl =335, F = $-5.656\,b_{si}$

Now it is considered that all indices are even, and then equation (3) becomes

For hkl = 200, F = 0. For hkl = 220, F = $-8\,b_{si}$. For hkl = 222, F = 0. For hkl = 400, F = $-8\,b_{si}$. For hkl = 422, F = $8\,b_{si}$. For hkl = 440,F = $8\,b_{si}$. For hkl = 442, F = 0. For hkl = 444, F = $-8\,b_{si}$.

From above deductions of structure factors it may be concluded that the allowed reflections follow the conditions:

h+k+l =2n+1

or, h+k+l = 4n

Where n is the positive integer.

Normally for Si the atoms are located in the (8a) site only. However, for our purpose of investigating the effect of change of atomic locations we have assumed the atoms to be located in all possible locations separately and also partially over two different locations. The allowed reflection condition for the corresponding composition have been calculated and listed table-1.

Table 1. The allowed reflection condition for corresponding composition of si atom sites

Lattice site in Wyckoff notation	Reflection conditions	Lattice site in Wyckoff notation	Reflection conditions	Lattice site in Wyckoff notation	Reflection conditions	Lattice site in Wyckoff notation	Reflection conditions
(8a)	h+k+l=2n +1 or h+k+l=4n	(8a)35% + (16c)65%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8b)20% + (16c)80%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8b)90% + (16d)10%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(8b)	h+k+l=2n +1 or h+k+l=4n	(8a)50% + (16c)50%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8b)25% + (16c)75%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)10% + (16d)90%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(16c)	h+k+l=2n+1 or h+k=2n k+l=2n l+h=2n	(8a)65% + (16c)35%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8b)35% + (16c)65%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)20% + (16d)80%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(16d)	h+k+l=2n+1 or h+k=2n k+l=2n l+h=2n	(8a)75% + (16c)25%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8b)50% + (16c)50%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)25% + (16d)75%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(8a)10% + (8b) 90%	h+k+l=2n+1 or h+k+l=4n	(8a)80% + (16c)20%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	8b)65% + (16c)35%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)35% + (16d)65%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(8a)20% + (8b)80%	h+k+l=2n+1 or h+k+l=4n	(8a)90% + (16c)10%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	8b)75% + (16c)25%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)50% + (16d)50%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(8a) 25% + (8b)75%	h+k+l=2n+1 or h+k+l=4n	(16c)10% + (16d)90%	h+k+l=2n+1 or h+k=4n k+l=4n l+h=4n	(8b)80% + (16c)20%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)65% + (16d)35%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(8a)35% + (8b)65%	h+k+l=2n+1 or h+k+l=4n	(16c)20% + (16d)80%	h+k+l=2n+1 or h+k=4n k+l=4n l+h=4n	(8b)90% + (16c)10%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)75% + (16d)25%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(8a)50% + (8b)50%	h+k+l=4n	(16c)25% + (16d)75%	h+k+l=2n+1 or h+k=4n k+l=4n l+h=4n	8b)10% + (16d)90%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)80% + (16d)20%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(8a)65% + (8b)35%	h+k+l=2n+1 or h+k+l=4n	(61c)35% + (16d)65%	h+k+l=2n+1 or h+k=4n k+l=4n l+h=4n	8b)20% + (16d)80%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8a)90% + (16d)10%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n
(8a)75% + (8b)25%	h+k+l=2n+1 or h+k+l=4n	(16c)50% + (16d)50%	h+k=4n k+l=4n l+h=4n	8b)25% + (16d)%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n		
(8a)80%+ (8b)20%	h+k+l=2n+1 or h+k+l=4n	(16c)65% + (16d)35%	h+k+l=2n+1 or h+k=4n k+l=4n l+h=4n	8b)35% + (16d)65%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n		
(8a)90%+ (8b)10%	h+k+l=2n+1 or h+k+l=4n	(16c)75% + (16d)25%	h+k+l=2n+1 or h+k=4n k+l=4n l+h=4n	8b)50% + (16d)50%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n		
(8a)10% + (16c)90%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(16c)80% + (16d)20%	h+k+l=2n+1 or h+k=4n k+l=4n l+h=4n	8b)65% + (16d)35%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n		
(8a)20% + (16c)80%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(16c)90% + (16d)10%	h+k+l=2n+1 or h+k=4n k+l=4n l+h=4n	8b)75% + (16d)25%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n		
(8a)25% + (16c)75%	h+k+l=2n+1 or h+k+l=4n,or h+k=4n k+l=4n l+h=4n	(8b)10% + (16c)90%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n	(8b)80% + (16d)20%	h+k+l=2n+1 or h+k+l=4n or h+k=4n k+l=4n l+h=4n		

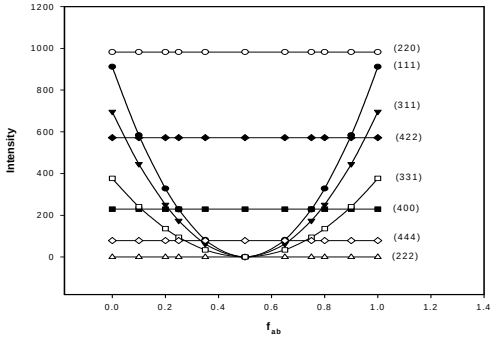

Figure-1: *Variation of intensities of different Bragg peaks with change of atom positions from (8a) to (8b).*

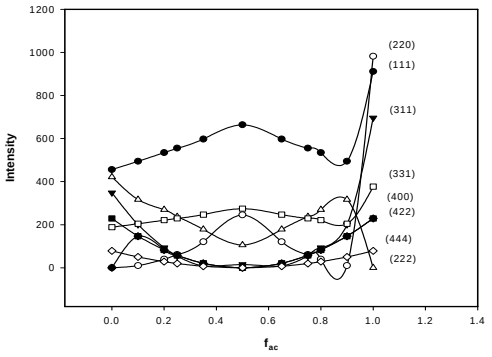

Figure-2: *Variation of intensities of different Bragg peaks with change of atom positions from (8a) to (16c).*

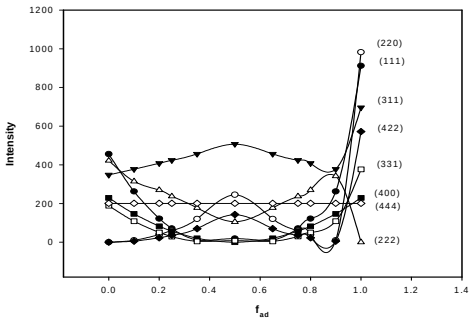

Figure-3: *Variation of intensities of different Bragg peaks with change of atom positions from (8a) to (16d).*

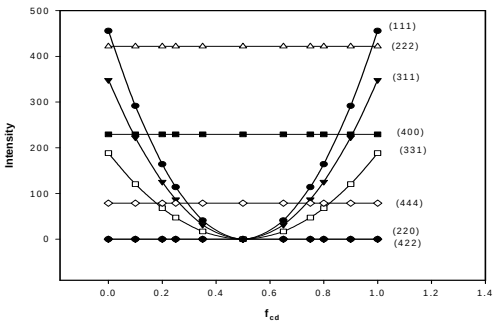

Figure-4: *Variation of intensities of different Bragg peaks with change of atom positions from (16c) to (16d).*

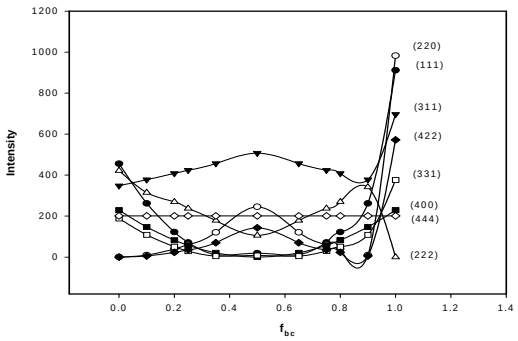

Figure-5: *Variation of intensities of different Bragg peaks with change of atom positions from (8b) to (16c).*

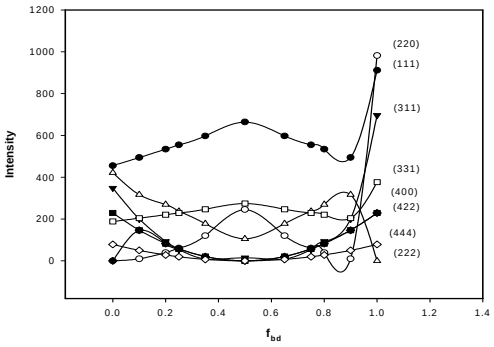

Figure-6: *Variation of intensities of different Bragg peaks with change of atom positions from (8b) to (16d).*

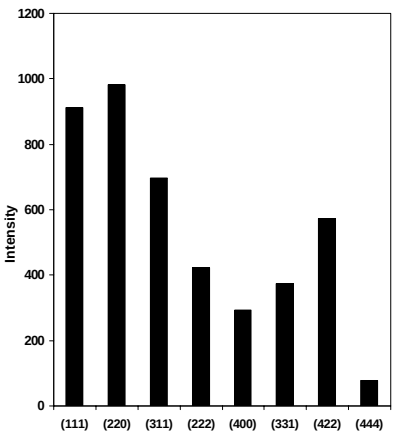

Figure-7: Maximum intensity for various peaks for different atom positions

Bragg intensities for various reflections have been found out for the different atom positions in for which structure factors have been calculated in table 1. This has been accomplished by simulating the diffraction patterns with the help of the computer program "FullProf". The simulation for all atomic positions has been done with a constant neutron wavelength (λ =1.5Å). Space group Fd3m has been used for generating the patterns for Si. Atom positions have been varied in the ratio obtained in table 1. All other parameters were kept fixed for all the calculations. The integrated intensities for various reflections have been obtained from the output of the program. Finally the intensity of the Bragg peak (111), (220), (331), (222), (400), (331), (422) and (444) are plotted in Figures 1 to 6.

Fig. 1 shows the variation of intensities of Bragg peaks when the atoms migrate from (8a) to (8b). The fraction of the atoms migrated from (8a) to (8b) has been denoted by f_{ab}. It is observed that the intensity for the reflection of even indices remains constant with variation of $f_{ab.}$ The intensity for the reflections of odd indices are affected by the variation of f_{ab}. The intensity for all odd reflection falls to zero while f_{ab} becomes one half. And the odd reflection show the maximum intensity for the value of f_{ab} either zero or unity.

Fig. 2 shows the variation of intensities of Bragg peaks when the atoms migrate from (8a) to (16c). The fraction of the atoms migrated from (8a) to (16c) has been denoted by f_{ac}. It is observed that the intensity for all reflection either even or odd indices are randomly varies with the variation of $f_{ac.}$ There is no reflection, which smoothly changes with the variation of $f_{ac.}$ Also it is observed that all reflection has non-zero intensity.

Fig. 3 shows the variation of intensities of Bragg peaks when the atoms migrate from (8a) to (16d). The fraction of the atoms migrated from (8a) to (16d) has been denoted by f_{ad}. It is observed that there is no reflection, which smoothly changes with the variation of $f_{ad.}$

Fig. 4 shows the variation of intensities of Bragg peaks when the atoms migrate from (16c) to (16d). The fraction of the atoms migrated from (16c) to (16d) has been denoted by f_{cd}. It is observed that the intensity for the reflection of even indices remains constant with variation of $f_{cd.}$ The intensity for all odd reflection falls to zero while f_{cd} becomes one half. And the odd reflection show the maximum intensity for the value of f_{cd} either zero or unity.

Fig. 5 shows the variation of intensities of Bragg peaks when the atoms migrate from (8b) to (16c). The fraction of the atoms migrated from (8b) to (16c) has been denoted by f_{bc}. It is observed that Fig.5 is identical to Fig. 3.

Fig 6 shows the variation of intensities of Bragg peaks when the atoms migrate from (8b) to (16d). The fraction of the atoms migrated from (8b) to (16d) has been denoted by f_{bd}. It is observed that Fig. 6 is identical to Fig.2.

The intensity of the peak for even indices is independent of f_{ab} and $f_{cd,}$ this is because the structure factor does not change when the atoms migrate from (8a) to (16c). Whereas the intensity of the peak for odd indices smoothly vary with f_{ab} , f_{cd} and randomly vary with f_{ac}, f_{ad}, fbc, f_{bd} the reason is that the structure factor smoothly vary with f_{ab}, f_{cd} and randomly vary with f_{ac}, f_{ad}, fbc, f_{bd}.

Examining the intensity curves for the different planes it can be noted that

1. The peaks (111), (311), (331) have maximum intensity when 100% atoms lie in either (8a) or (8b) locations.
2. The peaks (422), (220) have maximum intensity when 100% atoms lie in either (8a) (8b) position or any combination of the two locations.
3. The peaks (222) have maximum intensity when 100% atoms lie in either (16c) or (16d) locations.
4. The peaks (400) and (444) have maximum intensity when 100% atoms lie in any one of the location (8a), (8a), (16c), (16d).
5. The variations of intensity are same while the atoms migrated either (8a) to (16c) or (8b) to (16d) location.
6. The variations of intensity are same while the atoms migrated either (8a) to (16d) or (8b) to (16c) location.

The maximum intensity for all the peaks are compared in Fig. 7. It is observed that the (220) peak have highest intensity among the eight peaks and the (444) peak has the lowest intensity. The intensities of the (111) reflection is very close to that of (220) reflection. The intensities of (311) and (422) reflection are again comparable and fairly good. The intensity of (222) and (331) are also comparable magnitude.

CONCLUSION

The strength of intensity of Bragg reflections depends on the values of their structure factors. Again, the magnitude of structure factor is dependent on the positions of the atoms in the crystal lattice. The atoms in the Si crystal are specifically located in the (8a) site under Fd3m space group. The occurrence of a particular reflection on the pattern is restricted by certain conditions depending on the value of its structure factor. The variation of atoms from its specific locations has been investigated. The knowledge of the effect of deviation of atomic chemical species present in the system, there are often some deviations in atomic locations. Though in the

present study the effect of deviations in atomic positions on the diffraction pattern is very important in crystallographic research. In practice depending on the preparation conditions and also on the locations has been investigated in terms of a particular crystal system, but it will be helpful in understanding the consequences of deviations in other crystal systems as well.

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