

Effect of carbon wt% on the iron x-ray diffraction pattern and the volume of iron unit cell.

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Abstract

From standard x-ray diffraction chart for iron noticed that the effect of increasing in carbon wt% are accompanied with the change in the volume of the iron unit cell, after diffusion of carbon atoms it takes interstitial position between irons atoms, this will increase the edge length of the unit cell by follow the relationship ($\Delta \vec{c} = 0.11285 \times C \text{ wt\%}$), a permanent strain happens with the change in the mean of the lattice spacing.

This relation between carbon wt% and the volume of iron unit cell can be use to predict the carbon which is present in the iron alloy. The diffraction pattern act as an empirical fingerprint for carbon % and their phases.

Introduction

X-ray diffraction techniques are some of the most useful in the characterization of the crystalline materials. Techniques can be used to identify the phases present in the samples. Provide information on the physical state of the sample, such as grain size, texture and crystal perfection. These techniques cover various investigations including qualitative and quantitative phase, its use as a phase characterization because it can routinely differentiate between phases having the same chemical composition but different crystal structure (polymorphs). Several properties like magnetic properties of ultra Fe-thin films depend upon the crystalline phase of the material; this phase can be different for the first few layers compared with subsequent layer. These studies confirmed theoretical prediction that the magnetic properties of Fe are a function of lattice parameter (Dekadjavi *et al.*, 2005).

The Change in the lattice volume by compression of solid modifies their crystal and electron band structures with related properties and often produced denser form (Ovsyannikov *et al.*, 2010).

X-ray diffraction experiments are generally taken to be a reliable measure of the average lattice distance in crystals. This assumption can be misleading when determining hydrogen induced volume changes. For the sample volume of

Fe/V(001) super lattice while expanding the lattice by in-situ hydrogen loading serve as an illustration of this counter intuitive effect (palsson *et al.*, 2008).

Surface X-ray diffraction (SXRD) can be used in the study of the geometric structure of O/Fe (001). The adsorption a foreign species on a crystal surface usually induces atomic relaxations and modifications of surface electronic states thereby affecting the surface physical and chemical properties (parihar *et al.*, 2010).

When high purity iron alloyed with carbon and the mixture slow cooled the density have a linear relation with carbon wt%, from 0 to 4.17 C wt% it is found to follow the relationship (Xayser *et al.*, 1975):

$$\rho^{-1} \left(\frac{\text{cm}^3}{\text{g}} \right) = 0.12698 + (5.03 \times 10^{-1}) \times (\text{carbon wt \%}] \quad \dots (1)$$

A crystal is a three-dimensional repetition of building blocks called unit cells. The unit cell volume is (Blakemore, 1989):

$$V = (\overline{a} \times \overline{b}) \cdot \overline{c} \quad \dots (2)$$

Where a, b and c are the three vectors of the basis of the unit cell.

A specification of the shape and size of a unit cell and of the distribution of matter within it gives a complete crystallographic description of a crystal by miller indices (hkl). By using radiation of a wavelength comparable with atomic dimensions. Diffraction gives us information in Fourier form in term of average spacing of lines and planes of atoms in a solid, the angles between lines and planes, the symmetries of point groups and the location of particular species of atoms. X-rays are still the principal source of new information about the crystallography of solids and are supplemented by electron and neutron diffraction. Thus the condition for efficient specular reflection is (Blakemore, 1989):

$$2d \sin\theta = n\lambda \quad \dots (3)$$

Where n is an integer denoting the order of diffraction, λ is the x-ray wavelength, d is the lattice spacing of crystal planes [hkl], a is the lattice parameters and θ is the diffraction angle. For the monochromatic x-rays produced by the metallic anodes in x-ray tube. Any change in the lattice spacing d results in a corresponding shift in the diffraction angle 2θ . If the lattice spacing is made to increase (by some means, e.g. alloying) therefore the diffraction angle 2θ will decrease(Blakemore , 1989) .

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}} \quad \dots (4)$$

Results

In this study x-ray diffraction data were compelled from reference (JCPDS, 1997), and it was used as the basis for theoretical calculation, eq. (5) and eq. (6) were used in the calculations.

Table (1): the X-ray diffraction data (JCPDS, 1997).

No. of pdf [7]	C %	X-ray three strongest lines distance (Å ^o)			\vec{a} Å	\vec{b} Å	\vec{c} Å	Iron Unit cell Volume (Å ^o) ³	ΔV %
340529	0	1.84	1.97	2.12	2.866	2.866	2.866	23.55	0
441290	0.604	2.05	2.02	1.17	2.859	2.859	2.937	24.01	1.9532
441291	0.8875	2.06	2.02	1.17	2.856	2.856	2.96	24.14	2.505
441292	1.0023	2.06	2.02	1.17	2.854	2.854	2.983	24.3	3.1847
441293	1.3529	2.07	2.01	1.17	2.847	2.847	3.018	24.46	3.8641
441289	1.575	2.08	2.01	1.17	2.846	2.846	3.053	24.73	5.0106

Table (2): gives theoretical calculation of the density of Iron and Carbon as mixture of two phases.

C %	ρ_{Mixture} (g/cm ³)	Δ ρ_{Mixture} %	Volume (Å ^o) ³	Mass of unit cell (g)	Δ m Mixture %
0	7.8753	0	23.55	1.8546×10^{-22}	0
0.604	7.7581	-1.4	24.01	1.86272×10^{-22}	0.43783
0.8875	7.7043	-2.1713	24.14	1.859818×10^{-22}	0.28135
1.0023	7.6826	-2.447	24.3	1.86687×10^{-22}	0.82055
1.3529	7.6176	-3.2722	24.46	1.863265×10^{-22}	0.46721
1.575	7.5769	-3.789	24.73	1.873767×10^{-22}	1.03348

$$\rho_{\text{Mixture}} = \frac{100 \times \rho_1 \times \rho_2}{x_1 \rho_2 + x_2 \rho_1} \quad \dots (5)$$

Where: ρ_1 is the density for pure Iron (7.8753 g/cm³), ρ_2 is the density for carbon as graphite (2.25 g/cm³), x_1 is the weight percent of iron, x_2 is the weight percent of carbon.

$$\text{Mass of unit cell (g)}_{\text{mixture}} = \rho_{\text{Mixture}} \times \text{Volume of unit cell} \quad \dots (6)$$

In table (3) reproduced some practical data from reference (5) to calculate the mass of the unit cell by using eq. (7).

Table (3): gives the density of high purity Iron with a carbon achieved in practical method by slow cooling (Xayser *et al.*, 1975).

C %	$\rho_{\text{Practical}}$ (g/cm ³) [5]	$\Delta \rho_{\text{Practical}}$ %	Volume (Å ³)	Mass of unit cell (g)	Δm Practical %
0	7.8753	0	23.55	1.8546×10^{-22}	0
0.604	7.8564	-0.23999	24.01	1.886321×10^{-22}	1.71
0.8875	7.84766	-0.35097	24.14	1.894425×10^{-22}	2.1473
1.0023	7.8441	-0.39617	24.3	1.906116×10^{-22}	2.7777
1.3529	7.8332	-0.53458	24.46	1.916×10^{-22}	3.3107
1.575	7.8264	-0.62093	24.73	1.935468×10^{-22}	4.3604

Mass of unit cell (g) Practical = $\rho_{\text{Practical}} \times \text{Volume of unit cell} \dots (7)$

The difference between the theoretical calculation and the practical results are shown in table (4).

Table (4): give the practical and theoretical value of the mass of the iron unit cell.

C %	Mass of unit cell achieved in practical method by slow cooling (g)	$\Delta m_{\text{Practical}}$ %	Mass of unit cell given by theoretical method as mixtures (g)	Δm Mixture %
0	1.8546×10^{-22}	0	1.8546×10^{-22}	0
0.604	1.886321×10^{-22}	1.71	1.86272×10^{-22}	0.43783
0.8875	1.894425×10^{-22}	2.1473	1.859818×10^{-22}	0.28135
1.0023	1.906116×10^{-22}	2.7777	1.86687×10^{-22}	0.82055
1.3529	1.916×10^{-22}	3.3107	1.863265×10^{-22}	0.46721
1.575	1.935468×10^{-22}	4.3604	1.873767×10^{-22}	1.03348

Table (5) shows the change in the value of $\Delta V\%$, $\Delta \rho_{\text{Mixture}}\%$, $\Delta \rho_{\text{Practical}}\%$, $\Delta m_{\text{Mixture}}\%$ and $\Delta m_{\text{Practical}}\%$ with respect to Carbon wt %.

Table (5): give the value of ΔV %, $\Delta \rho_{\text{Mixture}}$ %, $\Delta \rho_{\text{Practical}}$ %, $\Delta m_{\text{Mixture}}$ % and $\Delta m_{\text{Practical}}$ % with respect to C wt %.

C %	ΔV %	$\Delta \rho_{\text{Mixture}}$ %	$\Delta \rho_{\text{Practical}}$ %	$\Delta m_{\text{Mixture}}$ %	$\Delta m_{\text{Practical}}$ %
0	0	0	0	0	0
0.604	1.9532	-1.4	-0.23999	0.43783	1.71
0.8875	2.505	-2.1713	-0.35097	0.28135	2.1473
1.0023	3.1847	-2.447	-0.39617	0.82055	2.7777
1.3529	3.8641	-3.2722	-0.53458	0.46721	3.3107
1.575	5.0106	-3.789	-0.62093	1.03348	4.3604

Figure(1) shows the effect of carbon wt% on the change of the Iron unit cell edge length.

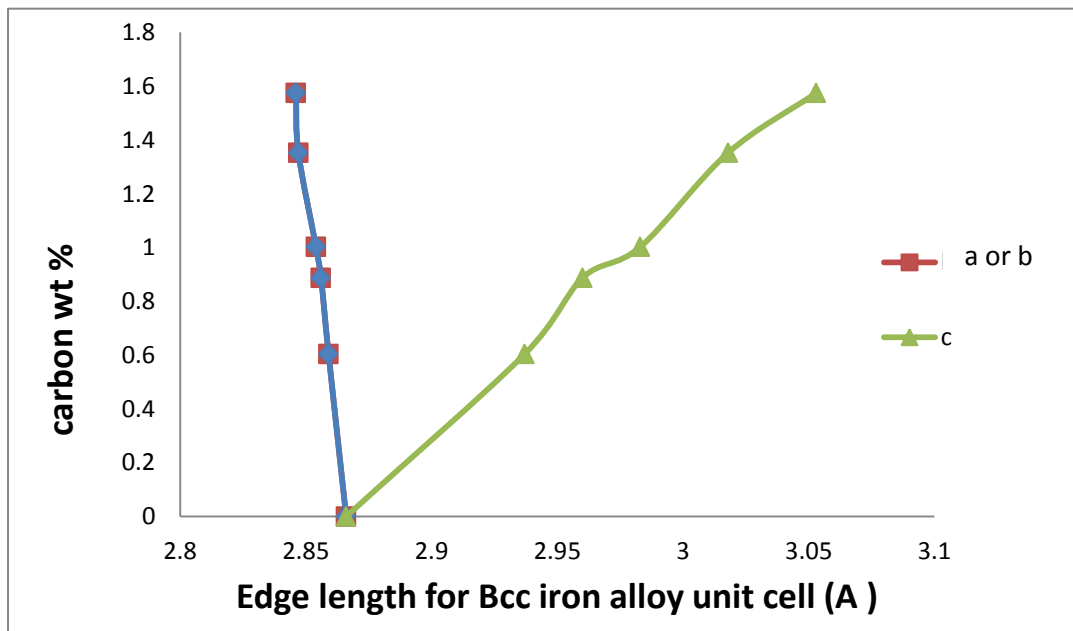


Fig. (1): carbon wt% as a function to the Iron unit cell edge length.

Figure (2) shows the effect of carbon wt% on the change in the volume of the iron unit cell.

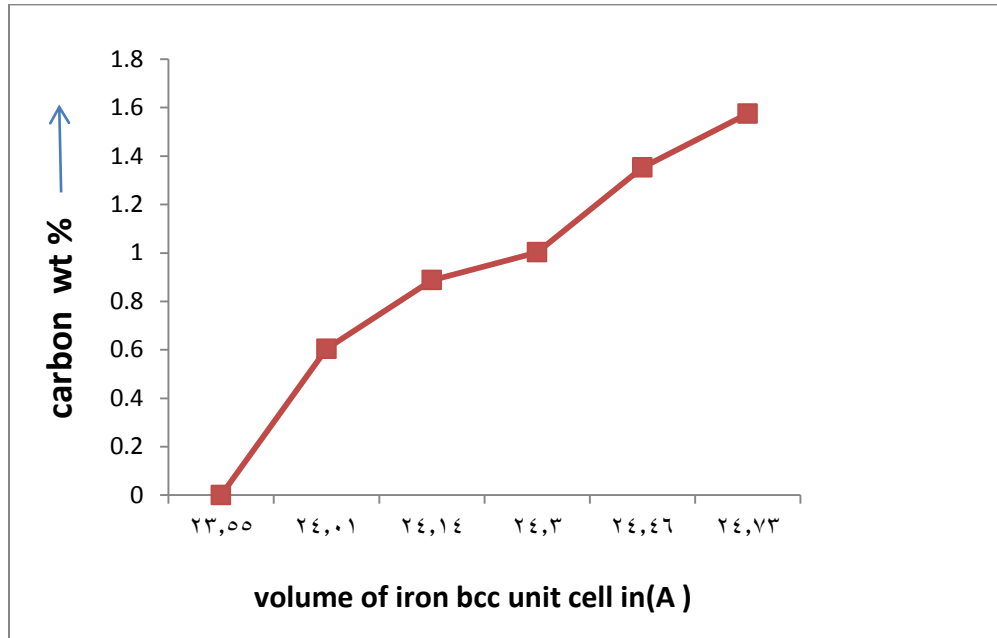


Fig. (2): carbon wt% as a function to the volume of the iron unit cell.

Figure(3) shows the effect of the carbon wt % on the the volume unit cell percent change.

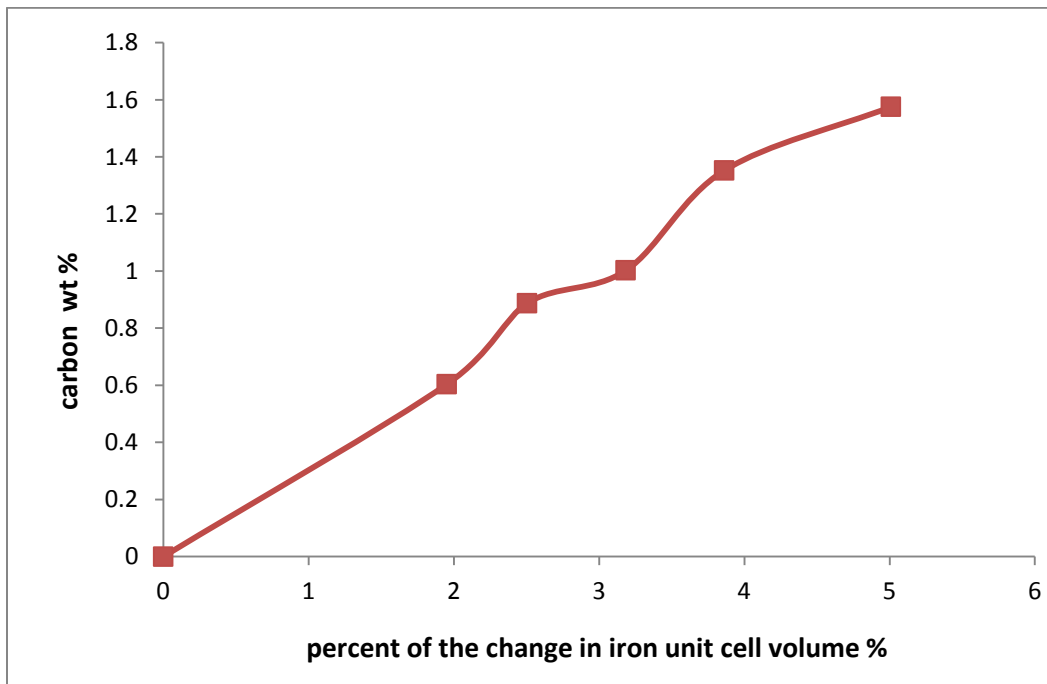


Fig. (3): carbon wt % as a function to ΔV %.

Figure(4) shows the effect of carbon wt% on the density of Iron.

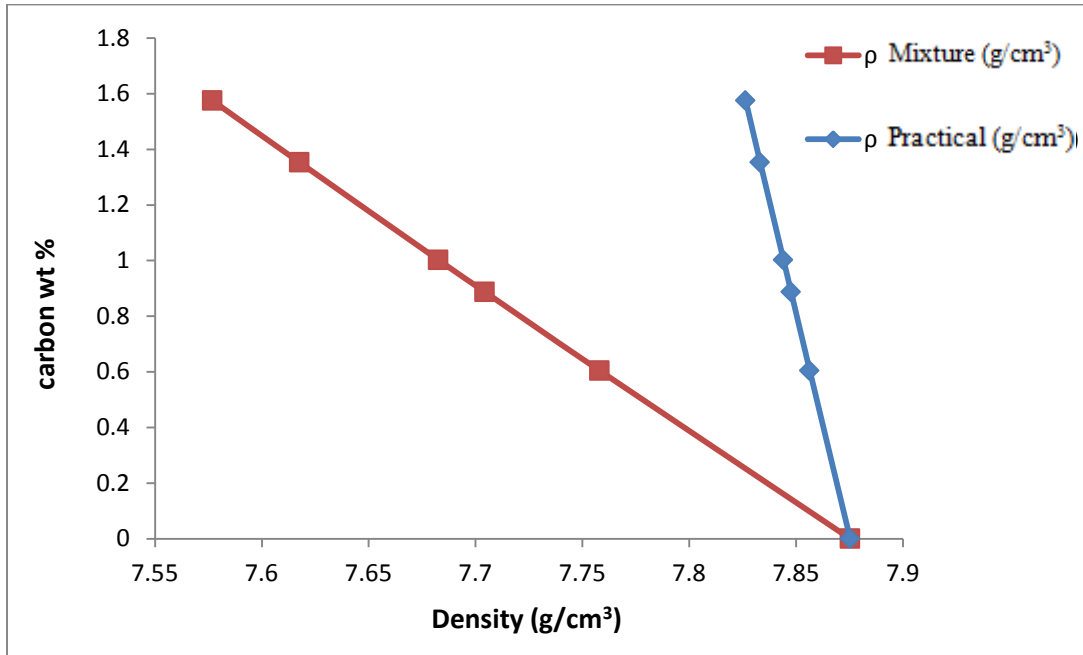


Fig. (4): carbon wt% as a function to the density of Iron.

Figure(5) shows the effect the Carbon wt % on the change in the value of ΔV %, $\Delta \rho$ Mixture %, $\Delta \rho$ Practical %, Δm Mixture % and Δm Practical % .

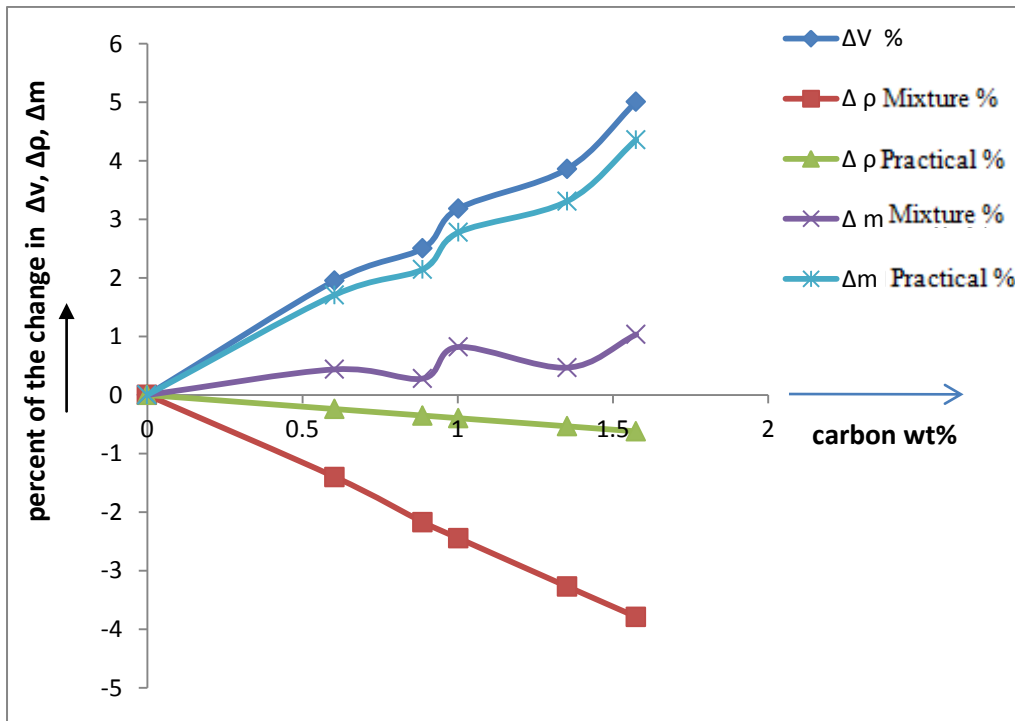


Fig. (5): ΔV %, $\Delta \rho$ Mixture %, $\Delta \rho$ Practical %, Δm Mixture % and Δm % as a function to the Carbon wt %.

Figure(6) shows the effect of the carbon wt% on the mass of Iron unit cell.

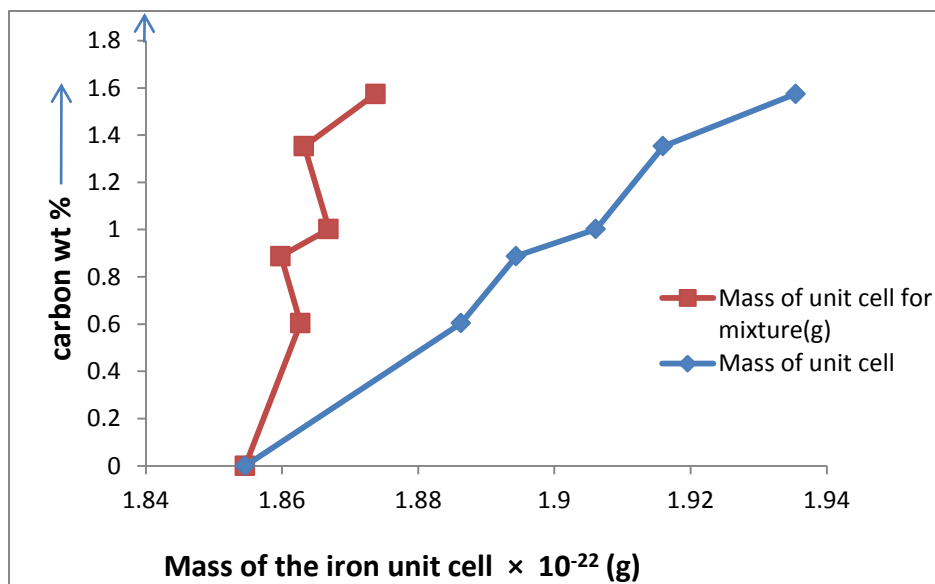


Fig. (6): mass of Iron unit cell as a function to the carbon wt % .

Discussion

A crystalline material is a three-dimensionally periodic arrangement of atoms in space. This arrangement is the best depicted by describing a unit cell having all the fundamental properties of the crystal as a whole, that is the basic repeating unit this unit cell is always a parallelepiped having typical edge dimensions of 2 to 20 Å. The arrangement of atoms depends on the type of atoms, the nature of their bonds, and their tendency to minimize the free energy by a high degree of organization, this organization usually results in some degree of geometric symmetry and unit cell shapes.

Shapes and symmetry controlled by the unit cell. Thus a goal of X-ray diffraction is to characterize the unit cell, that is to determine its size, shape, symmetry and the arrangement of atoms these characterizations can be determined from the collection of angles at which diffracted X-rays beams are detected and the interpretation of the intensities of the diffracted beams, the former is the geometry of the unit cell the latter is the crystal structure.

The carbon atoms have interstitial positions in the iron lattice. After cooling they still have their interstitial positions in the solid solution. This will distort the iron B.C.C cubic lattice to orthorhombic crystal structure, carbon atoms have the same position on the c axis, therefore the Iron unit cell will suffer an extension in c direction and shrinkage happening at a-axis and b-axis. All of this makes a change in the volume of the Iron unit cell with the increase in carbon wt%.

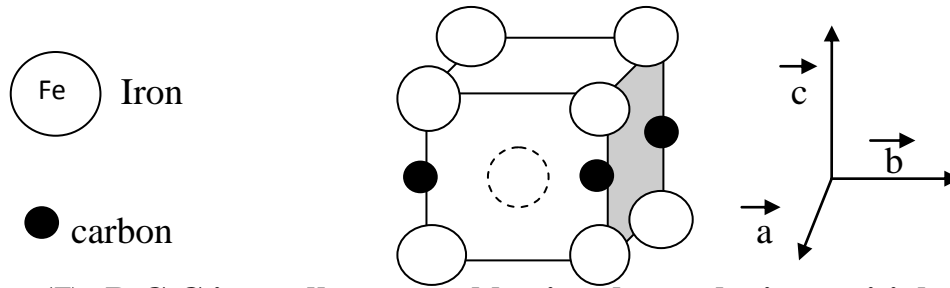


Fig. (7): B.C.C iron alloy crystal lattice shows the interstitial carbon atom.

The density also is changed with the change in the volume and the carbon wt %, table (5) gives us good comparison about the change in ΔV %, $\Delta \rho$ Mixture %, $\Delta \rho$ %, Δm Mixture % and Δm % with respect to C wt %.

Measuring the change in the angular position of the diffraction peak for three orientations of the sample defined by the angle enables the calculation of the strain in lattice edge. Because only the changes in the mean lattice spacing are measured by using x-ray diffraction for the determination of change in the atomic dimension. Figure (1) shows that there is a simple relationship between edge length of c axis and carbon wt% it's increased according to the equation:

$$\text{Carbon wt \%} = 8.86154 \times ((\text{length of C axis}) - 2.866)$$

This equation can be used to predict the carbon wt % by insert the value of c axis for Iron unit cell by using x-ray diffraction data, when carbon wt % increase the volume also increase, the change in the density of Iron by slow cooling is very small ,because the diffusion of the carbon atoms into the unit cell increase the mass of unit cell this make the practical density to decrease in small rate of change; but the theoretical density of the separated mixture decreases at high rate with increased in the value of carbon wt% .

Conclusion

1- X-ray diffraction can be used as finger print to predict the carbon wt% in carbon steel by using equation.

2-At low carbon wt% in carbon steel the density of the mixture cannot be used because the carbon atoms are very small with respect to iron atoms, carbon atoms are diffusion in the lattice easily specially at high temperature to produce ferrite (α -Iron) bcc crystal structure, ferrite (α -Iron) is stable equilibrium low temperature phase and cementite phase inter metallic. When Iron contain high carbon wt% its complex orthorhombic crystal structure. Also there is a laminar pearlite a metastable aggregate of ferrite and cementite due to eutectoid transformation of austenite; but if there is some element like silicon present into Iron alloy it will be

assist to produce carbon free as graphite hexagonal crystal structure, steel does not have any graphite causing it to be denser than either gray iron (7.2 g/cm^3) or ductile iron (7.06 g/cm^3).

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تأثير النسبة المئوية الوزنية للكربون على مخططات الأشعة السينية للحديد وعلى حجم وحدة الخلية

علي إسماعيل صالح

قسم الفيزياء/كلية العلوم _ جامعة كركوك

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الخلاصة

من مخطط حيود الأشعة السينية القياسي للحديد يمكن ملاحظة تأثير الزيادة في النسبة المئوية للكربون على الحديد حيث تكون مصحوبة بتغيير في حجم خلية الوحدة لمادة الحديد فبعد الانتشار تأخذ ذرات الكربون موقعا فراغيا بينيا بين ذرات الحديد وهذا سيؤدي في طول حافة خلية الوحدة وفق العلاقة التالية ($\Delta c = 0.11285 \times \text{Carbon wt\%}$) و يحدث انفعال دائم نتيجة التغيير في متوسط البعد للمستويات المتعاقبة في المشبك البلوري. هذه العلاقة بين النسبة المئوية للكربون وحجم وحدة الخلية يمكن أن تستعمل لتوقع نسبة الكربون التي تتواجد في السبيكة الحديدية عن طريق معرفة مخطط حيود الأشعة السينية كطبع إصابع تجريبي للنسبة المئوية للكربون المتواجد واطارة.