Structure and Properties of Materials
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Week-01
Lecture-02

So, good morning everybody. So far we have discussed different types of crystal structure of different materials and how their binding with each other, their geometric formation by arranging the atoms and all this we have discussed. Now we will try to shift the next part of this course that is called interstitial sites.

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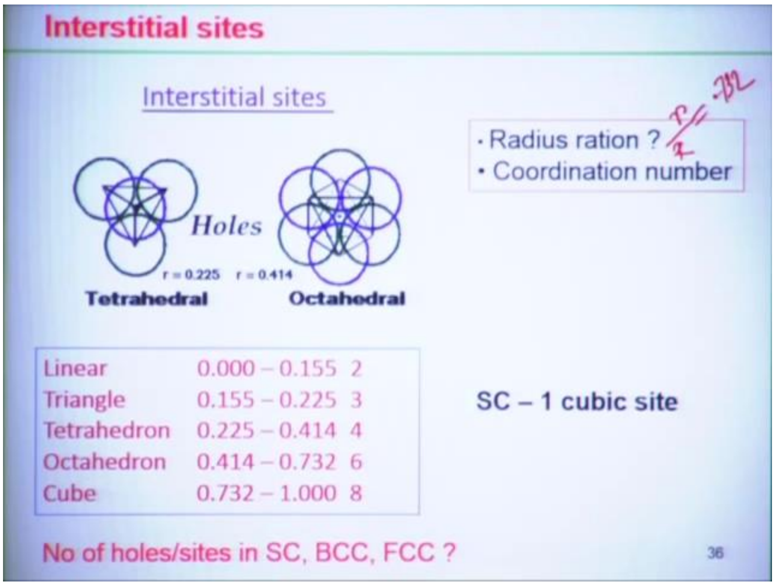

Interstitial sites

Interstitial sites

- Radius ration ? r/R .732
- Coordination number

Linear	0.000 – 0.155	2
Triangle	0.155 – 0.225	3
Tetrahedron	0.225 – 0.414	4
Octahedron	0.414 – 0.732	6
Cube	0.732 – 1.000	8

SC – 1 cubic site

No of holes/sites in SC, BCC, FCC ?

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We have observed that in case of simple cubic or body centred cubic or face centred cubic maximum part of that unit cell is occupied by the atoms, but there exist few holes (we de) that is corresponding to the with the coordination of different atoms and that positions is generally called the interstitial sites of the atoms. Now, the interstitial sites can be defined based on the coordination (of) respect to the surrounding atoms.

For example, if we start with the, from the very simple interstitial site for cubic structure. If we see the cubic structure the 8 cornered atoms exist within the cube itself. Now the cornered atoms are attached along the edge. So at the body centred that space (())(2:02) and we will theoretically try to find out what is the specific size of a sphere that can be exactly fit in the body of the simple cubic structure.

But in this case it is necessary to know that the ratio of the size where we are representing the size equivalent to the sphere and the radius of the atom. Based on this ratio there are formation of the different type of crystal structure and specifically we can found out in case of compound material. For example, in case of cubic structure the (maxi) the radius ratio that is we can say that small r by capital R. The small r represents the exactly, exactly size of the sphere means the size of the site and capital R is the size of the atom.

That ratio if we calculate then it becomes point 732 in case of cubic structure. The derivation for the same will be discussed the later but how this ratio can be found out. Now if we look into the other sites, for example tetrahedral sites, octahedral sites; in this case the tetrahedral sites having the coordination number 4.

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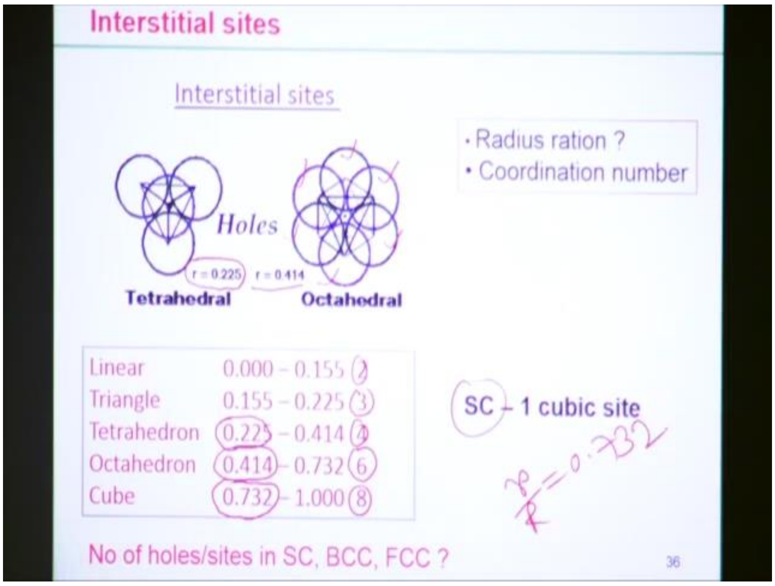

Interstitial sites

Interstitial sites

- Radius ration ?
- Coordination number

Linear	0.000 – 0.155 ②
Triangle	0.155 – 0.225 ③
Tetrahedron	0.225 – 0.414 ④
Octahedron	0.414 – 0.732 ⑥
Cube	0.732 – 1.000 ⑧

SC – 1 cubic site

$\frac{r}{R} = 0.732$

No of holes/sites in SC, BCC, FCC ?

So in case of octahedral site if we look, the coordination number is 6. There exists 3 atoms and above there is exist the another 3 atoms, so the interstitial site is having the coordination number 6.

In this case the radius ratio is 0 point 414 that means the interstitial if the site of the interstitial site is like a sphere so the radius ratio of the sphere and the atom is point 4 1 4 when it is exactly fitting in that space. But in case of tetrahedron when exactly (s) fitting the interstitial site, the radius ratio in this case is (point 22) point 225 and in case of octahedron it is point 414. In case of cubic site it is 0 point 732. So, depending upon the atomic arrangement the interstitial site we have the different coordination number like 4, 6, 8 and it is hardly found, the coordination number of 3 or 2.

But, the radius ratio actually varies over a range point 225 to point 414 in case of tetrahedron, but in case of octahedron it is the next stage point 414 to point 732 but point 732 is exactly the size of the (Inters) radius ratio in case in case of cubic site. So it is important to know the why the radius is so varies over a range depending upon the stability and the structure itself. But, at the same time it is important to know the number of holes in simple cubic, BCC and FCC structure we will try to investigate subsequently. But if we start with the simple cubic structure, it is having only one cubic site where the radius ratio is point 732.

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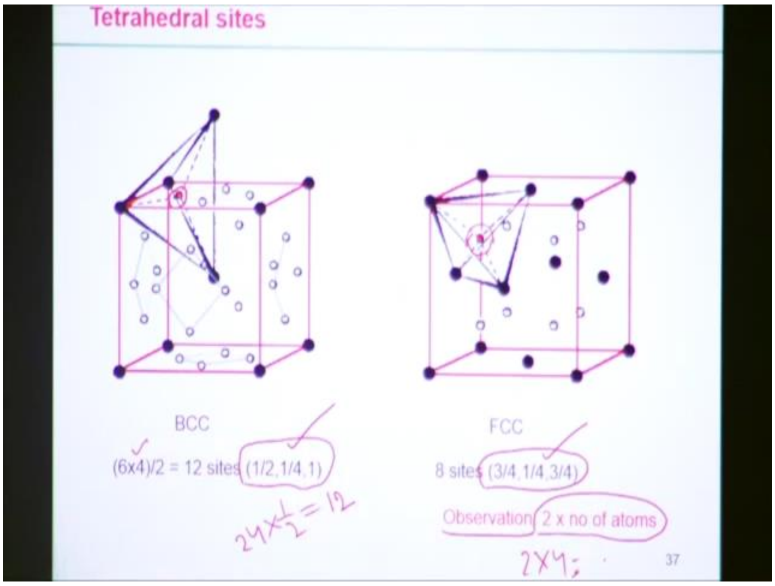

Tetrahedral sites

BCC

(6x4)/2 = 12 sites (1/2,1/4,1)

$24 \times \frac{1}{2} = 12$

FCC

8 sites (3/4,1/4,3/4)

Observation 2 x no of atoms

2×4;

Now we will try to investigate the, what are the tetrahedral sites exist in BCC and FCC (struc) structure. Let us look into first the BCC structure. If we see the the BCC structure see this tetrahedral site actually makes the coordinate with 4 surrounding atoms. So this forms actually tetrahedral sites in BCC structure and on the face there exist 4 such tetrahedral sites in BCC structure so if we estimate there are 6 faces and each faces there are 4 tetrahedral sites so there exist 24 tetrahedral sites.

But if we want to estimate the actual number of the tetrahedral sites that means that contribute to the unit cell then it becomes that looking to the sharing of the tetrahedral sites as (corres) in the surrounding unit cell. So here the 50 percent of the volume of the tetrahedral site exist within the unit cell. So total 24 into sharing is the 50 percent so then there exist total number of 12 sites such sites in BCC structure and position of the tetrahedral site can be seen that half along the X axis distance, along the Y axis which is 1 fourth distance, along the Z axis it is one distant. So this is the position which indicates the position of the tetrahedral sites in BCC structure.

But as I told that, again the tetrahedral sites may exist in FCC structure as well, but the position of the tetrahedral site in FCC structure is different from the BCC structure. Here if we see, this tetrahedral sites marked in the red colour that actually exist full volume inside the unit cell, so in FCC structure there exist 8 such interstitial sites and the position of the sites is the 3 fourth from the X axis, 1 fourth with respect to Y axis and 3 fourth with respect to the Z axis. So this is the typical position of the tetrahedral sites in (BCC) FCC structure.

Now if we observe that actually FCC number of FCC sites, here it is 8 sorry number of tetrahedral sites in FCC structure is 8 but we can found out the this co-relation, but this is simply observation that is equal to the 2 times of the total number of atoms. So we know that in FCC structure total number of atoms is 4 and so there exist total number of 8 such tetrahedral sites in case of FCC structure, okay?

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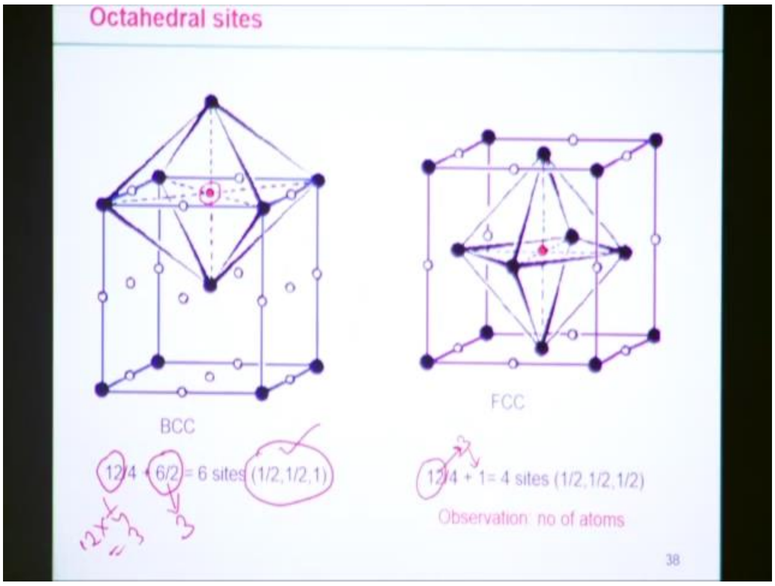

Octahedral sites

$12/4 + 6/2 = 6$ sites $(1/2, 1/2, 1)$

$12 \times \frac{1}{4} = 3$

3

$12/4 + 1 = 4$ sites $(1/2, 1/2, 1/2)$

Observation: no of atoms

So next slide, we will try to estimate octahedral sites in case of BCC and FCC structure. In octahedral sites that simply indicates the having coordination number 6. So in BCC structure we find out that there existence of the one octahedral site exactly at the face centre. The position of this octahedral site is the half from the X axis and half from the Y axis and 1unit from the Z axis. So sharing of such tetrahedral sites is that only the 50 percent.

Since there exists 6 faces and sharing is the 50 percent volume within the unit cell so in such case total number of octahedral sites in BCC is 3, but at the same time along the meet of the edges there exist also another tetrahedral sites in case of BCC structure. And if we try to investigate what is the total number of sites here the total number of sites along the edges is 12 but sharing volume within the unit cell is only the 25 percent (as if) that is 1fourth. So in this case there exist 3 number of such octahedral sites, so total number of octahedral sites in BCC structure is 6.

Similarly if we try to investigate what is the number of octahedral sites in case of FCC structure we found that along the edges also there exist such 12 number of octahedral sites but volume sharing is only 1 fourth so that is total number is 3 and along at the body centred there exist one octahedral sites so total 4 sites exist in case of FCC structure. So observation here is that octahedral sites in FCC structure is equal to the number of atoms.

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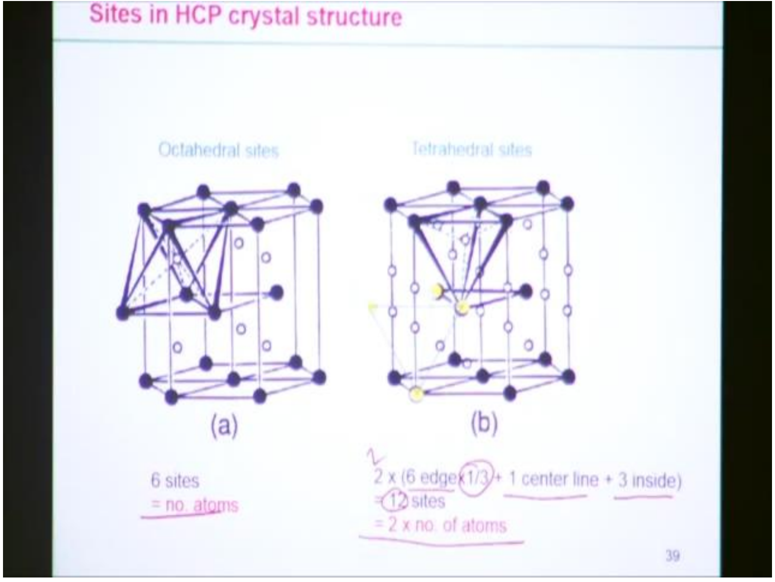

Sites in HCP crystal structure

6 sites
= no. atoms

2 x (6 edge x 1/3 + 1 center line + 3 inside)
= 12 sites
= 2 x no. of atoms

But in case, the similar investigation can be carried out in case of HCP crystal structure. if we look into that octahedral sites exist in HCP crystal structure and that the total number is 6 and all the 6 sites are existent within the volume of the unit cell. So here 6 number of octahedral sites in HCP crystal structure which is again equal to the number of atoms in case of HCP structure. So this is 1 observation and secondly in tetrahedral sites in case of HCP structure if we found out that there are 6 edges and along the edges is sharing is only 1 third.

There exists (once) long one centreline and 3 such sites exist inside the volume. But this number of sites with respect to the symmetric part of this things, if we divide the total volume in HCP structure is a symmetric with respect to the centrepoint then multiplied by 2 is actually represents the total number of tetrahedral sites exist in case of HCP structure. So here total number is 12. But typical observation here is that number of atoms in this case is the 50 percent of the number of tetrahedral sites. That means total number of tetrahedral sites equal to 2 times of the number of atoms in case of HCP crystal structure.

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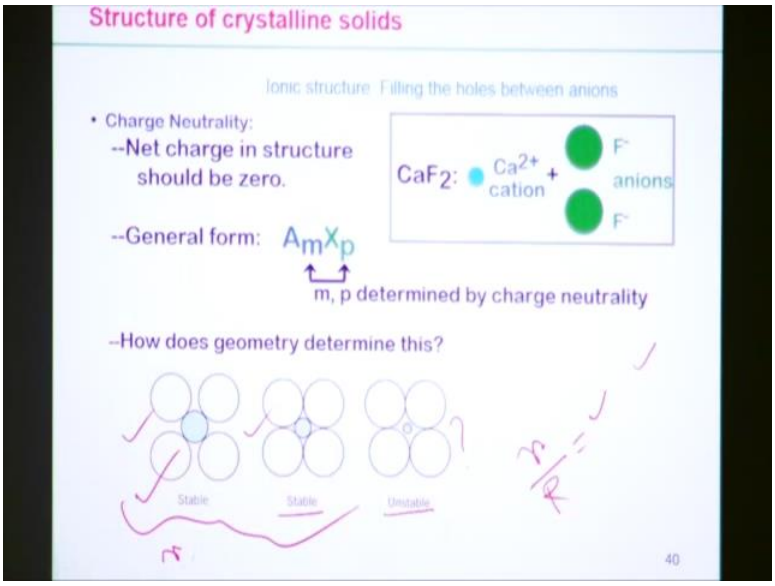

Structure of crystalline solids

Ionic structure: Filling the holes between anions

- Charge Neutrality:
  - --Net charge in structure should be zero.
  - --General form: A_mX_p
    m, p determined by charge neutrality
  - --How does geometry determine this?

CaF_2: Ca^{2+} cation + F^- F^- anions

Now we come to that point, the structure of the crystalline solids. So we did the regular investigation what is the total number of interstitial sites and what is the atomic arrangement of the, atomic arrangement within the unit cell different type of crystal structure; now we will try to find out who the crystalline solids is formed looking into the prospective of the simple crystal structure of different materials.

So first step compound material is to find the structure to check the charged neutrality. So here will charge neutrality should be maintained. Then for example CaF2; Ca2 plus is having 2 cations and F is having 2F minus anions. But general form of the any kind of solids can be represent in this type a AmXp where m and p determined by the charged neutrality based on the valance electrons exist and outer cell of the structure. But, how the geometric stability can be found out by looking into the structure of the specific crystal? If we see that first structure actually the interstitial (s) site try to disperse the other atoms but still we can consider is a stable (s) structure if the ratio between the interstitial site and ratio of the atoms maintain upto certain level.

Second structure we see this is can be considered the stable structure; here the interstitial site, there atoms is exactly fitting in the interstitial sites. Third is the, the atoms are not exactly fitting the interstitial sites even it is smaller than that. So third can be considered as a unstable structure because that space cannot be remain vacant without fitting exactly or more than that of the such. So, first 2 can be considered as a stable structure.

So that is why when you try to find out that radius ratio actually that is beating in the interstitial sites and the atoms in the other existence the corner points (of) of a cubic or any other kind of structure; this we define the radius ratio over a range. So, first point indicates that atoms is exactly fitting in the interstitial sites and second site indicates that it is go, the (ra) ratio can go out to certain extent. So this is a case of first one, instead that produces the stable structure according to the r by R (r) ratio.

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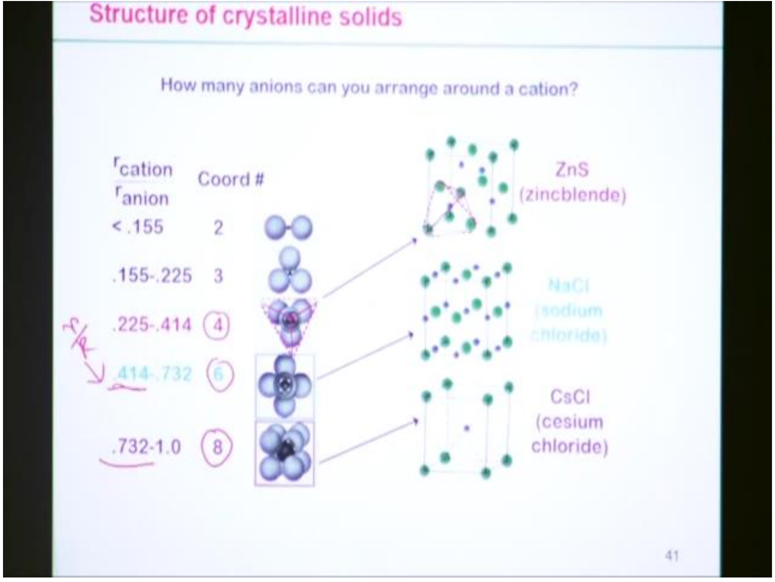

Structure of crystalline solids

How many anions can you arrange around a cation?

r/R

$\frac{r_{cation}}{r_{anion}}$	Coord #
< .155	2
.155-.225	3
.225-.414	④
.414-.732	⑥
.732-1.0	⑧

If we further investigate the structure of different crystalline solid, specifically the compound material if we see that how many anions can be arranged around a cation accordingly it can be, the stable structure and reformed. Now we try to investigate few (struct) structure of a compound materials, for example this zincblende so probably the ions can be Zn plus plus and S minus.

So in this case the cation and anion reformed and a smaller its size takes the interstitial positions and if we see that year the interstitial positions is created in such a way that the coordination number is falling as 4. So in this case the radius ratio between the atoms, positions in the interstitials part of the atoms in the other parts can follow this range, point 225 to point 414. So this is the stable structure in case of zinc sulphide, ZnS.

Now similarly (way) we can find out the initial structure as well if we see that interstitial positions are occupied and here it forms coordination number 6; that means accordingly the size and accordingly the radius ratio varies from point 414 to point 732. So first one indicates that interstitial position is exactly fitting by the atoms. If we consider the cesium chloride that it is actually positions there is a one interstitial site exactly at the body centre and here it creates the coordination number 8 so accordingly the radius ratio varies from point 732 to 1. So point 732 is the that value indicates the exactly fitting of the interstitial position.

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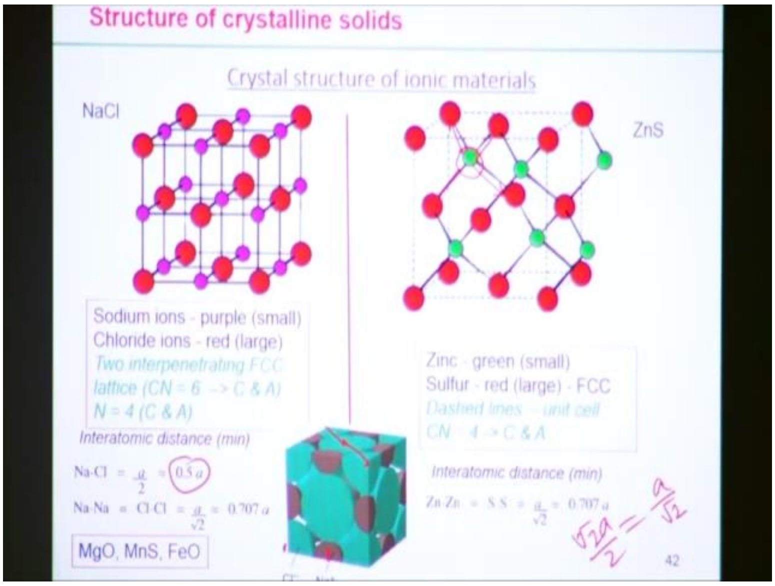

Structure of crystalline solids

Crystal structure of ionic materials

Sodium ions - purple (small)
Chloride ions - red (large)
Two interpenetrating FCC lattice (CN = 6 --> C & A)
N = 4 (C & A)

Interatomic distance (min)

$\text{Na-Cl} = \frac{a}{2} = \boxed{0.5\,a}$

$\text{Na-Na} = \text{Cl-Cl} = \frac{a}{\sqrt{2}} = 0.707\,a$

MgO, MnS, FeO

Zinc - green (small)
Sulfur - red (large) - FCC
Dashed lines - unit cell
CN - 4 -> C & A

Interatomic distance (min)

$\text{Zn-Zn} = \text{S-S} = \frac{a}{\sqrt{2}} = 0.707\,a$

$\frac{\sqrt{2}a}{2} = \frac{a}{\sqrt{2}}$

Now, we will try to incorporate the details discussion on the different types of structure. First we will look into the structure of NaCl. Tracy at sodium ion basically purple in colour and smaller in size but chloride ion which is red colour but it is larger size because chloride ions having some extra (cell) extra electrons outside the cell. Because of that, it is having the larger in size. Now in this case specifically the overall structure of the crystal represents that 2 interpenetrating FCC (st) lattices were the coordination number both cation and anion are 6 here and number of atoms if we try to estimate here it is 4. So that is number of cations is 4 and number of anions also 4.

Now if we try to find out the inter-atomic distance between Na and Cl that can be found out looking into the arrangement of the atoms. So if we look into this bottom figure, here if we see the corner atoms are the chloride ions in the longer edges there exist some sodium ions. So here between the Na and Cl is simply position from centre to centre point, this distance is basically half of the edge length that means half of the lattice parameter a. So point 5 a. But between sodium to sodium or between chloride to chloride ion, that we need to consider along the diagonal, face diagonal. So from here to here it is basically the total distance of the diagonal equal to root 2 a and half of this is the centre to (ce) centre distance between sodium to sodium ions that is corresponding to a by root 2.

Now if we look into that ZnS structure here the green colour represents smaller in size that is the Zinc and red coloured which is large in size that is Sulphur which is also having FCC structure. But dashed line indicates the unit cell here also the coordination number equal to 4. That coordination number, if we look into that, it is in continuous contact with the 4 surrounding atoms and both the cases either if we consider the cation or if we consider the anion, both the places we will be able to find out the coordination number is 4 in this case. Now interatomic distance between zinc to zinc or between sulphur to sulphur, it is along the half of the body diagonal, so that means a by root 2. These are the typical structure in case of compound material but it is very obvious the, this structure which is little bit different from the pure metals having the (s) simple cubic, BCC or FCC structure.

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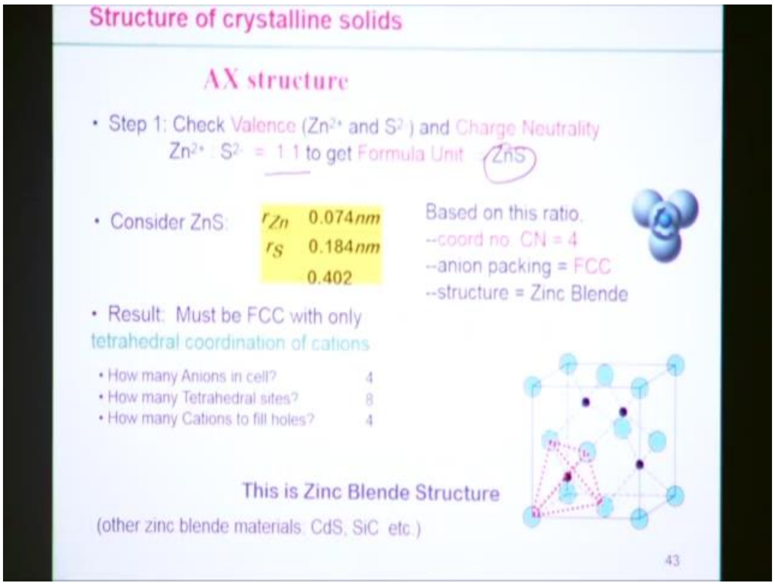

Structure of crystalline solids

AX structure

- Step 1: Check Valence (Zn^{2+} and S^{2-}) and Charge Neutrality
  Zn^{2+} : S^{2-} = 1:1 to get Formula Unit ZnS
- Consider ZnS:

r_{Zn}	0.074nm
r_S	0.184nm
	0.402

Based on this ratio,
--coord no. CN = 4
--anion packing = FCC
--structure = Zinc Blende

- Result: Must be FCC with only tetrahedral coordination of cations
  - How many Anions in cell? 4
  - How many Tetrahedral sites? 8
  - How many Cations to fill holes? 4

This is Zinc Blende Structure

(other zinc blende materials: CdS, SiC etc.)

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If we try to predict the AX structure, here first step is to check their valance electrons and then consider the charge neutrality we can find out the zinc plus plus and S minus minus is, ratio is 1 is to 1 therefore the formula stands like ZnS. Next step is to consider the ratio of the Zn plus plus and S minus minus. So that radius ratio is usually come point 402. So by looking into that, point 402 we can find out that what maybe the coordination number of interstitial sites. So in this case by looking into the standard table of the coordination number point 402 actually lies between this range point 225 to 414. So we can say that the coordination number should be 4 in this case.

Anion packing is that FCC and finally the structure is the Zinc blende structure. So, but in this case it is also necessary to investigate what is the total number of anions the cell, that is 4, how many tetrahedral sites exist, that is 8, and how many cations to fill the holes, that is the 4. So this is the way to investigate the structure, (was) looking into the other prospect like the valance (elect) electrons and the radius ratio between the anion and cation.

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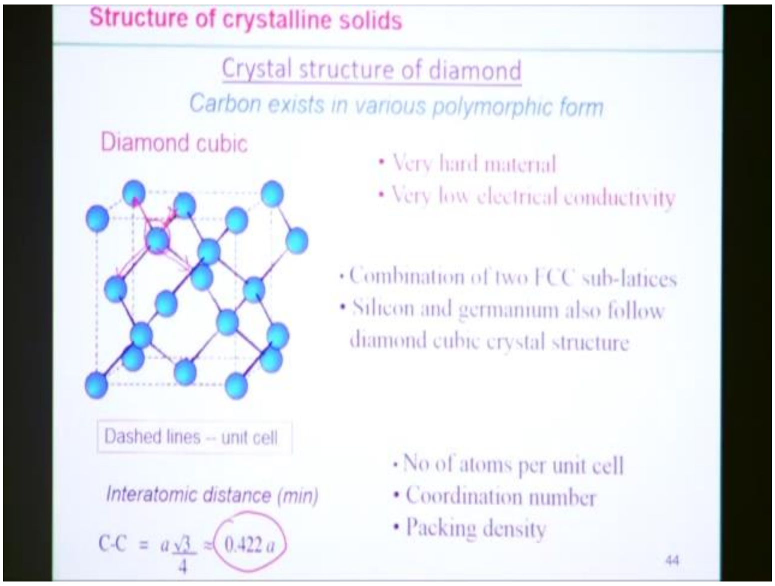

Structure of crystalline solids

Crystal structure of diamond

Carbon exists in various polymorphic form

Diamond cubic

- Very hard material
- Very low electrical conductivity

- Combination of two FCC sub-latices
- Silicon and germanium also follow diamond cubic crystal structure

Dashed lines -- unit cell

Interatomic distance (min)

$C\text{-}C = \frac{a\sqrt{3}}{4} \approx \boxed{0.422\,a}$

- No of atoms per unit cell
- Coordination number
- Packing density

Now, we will come to the structure of diamond cubic structure. So, it is also important to know because carbon is one of the important materials, and carbon exist in various polymorphic form. So first we will try to investigate the crystal structure of diamond. It is not necessary the polymorphic form of carbon can exist or the similar kind of structure. Diamond, as we know, it is a very hard material and having very low electrical conductivity and it is important to know that it is having very specific properties. Typically it is known for very hard material.

So looking into that properties if we try to investigate the crystal structure of diamond cubic structure, it is a combination of 2 FCC sub lattices and silicon and germanium also follow similar kind of structure. Now, if we look into the unit cell, here the coordination number is 4, because one atom is continuous contact with the another 4 atoms and interatomic distance between cc and be investigated as point 422a, where a is the lattice parameter. But, in details, the number of atoms per unit cell, coordination number, packing fraction we will try to discuss later (on) we will try to evaluate what are this all this parameters.

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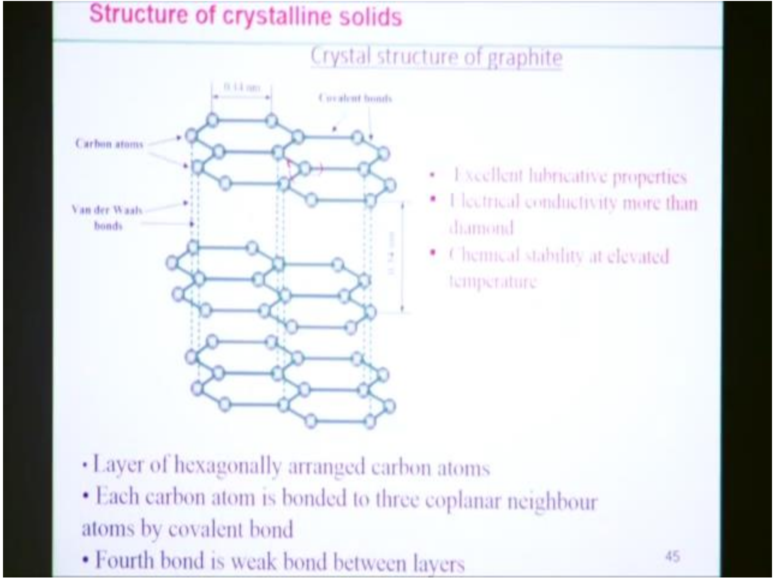

Structure of crystalline solids

Crystal structure of graphite

- Excellent lubricative properties
- Electrical conductivity more than diamond
- Chemical stability at elevated temperature

- Layer of hexagonally arranged carbon atoms
- Each carbon atom is bonded to three coplanar neighbour atoms by covalent bond
- Fourth bond is weak bond between layers

Now, we look into the another polymorphic form of carbon that is graphite. So in graphite if having the structure is looks like the carbon atoms exceptionally arrange but there is a layer wise, it is (bo) bounded by the covalent bonds. So, this type of structure means the graphite is having very good lubricative properties, good electrical conductivity and specifically more than diamond having chemical stability even at very high temperature. So if we see the structure is that the one carbon atom is connected the 3 carbon atoms, but (is) it is other way it is connected to the second layer by using the secondary bond that is called Van der walls bonds. So what the secondary bonds is generally weak in structure.

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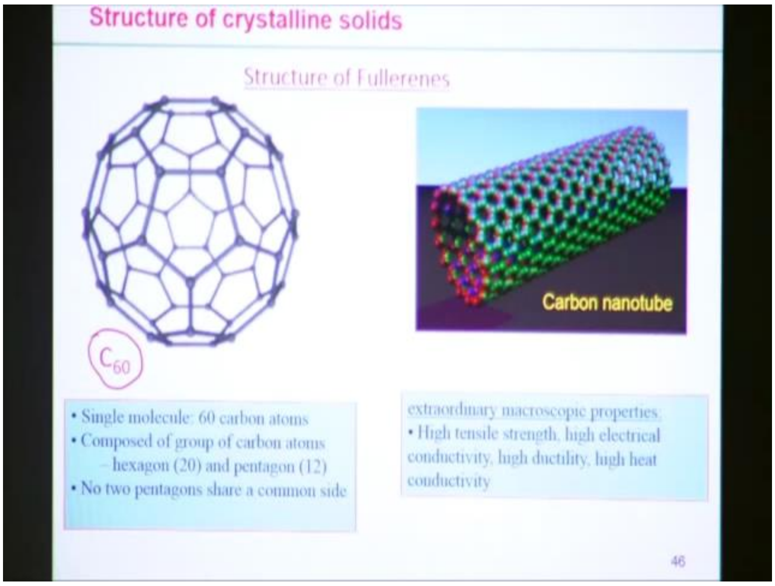

Structure of crystalline solids

Structure of Fullerenes

- Single molecule: 60 carbon atoms
- Composed of group of carbon atoms
  - hexagon (20) and pentagon (12)
- No two pentagons share a common side

extraordinary macroscopic properties:
- High tensile strength, high electrical conductivity, high ductility, high heat conductivity

Another polymorphic form that is called structure of Fullerenes that typically known as the single molecule having the 60 number of carbon atoms that is called the C60. So, typical characteristics of the structure is having the carbon atoms in the form of 20 hexagon and 12 pentagon but no 2 pentagons share a common side. So this is the typical structure of C60. Similarly another polymorphic form, this we know recently used or maybe nowadays widely used that is called carbon nanotube. It is also another polymorphic form of carbon.

Carbon nanotube is known, a very extraordinary properties like high tensile strength, electrical conductivity, high ductility, high heat conductivity and nowadays this is having the tremendous use of carbon nanotube. So detailed structure of these things it is a, may not be the scope of this course.

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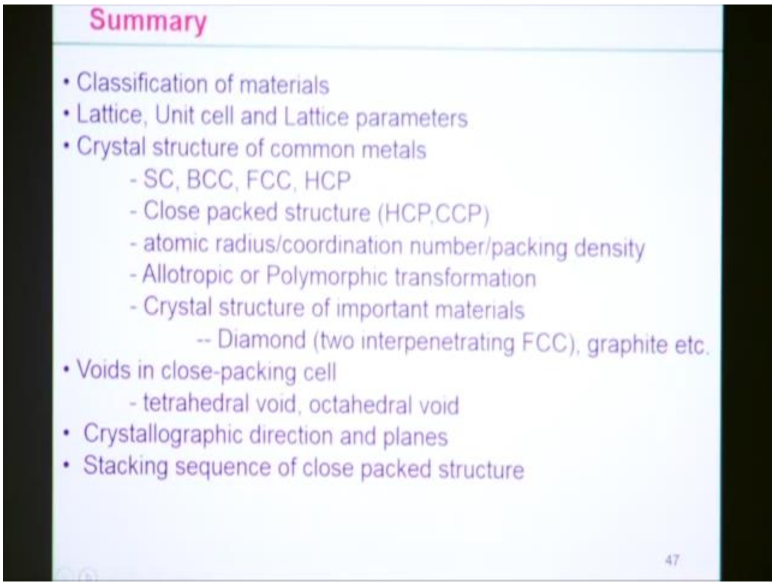

Summary

- Classification of materials
- Lattice, Unit cell and Lattice parameters
- Crystal structure of common metals
    - SC, BCC, FCC, HCP
    - Close packed structure (HCP,CCP)
    - atomic radius/coordination number/packing density
    - Allotropic or Polymorphic transformation
    - Crystal structure of important materials
        - Diamond (two interpenetrating FCC), graphite etc.
- Voids in close-packing cell
    - tetrahedral void, octahedral void
- Crystallographic direction and planes
- Stacking sequence of close packed structure

So, so far we have discussed the basic fundamental things of the crystal structure as well as the very basic parts of the atomic structure. Now, in sary we can say that first we looked into that classification of the different materials, what are the modern materials need, and the types of materials using nowadays. Secondly we actually went back to the very basic part of what is the lattice point, what is the unit cell, (how) how to the lattice parameter co-relation is happening in case of different type of simple cubic structures.

Next we try to demonstrate that different type of common structures of the metals like simple cubic, BCC, FCC, HCP structure; then we analyse that the close packed structure typically the hexagonal close packed structure and cubic close packed structure. So cubic close packed structure and hexagonal close packed structure (also) 1 certain (())(33:40) is having the similar type of atomic arrangements but if we consider the 3-D arrangement of the different stacking layer, that are different in case of hexagonal close packed structure.

The stacking layers actually varies in the form of 2 different types like AB, AB in that form. But in case of cubic close packed structure the stacking arrangement happens in the ABC, ABC in that form. So that are the difference between the close packed structure between HCP and CCP. Also it is mandatory to mention that cubic close packed structure, when you try to consider the stacking sequence in this case the stacking sequence should consider the normal to the plane 111 in case of FCC structure.

Now, then we have discussed the atomic radius, coordination number, relation between atomic radius and the lattice parameter and packing density or different type of crystal structure. Then we have discussed the allotropic and the more fixed transformation of 1 pure metal and as well as for compound materials. Then we discussed the crystal structure of the different type of important materials like diamond, graphite, etc.

We tried to find out what are the different interstitial sites exist in the simple cubic structure like BCC, FCC and HCP structures and what are the importance of the radius ratio and what (are), how to estimate the radius ratio is in case of different crystal structures. Then we focused on the crystallographic directions and planes and we try to represent the different direction in planes in case of simple cubic structure, hexagonal structure by the form of Miller Indices. Then we discussed the stacking sequence of the different close packed structure.

So hope with this (di) discussion on the basic crystal structure it will be beneficial understand the very basic (())(36:09) of the crystal structure. And now next part will be the, the to strengthening the knowledge of the (theo) theory so far we have discussed, we will try to focus on some numerical problems in the next part of this work. Thank you.

So after discussing about different theory or behind the different type of crystal structure of a specific material; that was the very basic understanding. Now we will try to focus on some problems to strengthen our knowledge on the different type of crystal structure and how to estimate or how to correlate the different parameters which generally used in the study of crystallography.

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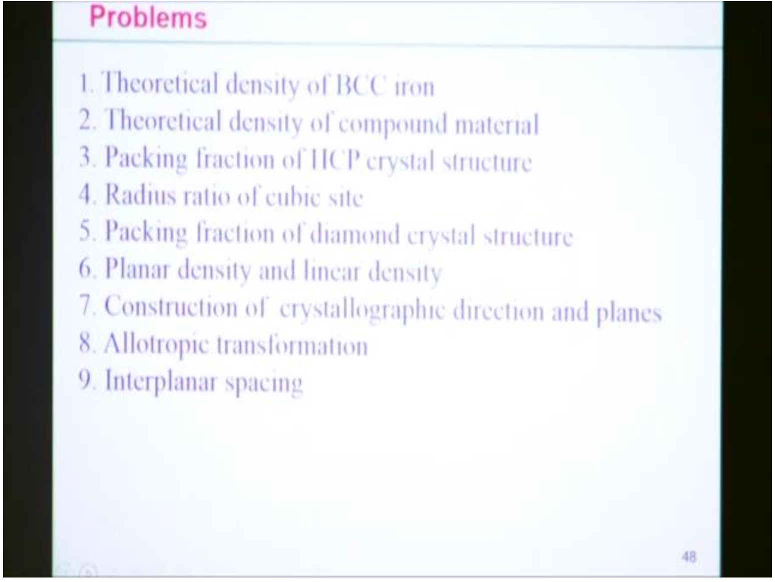

Problems

1. Theoretical density of BCC iron
2. Theoretical density of compound material
3. Packing fraction of HCP crystal structure
4. Radius ratio of cubic site
5. Packing fraction of diamond crystal structure
6. Planar density and linear density
7. Construction of crystallographic direction and planes
8. Allotropic transformation
9. Interplanar spacing

So we will try to focus on this, this type of typical problems like theoretical density of BCC iron; theoretical density if it is not pure metal; then what, how to estimate the packing fraction of the HCP crystal structure; radius ratio of the cubic site, how to estimate that; packing fraction of the Diamond crystal structure; what are the different type of planar density, linear density (once) on specific plane or 1 specific direction (on) of a unit cell; then how to construct the different crystallographic (d) direction and planes; finally the allotropic transformation and what is important (h) and how we can practically consider the allotropic transformation of material to design sensor and finally interplanar spacing how to estimate this in case of 1 specific to crystal structure.

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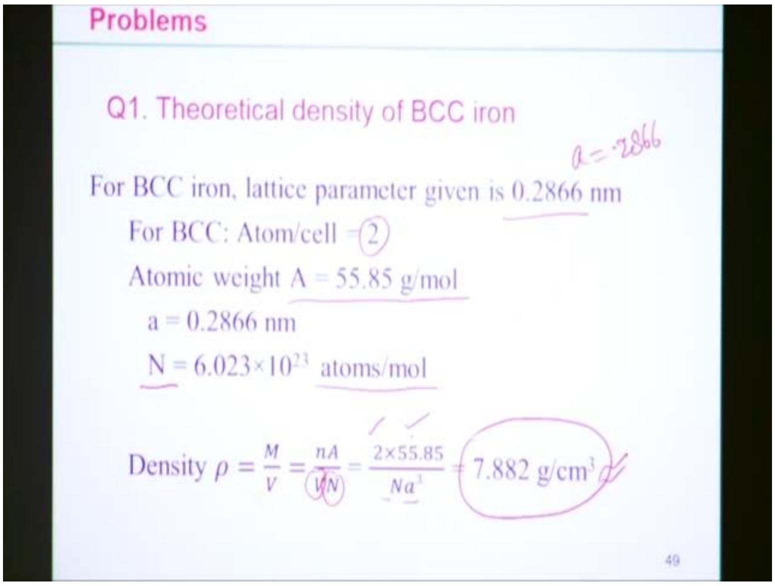

Problems

Q1. Theoretical density of BCC iron

$a = .2866$

For BCC iron, lattice parameter given is 0.2866 nm

For BCC: Atom/cell = $\textcircled{2}$

Atomic weight A = 55.85 g/mol

a = 0.2866 nm

N = 6.023×10^{23} atoms/mol

Density $\rho = \frac{M}{V} = \frac{nA}{VN} = \frac{2 \times 55.85}{Na^3} = \boxed{7.882 \text{ g/cm}^3}$ ✓

So first problem is that let us look into the theoretical density of BCC iron. So we have done through the theoretical part now we look that BCC iron, the lattice parameter is given point 2866 that is a equal to point 2866. Now we know (in) for BCC structure atoms per unit cell equal to 2 V have already estimated. Next, atomic weight of iron it is known to us 55 point 85 gram per mole and then N equal to Avogadro's number that is the unit is given atoms per mole. So density we can find out, the mass by volume; so mass can be represents in terms of what is the number of atoms per unit cell and what is the atomic weight and V is the actually volume of the unit cell and N is the Avogadro's number.

So from this we can find out that 2 is the number of atoms, a is the atomic weight, N is the Avogadro's number, a is the volume, and finally it is coming 7 point 882 grams per centimetre cube. So this is purely calculation from the BCC iron and by looking into the parameters of (crys) crystal structure of BCC iron. But practically if we try to find out the bulk of the material iron we find out density is almost near about this value. So this is the theoretical estimation. But one important thing is that here when we try to estimate these things we need to focus on the what are the units are given if necessary we can transfer the units and so my point is that units consistency should be maintained when you doing some numerical calculation related to this problem.

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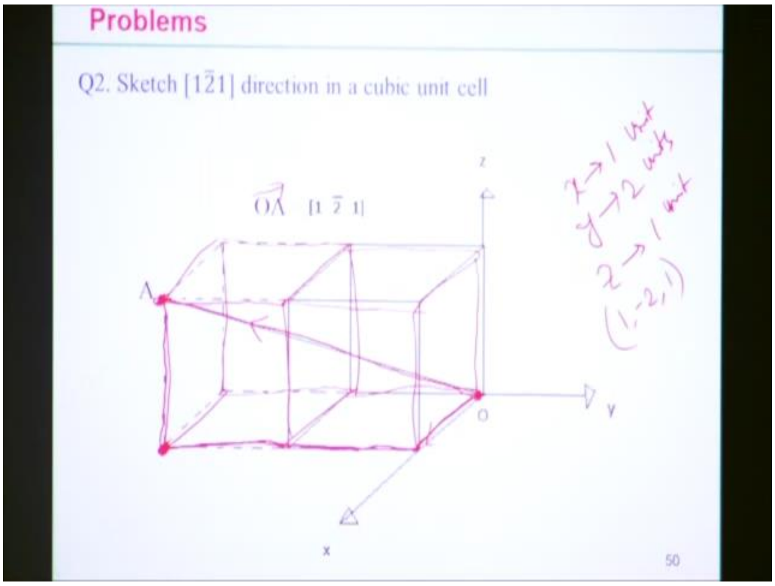

Problems

Q2. Sketch $[1\bar{2}1]$ direction in a cubic unit cell

Next problem, second problem; so a construct the 12 bar1 the direction in a cubic unit cell, how we can do that? So first, first thing is that we try to find out in the direction that what is the coordinates for that. So if we see along the X axis there is 1, along the X axis there is 1 unit. Along the Y axis it represents 2 units but that 2 units is along the negative direction of

Y. And the Z direction it is 1 unit. So we can construct in such a way that we can, first we can produce the 2 unit cell along the Y direction, but it should be the opposite to the Y direction. So first we need to chose the origin here and we need to define the axis X Y and Z. With respect to that axis first we can draw one unit cell with reference to the negative Y direction because we knew to produce the 2 units negative to the Y direction. And adjacent to (tho) we can draw another unit cell and now we try to represents this units along X Y and Z directions. So, O, it starts from 000 and final point is comes 1 minus 21, that is the coordinate of the final point, say point A.

So here along the X axis we move 1 unit so upto this point; next negative to the Y direction we can move 2 units this is one unit and next we move upto 2 unit, so now at this point. Next part is the we (move) need to move 1 unit along the positive Z direction, so from here to up to that point a. So this is the final position, now we can join the line between O and A and that actually represents the direction OA within a cubic unit cell. So this very can construct the different direction within the unit cell.

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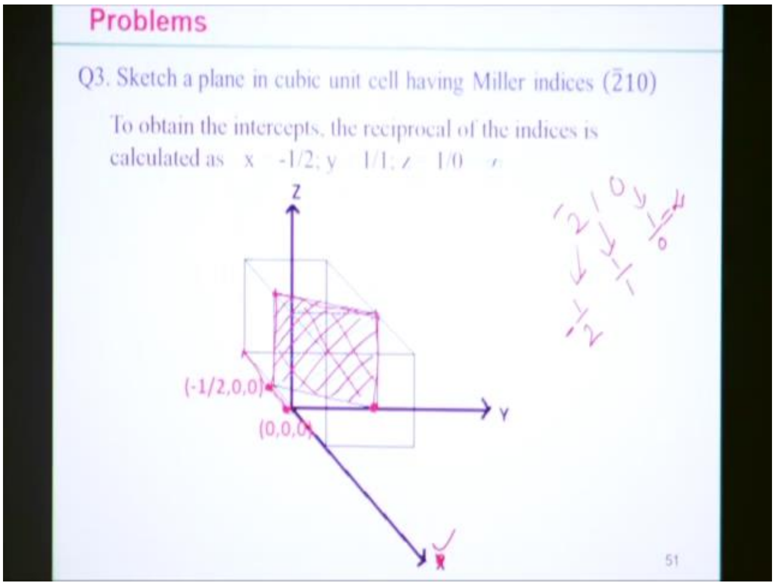

Problems

Q3. Sketch a plane in cubic unit cell having Miller indices $(\bar{2}10)$

To obtain the intercepts, the reciprocal of the indices is calculated as x = -1/2; y = 1/1; z = 1/0 = ∞

Now third problem we can focus the construction of the plane in a cubic unit cell having Miller Indices 210. So in this case the, you are trying to construct the 1 plane within the unit cell. So here the Miller Indices of the plane is given 2 bar 10. So, first step is to find out the length of the intercepts along X Y and Z directions. So, if we assume first of all the X component so intercept length along the X direction is minus half, along the Y direction the intercept length is 1, along the Z direction intercept length we can consider as infinity.

So when we try to place or try to draw the plane first thing we need to find out the intercept length along the Y direction that is negative of half, it should be (also a) here it is X axis (oh ok), so along the X axis it is minus half, so if this is the origin so opposite to X axis we; if this is the unit length, so we consider this point is equal to half of along the (opposite) along the X axis in the negative direction; and (s) with respect to the Y axis, this is the intercept length is this, because along the Y direction this is the unit 1 unit.

But since intercept length along the, with respect to the Z axis is infinity, that means the plane should be parallel to the Z axis. So we extend along the Z axis but it is, should be the parallel. Now we can construct the plane like this, so if we check it at this plane is having intercept length with respect negative X axis is (point half) minus half, positive Y axis is 1 and parallel to the Z axis. So this is the plane or having the Miller Indices 2 bar 10. So similarly (we can) we can construct the several planes in case (of) in, within the unit cell if we know the Miller Indices of that.

But steps; in this case the steps can be followed like that; first step is to find out the intercept length and then we can point out the intercept length but looking into that point then we can draw the plane with respect to the specific points. But, careful, it is different from the construction of the direction, because in construction of the direction it is not necessary to find out the step as a, like finding the reciprocals; we can directly plot, find out the coordinate and we can directly plot the direction in a unit cell. But in case of plane, first we need to find out the intercept then we can represents the plane according to the intercept length.

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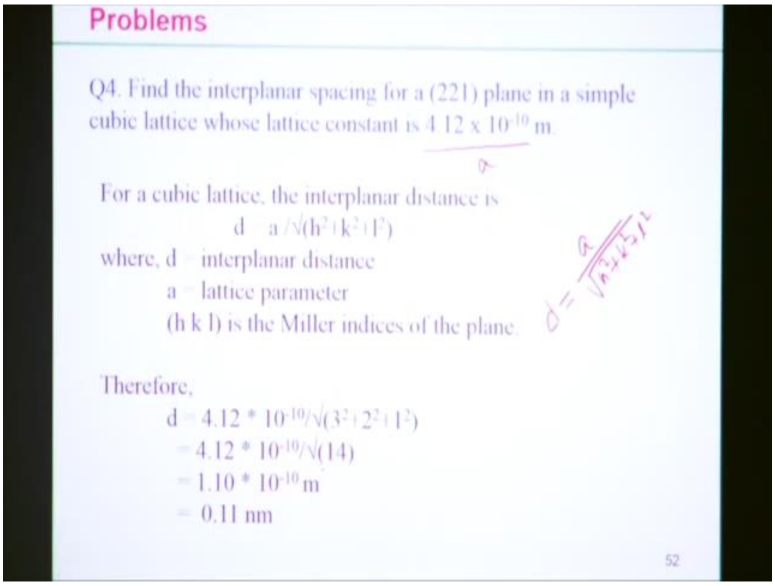

Problems

Q4. Find the interplanar spacing for a (221) plane in a simple cubic lattice whose lattice constant is 4.12×10^{-10} m.

a

For a cubic lattice, the interplanar distance is

$$d = a/\sqrt{(h^2+k^2+l^2)}$$

where, d = interplanar distance

a = lattice parameter

(h k l) is the Miller indices of the plane.

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

Therefore,

$$d = 4.12 * 10^{-10}/\sqrt{(3^2+2^2+1^2)}$$
$$= 4.12 * 10^{-10}/\sqrt{(14)}$$
$$= 1.10 * 10^{-10}\ \text{m}$$
$$= 0.11\ \text{nm}$$

Now we shift to the next problem. Find the interplanar spacing for a 221 plane in simple cubic lattice pose lattice constant is 4 point 12 into 10 to the power minus 10 m. So interplanar distance that we have already discussed, that distance can be like this; a by root of h square, l square, where h, k, l is the Miller Indices of the plane and d is the interplanar distance and a is the lattice parameters. So, lattice parameter is given, Miller Indices also given then we can find out the distance just to focus on that what units we are using. So, in terms of meter, in terms of nanometre we can represent.

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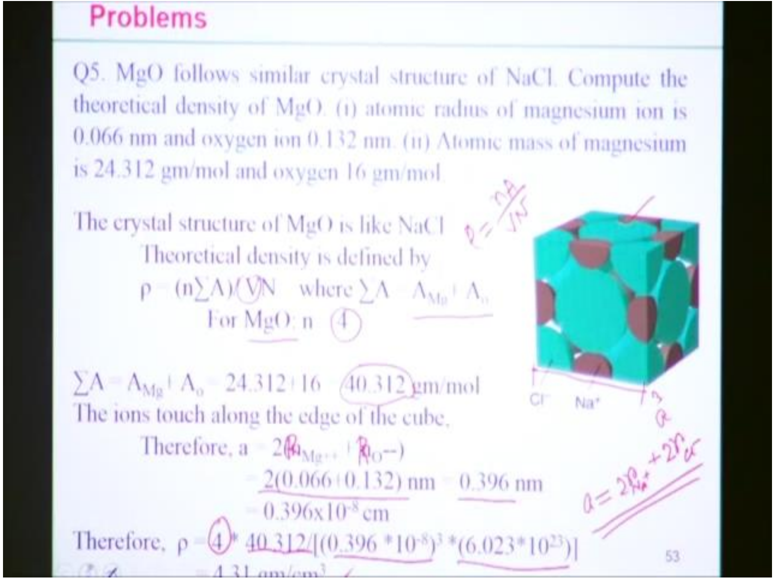

Problems

Q5. MgO follows similar crystal structure of NaCl. Compute the theoretical density of MgO. (i) atomic radius of magnesium ion is 0.066 nm and oxygen ion 0.132 nm. (ii) Atomic mass of magnesium is 24.312 gm/mol and oxygen 16 gm/mol

The crystal structure of MgO is like NaCl

Theoretical density is defined by

$\rho = (n\sum A)/(VN)$ where $\sum A = A_{Mg} + A_o$

For MgO: $n = \boxed{4}$

$\sum A = A_{Mg} + A_o = 24.312 + 16 = 40.312$ gm/mol

The ions touch along the edge of the cube,

Therefore, $a = 2(R_{Mg++} + R_{O--})$

$= 2(0.066 + 0.132)$ nm $= 0.396$ nm

$= 0.396 \times 10^{-8}$ cm

Therefore, $\rho = 4 * 40.312/[(0.396 * 10^{-8})^3 * (6.023 * 10^{23})]$

$= 4.31$ gm/cm^3

$\rho = \frac{nA}{VN}$

$a = 2r_{Na^+} + 2r_{Cl^-}$

Problem 5, we can see that magnesium oxide follows the similar crystal structure of NaCl; the structure is, we can observe from the figure. Now we need to find out the theoretical density of magnesium oxide; all the data are given, atomic radius of magnesium ion, atomic radius of oxygen ion, atomic mass of magnesium, atomic mass of oxygen, this all (are) are provided now we need to find out the theoretical density. We will be following the similar procedure (wh) what we did for pure metals. But here we need to be careful when we try to applying the formula of theoretical density of any compound material, see that is, was given like that; nA by V into N.

So n equal to number of atoms within the unit cell, A is the atomic mass or atomic weight and V is the volume of the unit cell, and (n) N is the Avogadro's number here. But here since in this compound structure the number of anions and number of cations, I, that means magnesium ion and oxygen ion, the number is the same that is total n equal to 4. But since we have the different values of the atomic mass or different values of the atomic radius in case of magnesium oxide so, A can be represented like that, is that consists of AMg plus, magnesium plus, atomic mass of oxygen. So that can be found out that total is the 40 point 312 grams per mole, but here magnesium oxide number, total number of atoms equal to 4. But, that is equal to for both anion (and) as well as cation.

Now, how to estimate the volume V in this case? To estimate the volume we know simply if we know the lattice parameter a, the volume indicates the a cube. But, how radius of the individual ions and the lattice parameters can be correlated? So if you see along the edge if the orientation of the atoms is like that, that a is equal to twice, 2 times of r sodium ion plus times of r chlorine ion, chloride ion. And here which is same for the magnesium oxide so where the Mg plus plus and n minus minus, so here it should be the, I think, r, r. So if we add it and then it becomes, point 396 nanometre and from here we can find out the edge lengths or maybe lattice parameter and from that we can find out the volume. Once the volume is found out, so this is the volume and this is the Avogadro's number and this is number of atoms and this is the atomic mass. So we can find out, this is the theoretical density of magnesium oxide.

So it is almost equal, equivalent to the similar procedure what we followed in case of pure metal, but we should be very careful when we try to estimate the atomic mass, that is consist of both the magnesium as well as (ox) oxygen ion but at the same time we need to know what are the number (of) is there any difference or obviously it should be the same, the number of anions and cations there, and how to link between the lattice parameter and the radius of the ions. So looking into the available parameter we can find out the theoretical density of compound material in case of magnesium oxide here.

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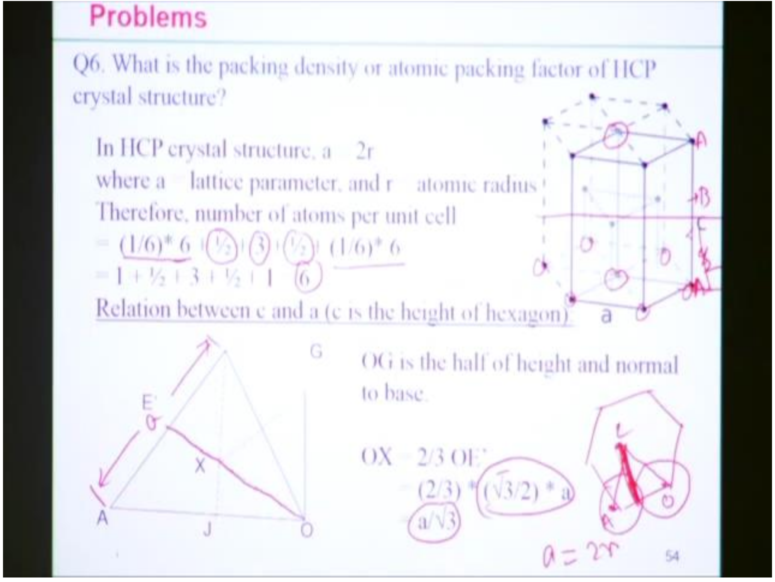

Problems

Q6. What is the packing density or atomic packing factor of HCP crystal structure?

In HCP crystal structure, a = 2r
where a = lattice parameter, and r = atomic radius
Therefore, number of atoms per unit cell
= (1/6)* 6 + (½) + (3) + (½) + (1/6)* 6
= 1 + ½ + 3 + ½ + 1 = (6)

Relation between c and a (c is the height of hexagon)

OG is the half of height and normal to base.

OX = 2/3 OE'
= (2/3) * (√3/2) * a
= a/√3

a = 2r

Next problem, we will try to theoretically estimate that what is the packing density or atomic packing factor for HCP crystal structure. If we look in the HCP crystal structure, here along the base, hexagonal, 2 atoms are in continuous contact so from here we can easily correlate between the lattice parameter a and the radius of the atom which is a equal to 2r where a is the lattice parameter and r is the atomic radius. Now what is the total number of atoms for unit cell, here we can find out that along the corner are 6 atoms but sharing volume of the atoms within the unit cell is only 1 sixth.

This is the case for the bottom surface, this is the case for the upper surface and 3 atoms inside exist the, this is the stacking sequence layer A and 3 atoms stacking sequence layer B, again it is stacking sequence layer A; so in this case the, on the stacking sequence at the layer B there exist 3 atoms which completely inside the unit cell. So, that is why 3 comes here and another 2 these atoms and that base atoms actually half of the atoms exist inside the unit cell one from base, another from the upper side. So, total numbers of atoms within the unit cells comes as 6.

Now we need to find out since in this cell there are 2 parameters are there a and c, so it is necessary to find out the correlation between a and c. So first if we look into on the base, OG is the half of the height and (n) normal to the base. So OG we consider the half of the height, which is basically c by 2. You can find out the OX, OX basically we are (co) we are focusing on this part A, O and some C for example.

So here, if we find out the OX; OX which is equal to 2 third of the OE so OE can be found out, this is this length, so OE is basically root 3 by 2 into lattice parameter a; actually this is the base A. So, OE is the root 3 by 2 into A and OX is the, is of course OX is the 1, 2 third of the OE or the EX equal to one third of the OE. So here it is coming a by root 3.

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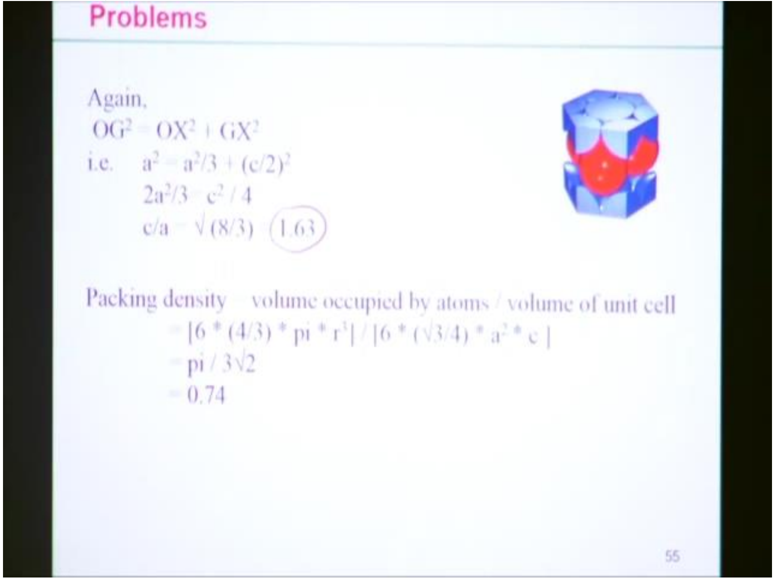

Problems

Again,

$OG^2 = OX^2 + GX^2$

i.e. $a^2 = a^2/3 + (c/2)^2$

$2a^2/3 = c^2 / 4$

$c/a = \sqrt{(8/3)} = \boxed{1.63}$

Packing density = volume occupied by atoms / volume of unit cell

$= [6 * (4/3) * pi * r^3] / [6 * (\sqrt{3}/4) * a^2 * c]$

$= pi / 3\sqrt{2}$

$= 0.74$

And again if we look into that triangle, OG, OX and GX, OG, OX and GX looking into this triangle, but, this triangle we are considering that OG actually, the distance along the Z axis of this HCP structure and the OG actually represents the half of the distance along the Z axis. That means if along the Z axis the parameter is C, basically OG represents the half, C by 2. Hear OG square equal to OX square plus GX square. So OG we have already estimated that is a square equal to OX; OX equal to a by root 3, so a square by 3 and GX equal to C by 2 square if we look into the OG square, it is the equal to the a square.

So from here we can find out the c by a ratio is basically 1 point 63. But we can find out the packing density actually volume occupied by atoms, volume of unit cell; divided by volume of unit cell we can find out the packing density in this case, but first before that we need to estimate the c by a ratio. If we find out this and other terms can be proceed as usual.

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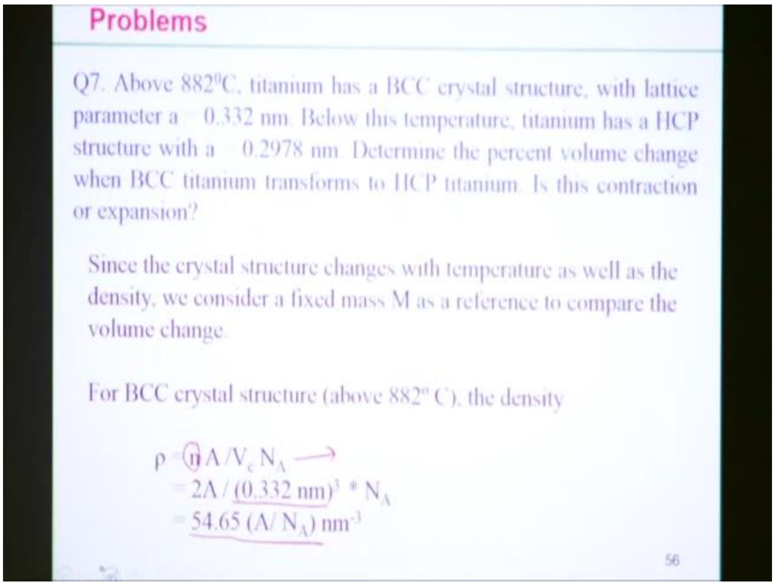

Problems

Q7. Above 882^{0}C, titanium has a BCC crystal structure, with lattice parameter a = 0.332 nm. Below this temperature, titanium has a HCP structure with a = 0.2978 nm. Determine the percent volume change when BCC titanium transforms to HCP titanium. Is this contraction or expansion?

Since the crystal structure changes with temperature as well as the density, we consider a fixed mass M as a reference to compare the volume change.

For BCC crystal structure (above 882^0 C), the density

$$\begin{aligned}\rho &= \textcircled{n} A / V_c N_A \longrightarrow \\ &= 2A / \underline{(0.332\ \text{nm})^3} * N_A \\ &= \underline{54.65\ (A/N_A)}\ \text{nm}^{-3}\end{aligned}$$

Now we come to that point that is next problem which is allotropic, related to the allotropic transformation, when there is a change of the structure from BCC to (s) any other crystal structure it is associated to some other change of the volume. For example 1, if we consider the titanium is a BCC crystal structure and 882 degrees centigrade with lattice parameter a equal to point 332. Below this temperature, titanium has a HCP structure were lattice parameter is different.

Now we need to find out the percentage of volume change when BCC titanium transforms to the HCP titanium, we need to find out whether it is contraction or expansion. Okay, let us see how to solve this problem. Since the crystal structure changes with temperature as well as the, there is a, there may be the change in the density, so, we need to consider the some reference when, maybe here we can consider the fixed mass as a reference to compare the change of the volume.

In case of BCC crystal structure above 882 degrees centigrade the density can be calculator like that from the formula of the theoretical density calculation but here in case of BCC structure, total number of atoms is 2, and A is the atomic mass and BCC, Vc is the volume of the unit cell that corresponding lattice parameter is given so from there we can find out the volume and Avogadro's number. So finally it can be estimated that 54 point 65 and the ratio a by Na, that gives atomic mass by Avogadro's number, suppose the unit in, representing in terms of nanometre.

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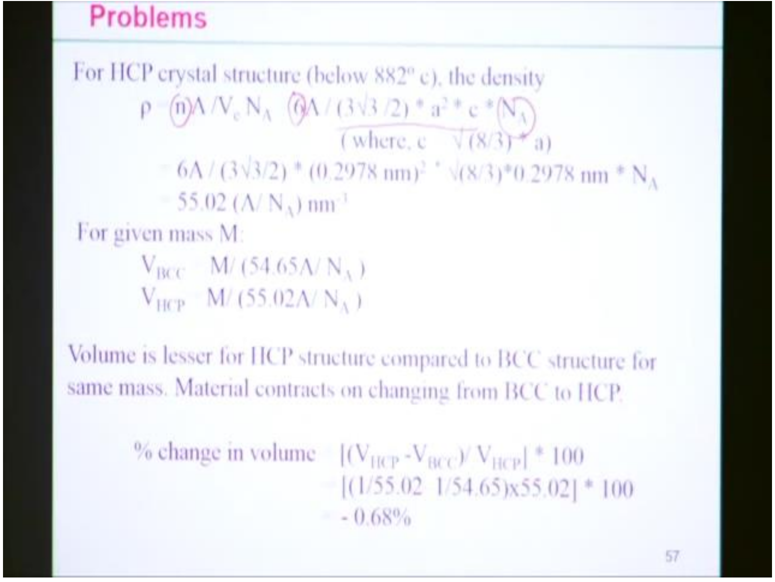

Problems

For HCP crystal structure (below 882° c), the density

$\rho = (n)A / V_c N_A = (6)A / (3\sqrt{3}/2) * a^2 * c * (N_A)$

(where, $c = \sqrt{(8/3)} * a$)

$= 6A / (3\sqrt{3}/2) * (0.2978 \text{ nm})^2 * \sqrt{(8/3)} * 0.2978 \text{ nm} * N_A$

$= 55.02 \, (A / N_A) \text{ nm}^{-3}$

For given mass M:

$V_{BCC} = M / (54.65A / N_A)$

$V_{HCP} = M / (55.02A / N_A)$

Volume is lesser for HCP structure compared to BCC structure for same mass. Material contracts on changing from BCC to HCP.

% change in volume $= [(V_{HCP} - V_{BCC}) / V_{HCP}] * 100$

$= [(1/55.02 - 1/54.65) x 55.02] * 100$

$= - 0.68\%$

Now this is the theoretical density estimation of (BCC) BCC structure but when there is a change of the temperature exist in the HCP structure then similar way we can find out the theoretical density where we need to know that number of atoms are different in this case, maybe in HCP crystal structure, total number of atoms is 6, A is the atomic mass. Here we can estimate the volume of the unit cell in case of HCP structure and Avogadro's number is given as Na.

Now here if we find out this things we will find out that (50), the density is coming 55 point 02, A by Na nanometre the power minus 3. So this are the 2 different densities assuming the 2 different type of crystal structure. Now over a fixed mass the volume (assume) in case of BCC structure will be the mass by density, in case of HCP structure similar we can find out the volume. So, obviously the, for the same mass, the volume of BCC and volume of (BCC) HCP structure are different. So in this case the volume is less, in case of HCP structure as compared to the (BCC) BCC structure and it is obvious from the, these 2 calculation.

Now material constants like atomic mass, total mass and Avogadro's numbers remain constant so change of the volume can be estimated that, this is the change of the volume with respect to the final volume and in terms of percentage we can estimate is around minus 0 point 68 percentage. So there is a volume (con) contraction but at the same time we found that change of the volume percentage is very less, only minus point 68 percent. But (it he) it may be very important in case of any structural changes when there is a change of the temperature in case of (titanium) titanium.

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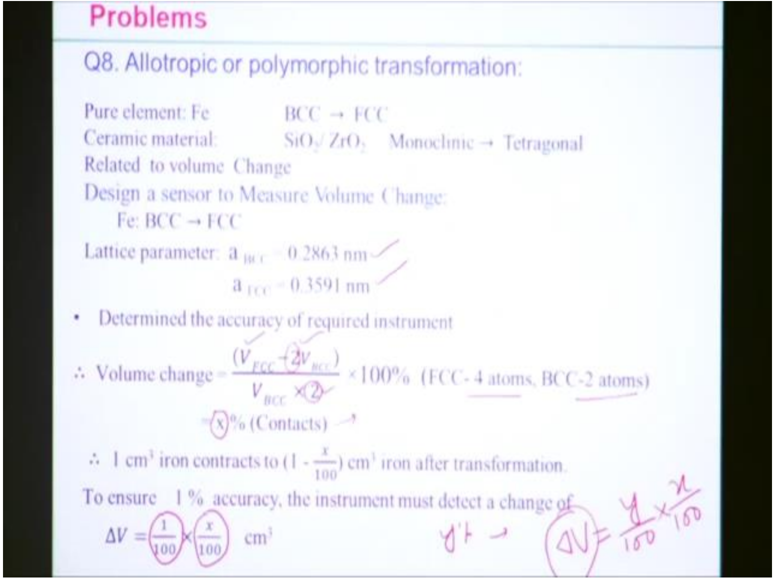

Problems

Q8. Allotropic or polymorphic transformation:

Pure element: Fe BCC → FCC
Ceramic material: SiO_2/ ZrO_2 Monoclinic → Tetragonal
Related to volume Change
Design a sensor to Measure Volume Change:
Fe: BCC → FCC
Lattice parameter: $a_{BCC} = 0.2863$ nm ✓
$a_{FCC} = 0.3591$ nm ✓

- Determined the accuracy of required instrument

$$\therefore \text{Volume change} = \frac{(V_{FCC} - \boxed{2}V_{BCC})}{V_{BCC} \times \boxed{2}} \times 100\% \quad (\text{FCC - } \underline{4 \text{ atoms}}, \text{ BCC } \underline{\text{-2 atoms}})$$

$$= \boxed{x}\% \text{ (Contacts)} \rightarrow$$

$\therefore$ 1 cm^3 iron contracts to $(1 - \frac{x}{100})$ cm^3 iron after transformation.

To ensure 1 % accuracy, the instrument must detect a change of

$$\Delta V = \boxed{\frac{1}{100}} \times \boxed{\frac{x}{100}} \text{ cm}^3 \qquad y\% \rightarrow \qquad \boxed{\Delta V} = \frac{y}{100} \times \frac{x}{100}$$

Another example for the allotropic and polymorphic transformation we can consider. In this case, in case of pure iron, that we know there is a change from BCC to FCC with respect to temperature and ceramic materials like SiO2, ZrO2 they also change the structure from monoclinic to tetragonal crystal structure. So of course it is associated with some volumetric changes. Now, looking into the change of the volume, it is possible to design the sensor. let us look into that how we can estimate this things.

So, look, take the example of iron and there is a change of the volume from crystal structure from BCC to FCC. BCC structure, the lattice parameter is given as point 2863 nanometre but FCC structure, the lattice parameter is given as point 3591 nanometre. Of course the same material, but they have 2 different lattice parameters of course there having the (s) crystal structure or atomic arrangements are different in these 2 cases.

Now when we try to find out the accuracy of required instrument we need to change the sense of the (volumic volume) of volume during the transformation from BCC to FCC or vice versa. Now, how we can estimate the volume change? Here, volume change from final to initial and here it is the, with respect to the initial volume, VBCC. If we see that here we are trying to put some reference (())(67:38) compare the change of the volume keeping the total number of atoms remains the same.

In FCC, total number of atoms is 4 but in BCC structure total number of atoms is 2. Therefore to compare with respect to the total number of atoms remains the same, even they change the crystal structure, we multiplying by the 2 in case of BCC structure to compare the volumetric change. So here also we multiplying the 2 since the ratio of the number of atoms in FCC and BCC is 2.

So now putting the other lattice, putting the lattice parameter if we estimate the volume change then we can find out some percentage change maybe we can see that if we estimate that suppose it is the coming as x; x maybe the numerical value but finally we estimate this thing with these parameters, maybe it may contracts. So volume contraction will be there. Suppose that there is a x percent of the volume contraction when there is a change of the structure from BCC to FCC in case of pure iron.

Now, if we, so that makes 1 centimetre (co) cube iron contracts to 1 minus x by 100 centimetre cube iron after transformation. Now if we try to use this information and if we try to design one sensor having 1 percent accuracy then the instrument must be detect a change of the volume should be, this is the, this comes to 1 by 100, that means this comes from the accuracy level of the instrument as per the requirement and second plot comes from the, that what is the volume change can be detected when there is a change of the crystal structure.

So, if it is defined that we need to ensure Y percent of the accuracy in the instrument then (what) what should be the age of the volume will be able to detect, that, then in that case delta V can be Y by 100 into that x by 100 that actually comes from the structure of the crystals, structure of the crystal when there is a change from one structure to another (change). So, that amount of the volume change will be able to, we will be able to detect it by the instrument. So these are the typical application of the crystal structure when you try to design a sensor.

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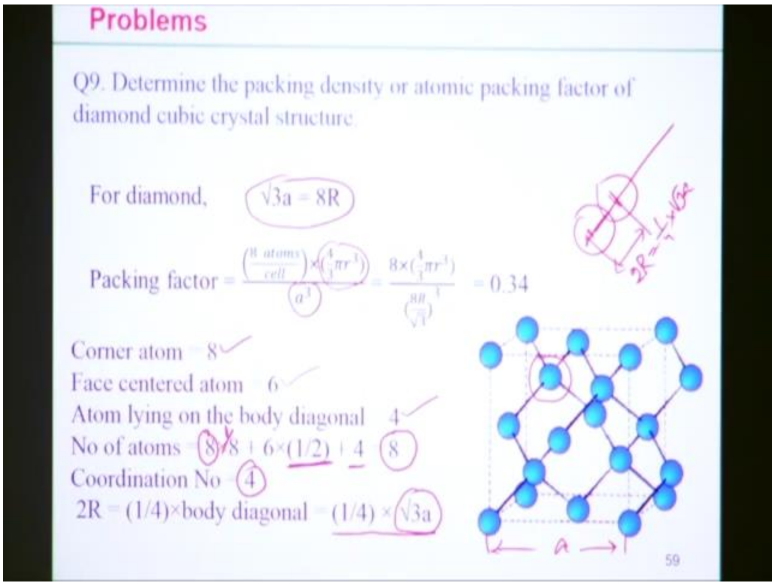

Problems

Q9. Determine the packing density or atomic packing factor of diamond cubic crystal structure.

For diamond, $\boxed{\sqrt{3}a = 8R}$

$$\text{Packing factor} = \frac{\left(\frac{8\ \text{atoms}}{\text{cell}}\right)\times\left(\frac{4}{3}\pi r^3\right)}{a^3} = \frac{8\times\left(\frac{4}{3}\pi r^3\right)}{\left(\frac{8R}{\sqrt{3}}\right)^3} = 0.34$$

Corner atom = 8 ✓

Face centered atom = 6 ✓

Atom lying on the body diagonal = 4 ✓

No of atoms = $\cancel{8}/8 + 6\times\underline{(1/2)} + \underline{4} = \boxed{8}$

Coordination No = $\boxed{4}$

2R = (1/4)×body diagonal = $\underline{(1/4)\times\boxed{\sqrt{3}a}}$

Here we will need to consider another problem related to that packing density or atomic packing fraction of diamond cubic crystal structure. First, we need to investigate what are the total number of atoms exist within the diamond structure. There are 8 corner atoms, there are 6 face atoms and atoms lying on the body diagonal is 4, so within unit cell there is a unit cell there may be the possibility of constructing the 4 diagonals within that cell, so along the 4 diagonals 4 atoms exist in diagonal structure.

So total number of atoms like that, total number of atoms is 8 but sharing of the volume of the cornered atoms is 1 eighth, so it should be 1 eighth plus 6 (fate) face atoms and sharing is half and plus 4 body diagonal atoms. So in this case total number of atoms is 8. Now what is the coordination number in this case here if we find out that coordination number is only 4 here. So that means one atom is connected to the 4 surrounding atoms in, continuously.

Now we need to find out what is the lattice parameter a and the atomic radius relation. So in this specific structure the body diagonal elements exist and (so) actually 1 fourth of the distance along the diagonal on the corner point. So along this corner points, so along the body diagonal on the corner points these 2 atoms are in contact but that is in 1 fourth of the total distance of body diagonal, so one fourth of the body diagonal so root 3a is actually the distance of the body diagonal or length of the body diagonal and this atoms exist at a 1 fourth distance.

So this is corresponding to the 1 fourth of the body diagonal distance and from this relation we can find out between the lattice parameter and radius. Now if we try to find out the packing fraction in this case here if we see there are 8 atoms per unit cell and total (vo) volume of 1 atom is this and here is the volume of the unit cell. So if we quote these values we can find out the packing fraction is the only point 34, although, it is obvious that the packing fraction of diagonal structure is very less point 34 percent only. Probably, this is because of the coordination number is very poor in this case (pro) only (f) coordination number is 4 and so most of the space within the unit cells remains vacant or we can say that may not be very compact structure it can form, diamond.

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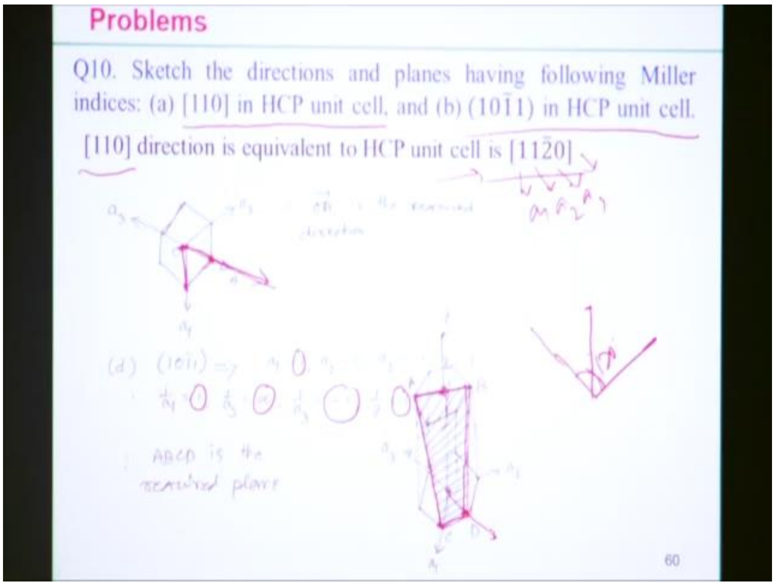

Problems

Q10. Sketch the directions and planes having following Miller indices: (a) [110] in HCP unit cell, and (b) $(10\bar{1}1)$ in HCP unit cell.

[110] direction is equivalent to HCP unit cell is $[11\bar{2}0]$

Next we try to focus on the problem like this. Sketch, so now we shifting to the construction of the directions and planes in case of HCP structure. So first direction first we need to show the Miller Indices of this 1110 direction in HCP unit cell and another is the 101 bar 1 in case of HCP unit cell, so that; so first problem it indicates the direction but if you see there are 3 elements is there, so actually this direction in 3 axis system which is equivalent to the 112 bar 0 in case of HCP cell so that we can easily convert it, if we know the relation between the 3 axis system to the 4axis system of HCP structure. So if we see that 1120 structure can be like that.

So along the a1 axis, if say, suppose this is the base and if we see that a1 axis, a2 axis component a3 axis minus 2 and Z axis or c axis is 0. That means it is existing on this specifically base plane. So we, unit distance along the a1 if we consider as a unit distance we start from the origin, unit distance along the a1, then unit distance along the a2, so here we try to move from (the it) this parallel to the a2 at this point and then unit (so) 2 units negative to the a3 direction which is equal to the, opposite to the this direction, a3. So here actually, if this is the; so it actually represents that; so now a3 we need to move negative to the 2 units along this direction.

Now if we join between this origin the point to that point, then it can be same that actually this direction indicates the opposite to the a3 axis. Okay, so OA is the required direction within the HCP unit cell. Now if we look into that specific plane and HCP unit cell, here if we see that 101 bar 1 is the unit cell, the first step is to find out what are the intercepts along the different axis where a1 equal to 1 unit, a2 equal to 0, a3 equal to minus 1 and Z equal to 1 the centre values, but reciprocals of that a1 that is 1, along the a2 reciprocals indicates 1 by 0 that means it is infinity, and a3 it is minus 1, and Z it is 1.

Now we will try to find out the, this intercepts along the different axis. So a1 we can find out the unit length, this point a2 is infinity that means the plane should be parallel to the a2 axis when a3 is the negative 1, so this direction actually indicates the negative direction. So this point is the intercept along the negative direction but of unit 1 and Z, along the Z direction it is the unit 1. So from here the, this unit 1 along the Z direction is this. Now if we construct this point and then that actually define the specified plane and you can investigate this, this (ac) plane actually parallel to the a2 axis, that is also satisfying, because it should be parallel to the a2 axis. So ABCD is required plane this case.

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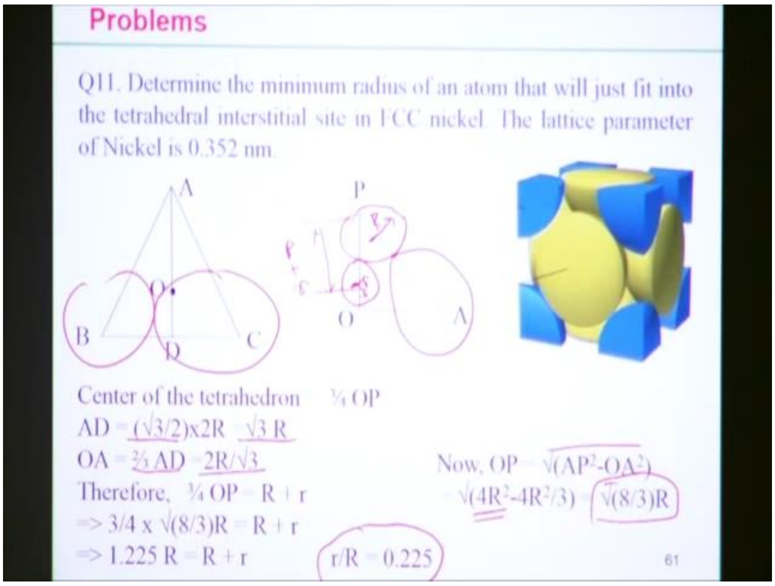

Problems

Q11. Determine the minimum radius of an atom that will just fit into the tetrahedral interstitial site in FCC nickel. The lattice parameter of Nickel is 0.352 nm.

Center of the tetrahedron = ¾ OP

AD = (√3/2)x2R = √3 R

OA = ⅔ AD = 2R/√3

Therefore, ¾ OP = R + r

=> 3/4 x √(8/3)R = R + r

=> 1.225 R = R + r

r/R = 0.225

Now, OP = √(AP²-OA²)

= √(4R²-4R²/3) = √(8/3)R

Another case if we, here there is a, how to find the minimum radius of an atom that will just fit into the (intersti) tetrahedral interstitial site in FCC nickel. The lattice parameter of nickel is given. So in case of tetrahedral site, tetrahedral site can be constitute among the 4 atoms and in between that atoms we can find the 1 site and we (need) it is also necessary to find out what is the exact size of the atom that (ex) exactly fitting in that tetrahedral site.

And we observe that tetrahedral site exist both in FCC as well as BCC structure. But here we need to find out the tetrahedral site in FCC structure. But basic point starts that if we look into that FCC structure there the several tetrahedral sites exist but if we look into, from the and the 1 plane is ABC and its same a point O, from the point O is represents the actually, height along the Z direction.

So, centre of the tetrahedron is basically exist over the 1 fourth of the distance OP. OP is the distance along the Z axis. Now if we see that AP, in this case the 2 atoms are in continuous contact and tetrahedral site probably exists here. So first, centre of the tetrahedron is the third fourth of the, this distance, this is, we see this as a capital R, this small r. Now on the base if we find out AD is the, from the triangular route we can find out the root 3 2 into A, A or in this case it is 2R because 2 atoms are in continuous contact. So here it is root 3 R.

So, OA is the 2 third of AD that is 2R by root 3. Therefore this distance is basically (s) from the Centre of the tetrahedral to this distance is basically R plus small r. So then, 3 fourth of OP is equivalent to the R plus small r. Now OP can be calculated from other way. So from the (triangular) AP square minus of OA square from here AP equal to 2R because along the AP 2 atoms are in continuous contact and here we can find out 4R square minus here OA, we have already estimated 4R square by 3, so root 3 8 by 3 R is the value of the OP. So we put it here, 3 fourth into root 3 8 by 3 R and from here we can find out r by R is equal to point 225. So this is the way we can find out the interstitial sites.

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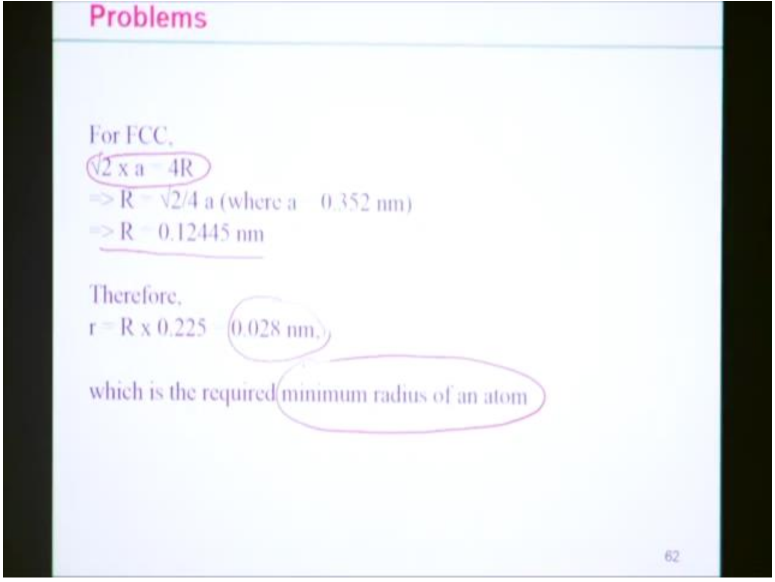

Problems

For FCC,

$\sqrt{2} \times a = 4R$

$\Rightarrow R = \sqrt{2}/4\ a$ (where $a = 0.352$ nm)

$\Rightarrow R = 0.12445$ nm

Therefore,

$r = R \times 0.225 = 0.028$ nm.

which is the required minimum radius of an atom

Now if we put this value in case of nickel then in case of FCC this is the relation exists over the face diagonal and from here we can find out the relation between the radius and the lattice parameter and since lattice parameter is known to us then putting this value we can find out the radius R here and finally that, put the radius here and we will be getting the radius of the interstitial site or maybe atom existence in the interstitial site exactly fitting this (point 0) point 028 nanometre which is the required minimum radius of an atom that produce the stable structure.

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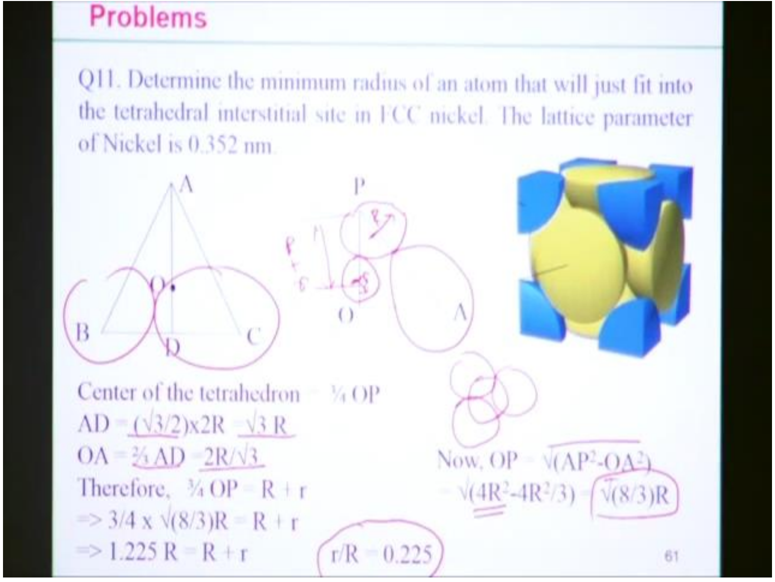

Problems

Q11. Determine the minimum radius of an atom that will just fit into the tetrahedral interstitial site in FCC nickel. The lattice parameter of Nickel is 0.352 nm.

Center of the tetrahedron = ¾ OP

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OA = $\underline{⅔\,AD}$ = $\underline{2R/\sqrt{3}}$

Therefore, ¾ OP = R + r

=> 3/4 x $\sqrt{(8/3)}$R = R + r

=> 1.225 R = R + r

$\boxed{r/R = 0.225}$

Now, OP = $\sqrt{(AP^2 - OA^2)}$

= $\sqrt{(4R^2 - 4R^2/3)}$ = $\boxed{\sqrt{(8/3)}R}$

So in this case just maybe, need to consider that atomic arrangement when you try to find the interstitial site that from the tetrahedral that means the having the coordination number of 4. So it is like that on the base there are 3 atoms and on the top between, there is a another 1 atom that actually constitute 1 tetrahedral interstitial site case of FCC and based on that we can do all this calculation to find out the radius ratio.

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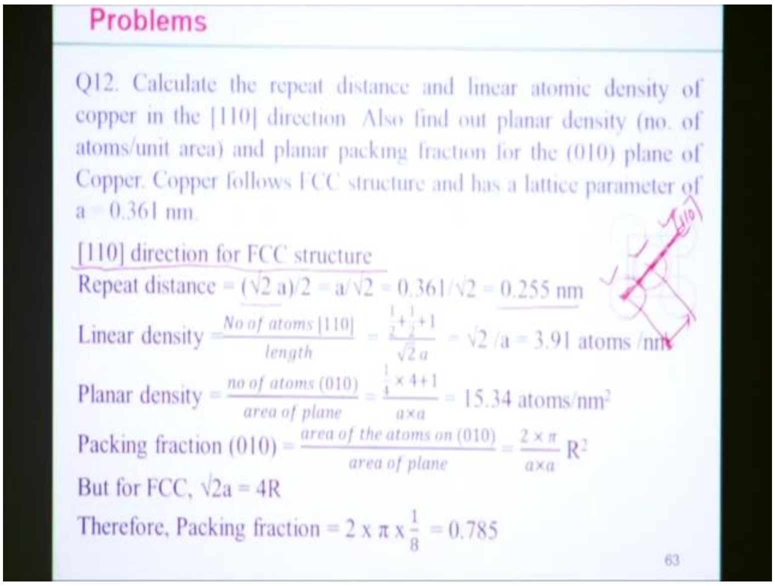

Problems

Q12. Calculate the repeat distance and linear atomic density of copper in the [110] direction. Also find out planar density (no. of atoms/unit area) and planar packing fraction for the (010) plane of Copper. Copper follows FCC structure and has a lattice parameter of a = 0.361 nm.

[110] direction for FCC structure

Repeat distance = ($\sqrt{2}$ a)/2 = a/$\sqrt{2}$ = 0.361/$\sqrt{2}$ = 0.255 nm

Linear density = $\frac{No\ of\ atoms\ [110]}{length} = \frac{\frac{1}{2}+\frac{1}{2}+1}{\sqrt{2}\,a} = \sqrt{2}/a = 3.91$ atoms /nm

Planar density = $\frac{no\ of\ atoms\ (010)}{area\ of\ plane} = \frac{\frac{1}{4}\times 4+1}{a\times a} = 15.34$ atoms/nm^2

Packing fraction (010) = $\frac{area\ of\ the\ atoms\ on\ (010)}{area\ of\ plane} = \frac{2\times\pi}{a\times a}R^2$

But for FCC, $\sqrt{2}$a = 4R

Therefore, Packing fraction = 2 x π x $\frac{1}{8}$ = 0.785

Now we will try to focus on this problem that idea about this thing what is the repeat distance, a linear atomic density of copper or planar atomic density. Let us look into this problem for copper having the FCC crystal structure. So first problem is that what is the repeat distance and a linear atomic density on specific direction, 110 direction; in FCC copper what is the repeat distance.

So, repeat distance is basically similar sequence of atoms, 1 specific direction. Since direction is specified here so 110 direction in FCC crystal structure actually indicates the face diagonal. So if we look into this figure, this is the 110 direction. So 1 atom exist at the corner point, next atom exist in this point. So in this case, repetition, repetitions can be considered as this distance which is half of the face diagonal. So, face diagonal length is root 2 a and half of this a by root 2. So, lattice parameter is given here, so we can find out point 255 nanometre is the repeat distance along the direction 110.

Now, linear density, linear density; when we try to focus on the linear density we need to consider along 1 specific linear direction, what is the number of atoms. So in this case along this direction 110 number of atoms can be represented so it is a only radius, radial only up to half of the atoms exist, then full atom exist; that is the representation along this line and half of the atom represented (as) along this line, so representations of the atoms along 1 specific line. So in that sense we can find out the total number of atoms is half (this) from this half from this and full from the middle one. So total 2 and a half and what is the total length; it is the length of the face diagonal root 2a and from here we can find out the 3 point 91 atoms per unit length per nanometre here.

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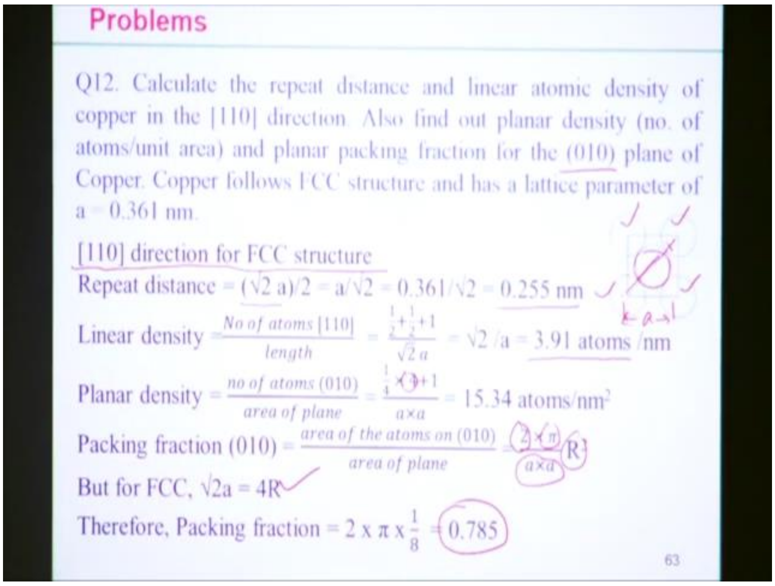

Problems

Q12. Calculate the repeat distance and linear atomic density of copper in the [110] direction. Also find out planar density (no. of atoms/unit area) and planar packing fraction for the (010) plane of Copper. Copper follows FCC structure and has a lattice parameter of a = 0.361 nm.

[110] direction for FCC structure

Repeat distance = $(\sqrt{2}\,a)/2 = a/\sqrt{2} = 0.361/\sqrt{2} = 0.255$ nm

Linear density = $\frac{No\ of\ atoms\ [110]}{length} = \frac{\frac{1}{2}+\frac{1}{2}+1}{\sqrt{2}\,a} = \sqrt{2}/a = 3.91$ atoms /nm

Planar density = $\frac{no\ of\ atoms\ (010)}{area\ of\ plane} = \frac{\frac{1}{4}\times 4+1}{a\times a} = 15.34$ atoms/nm^2

Packing fraction (010) = $\frac{area\ of\ the\ atoms\ on\ (010)}{area\ of\ plane} = \frac{2\times\pi R^2}{a\times a}$

But for FCC, $\sqrt{2}a = 4R$

Therefore, Packing fraction = $2 \times \pi \times \frac{1}{8} = \boxed{0.785}$

Now planar density; it is a number of atoms for unit area. So in this case we need to find out the planar density on 010 plane so here if we see that number of atoms on 010 plane, 010 plane or 100 or 001 plane is basically on the indicates an FCC structure on the face. Suppose this is the face, here if we find out what is the total number of atoms here, so this 4 cornered atoms, is representation here is the 1 fourth of each atom but there exist the number of atoms is 4 and 1 representation is this is the full atoms. So, total 1 plus 1, 2 number of atoms and what is the area of plane; area of plane equal to simply a square. So from here you can find out the 15 point 34 atoms per nanometre square length, is the planar density in case of FCC nickel (fa) sorry FCC copper.

Now, packing fraction on similar plane; here is the area of the atoms on that plane divided by the total area of the plane; that actually represents the fraction. So, here you can find out the area of the atoms, so it is a total number of atoms 2 and area of each atom equal to pi into R square, and a into a is the total area of the plane. So, here we need to know the relation between a and R, because only one parameter is given, a is given. So if we look into along the face diagonal, for FCC structure can find out this relation. So, this is root 2 a and at the same time this is 2R, R and R, so total 4 R equal to root 2 a.

So from here we can find out the relation between a and R if we put it here then we can find out the packing fraction. So, planar packing, but this packing fraction and this is corresponding to the planar packing fraction. So this fraction is corresponding to 1 specific plane and here also planar density is represented by the number of atoms per unit area but planar packing fraction is a, simply the ratio of the area occupied by the atoms and with respect to the total area of a specific plane. So these are the ways we can find out this calculation.

So I have discussed the different type of diverse problems (connec) which is connected to the theoretical discussions of this structure. Hopefully it will be understandable all these different kinds of numerical problems, but at the same time if we can go, or we can follow some reference book also we can find out lot of such numerical problems. But it is necessary to understand all the problems, or how to solve these problems for further understanding of the subjects for the (s) next module.

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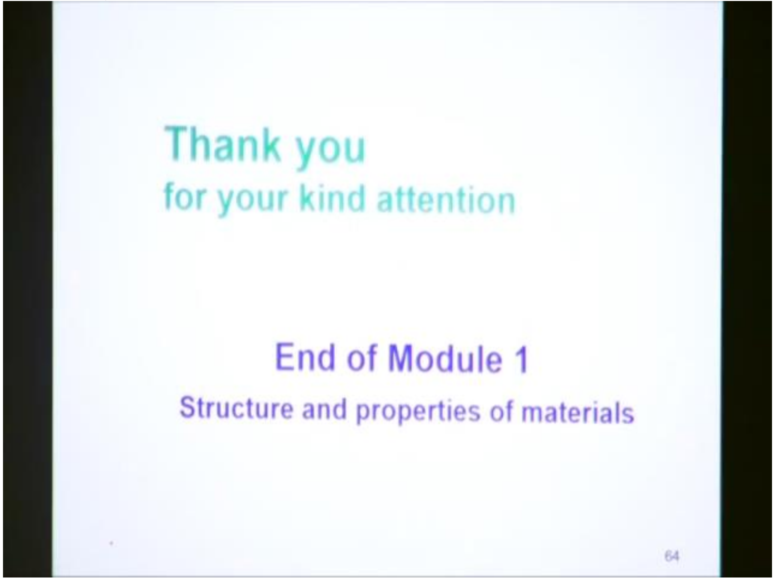

Thank you

for your kind attention

End of Module 1

Structure and properties of materials

So, this is the end of the module one that is, that was corresponding to the structure and properties of the materials. So next we will start in the next module. Thank you very much.