Advanced Ceramics for Strategic Applications
Prof. H. S. Maiti
Department of Mechanical Engineering
Indian Institute of Technology, Kharagpur

Lecture - 6
Crystal Structure (Contd.)

Let me continue my discussion with Crystal Structures, we were discussing about the silicate structures, we have discuss the seat silicate structures. And now, let me go to another topic in the same in the same subject that is the crystal structures of silicates and silica; to start with, we will look at the polymorphic forms of silica.

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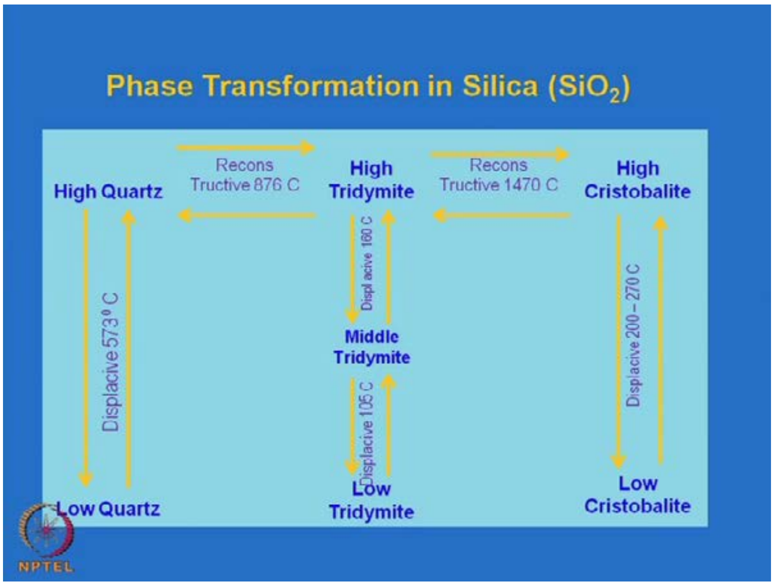

Phase Transformation in Silica (SiO_2)

High Quartz

Recons Tructive 876 C

High Tridymite

Recons Tructive 1470 C

High Cristobalite

Displacive 573° C

Displ acive 160 C

Middle Tridymite

Displacive 105 C

Displacive 200 – 270 C

Low Quartz

Low Tridymite

Low Cristobalite

Silica SiO 2 is basically composed of silicon oxygen tetrahedron, and we have seen how this silicon oxygen tetrahedron can be combined with other cations, and form a series of different silicates. But pure silica is also a very important raw material for this ceramics, not only for the traditional ceramic group, but silica sometimes is also important for advanced ceramic products in combination with other oxides. So, let us try to look at silica is a very complex material in some someway, because it has many different polymorphic forms, polymorphic forms means it is different crystal structures.

So, if you want to have a look at the different crystal structures, first of all let us try to understand, what are the different polymorphic forms pure silica may have. There are, the on the low temperature side, you have what we called high quartz or sometimes called beta quartz, and the still low temperature you have a low quartz. So, these are the low temperature regions, and then these are high temperature in the highest temperature is here.

So, you have low quartz which is alpha quartz sometimes called alpha quartz, and if we heat above 573 degrees centigrade which specific temperature, around about this you have a high quartz or sometimes is refer to as beta quartz, there is a density change, volumetric change. So, it is a kind of problem transformation for the industry, because whenever there is a volume change there is always a tendency of cracks, so making a densified material with pure silica is quite difficult.

There are techniques by which one can avoid that, but otherwise most of the time in the industry; this transformation is actually a very problematic phenomenon. There are different kinds of transformation in the whole gamete of different phases, low alpha quartz, beta quartz, then that beta quartz goes to high tridymite. High tridymite is another name of same composition, chemical composition yes I have to, but with the different structure.

Then if it is heated to still further distance transformation takes place around 876 degree centigrade, and then this around 1470, this goes to cristobalite, and then beyond that of course, silica melts are around 1710 1710 degree centigrade. Now, then this high tridymite, once again if you cool below about 160 degree centigrade, we will find another phase forms which is called beta, a middle tridymite and still below about 100 degrees, around 100 degrees centigrade it goes to low tridymite. Here also the cristobalite goes to a low cristobalite phase, which is different from the high cristobalite, but much lower temperature 270 degree centigrade around 200-270 degree centigrade.

In fact, these transformations are not always a thermodynamic transformation, some of them are different forms a trans I mean, not always an equilibrium transformation, there are some non equilibrium transformations also. Let us try to look at it, there are two types of transformation has been indicated in this table, one is called displacive transformation, this is called displacive transformation, this transformation from high quartz to high tridymite, the reconstructive transformation.

Then another reconstructive transformation takes place from high tridymite to high cristobalite, when these are cooled, these are this goes to the low cristobalite phase through a displacive transformation. Once again high tridymite when it is cool, it goes through a two different displacive transformation, one at around 160 degrees, and another at 105 degrees centigrade. Let us try to understand, what is the difference between a displacive transformation, and reconstructive transformation? We will discuss part of it later on in our topic on phase transformation, what is the mechanism of phase transformation, how one particular phase can transform to another particular phase.

Phase in this case we are basically referring to two different crystal structures, one crystal structure is changing of work to another crystal structure as a function of temperature. So, whenever the phase transformation taking place, a particular arrangement of atoms is getting changed to another geometric pattern of the atomic arrangement. And therefore, there is always what we call the mass transport, particular ion is moving from one position to another position and therefore, it can go through a process of what we call, a nucleation and growth phenomena.

If you talk about phase transformation, there are many mechanisms of phase transformation, one common phenomenon which takes place is nucleus and growth phenomena. Initially a small nuclei of a different crystal structure nucleus, and then more and more atoms join that particular structure and continue to go, so that is what you call the nucleus and growth phenomena. It involves a long range moment of a large number of atoms by atom is step by step manner, so it is a time dependent process, it is not only a temperature dependent process, but also a time dependent process. So, it is a kind of isothermal action; so it nucleus at a particular rate and then grew at a particular rate.

So, as time to seeds more and more transformation takes place, and you get 100 percent transformation only after alive in sufficient time at a particular temperature, there may be another mechanism, I use the similar phenomena can take place. One structure is changing over to another structure, but it is time independent, it does not take much long much very high long time. But, almost instantaneously through a cooperative moment of a large number of atoms, simultaneous moment large number of atoms, one particular geometry changes over to geometry.

And that is time independent and sometimes it is called a thermal process, the previous one the time dependent process is called isothermal process. And the second one they which is the time independent, sometimes called a thermal process and these two distinctions of phase transformations are very well known in material signs including ceramics. So, when we are talking about to this two transformations here, in reference to you see transformation of silicon, then you have a displacive transformation this is actually a time independent phenomena that means, is a very fast process.

And that is a thermal process, and also it is sometimes another way of looking at it is it is diffusion less transformation it is diffusion less transformation; that means, no long range moment of atoms, it is some kind of Cr moment, a small distance of moment by atom of the atoms. But, cooperative moment of atoms can change over from one geometric to another, and that is what we call the displacive transformation, and it is extremely difficult to coincide this transformation or avoid this transformation.

So, these are displacive that is the characteristics of a displacive transformation, where as the so called nucleation and growth type of phenomena is refers to as a reconstructive transformation; so that is the a kind of terminology. Normally ceramist uses these two terminology displacive transformation and reconstructive transformation, whereas metallurgist uses this and less transformation or a thermal transformation, and isothermal transformation.

So, that is the basic difference, may be we will discuss these things at related, states when talk about phase transformation. So, silica is very unique system that will where many displacive transformations takes place, as well as some reconstructive transformation take place to the reconstructive transformation take place, these are time dependent, but these are other transformations are time independent.

And they are not as I mentioned few minutes back that they not always a equilibrium transformation, some non equilibrium transformations also take place, these transformations do not take place until unless heated to high temperature, and then cool it back. For example, if you try to heat it to re high temperature, cristobalite sometimes depending on the rate of cooling, either it goes to the low cristobalite phase or it can go to the low tridymite phase right. So, there are some glass formations also, you know silica is one oxide which is easily forms glass.

So, once it forms a glass then of course, again the transformation becomes non equilibrium transformations, and then depending on the cooling rate, depending on the other impurities present many different cases situations may arise. So, otherwise these are the phases present in silica, and you get different kind of transformation as well as different temperatures, so that is all so for as silica transformations are considered.

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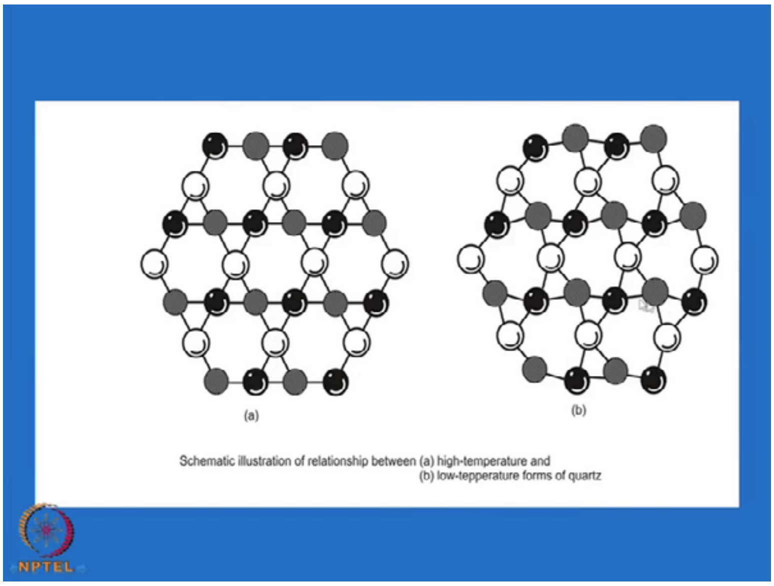
(a)

(b)

Schematic illustration of relationship between (a) high-temperature and (b) low-tepperature forms of quartz

Keeping this in mind we have some structures, these structures are to start with low quartz and high quartz, low temperature form of the quartz, this is the low temperature form of the quartz, and on the left you have high temperature form of the quartz. So, the basically a silica oxygen network these are stated differently, because they are at different planes, there are not in the seat only this is only one section and they have been given difference shades, because they are different depths. So, these are the kind of native work, only difference between this structure and this structure we will see, these area an regular hexagon, these are all regular hexagons.

Whereas, here the there is a slide deformation, there is no regular hexogen is more pentagon and then, so it is a combination of tetraha triangles and pentagons, so there is a distortion. And if you want to change this to this is actually slide displacement slide displacement of the individual atoms, and that is why this transformation this transformation is quite easy, at a particular temperature suddenly the atomic positions change, but not to a great distance, the atoms will not diffuse from over longer distance.

So, it is all within the inter atomic spaces, the moments are all with in the inter atomic spacing and that is why this is one of the examples of the displacive transformation, so it is much easy. So, and none of this displacive transformations very easy to stop or coinside transformation, if a reconstructive transformation, nucleons and growth phenomena, then if you coins them very fast or you can change the temperature particularly from high temperature to low temperature, the transformation can be or the phase can be quartz.

That means, high temperature fields can be available at room temperature, we will the kinematics is slow, so you are not allowing by co-in seat it fast or rapidly cooling it, we are not allowing enough time for the atoms to move. And therefore, the high temperature phase can be available at the room temperature or at your temperature, although it is not a thermodynamic phase table situation.

However, any displacive transformation would you do not take, do not involve, so much of larger distance moment of the atoms. Then you can you cannot co-in seat you cannot co-in seat, so even if (( )) rapid heating or rapid cooling the transformation will take place, and that happens when this particular situation between alpha and beta quartz transformations.

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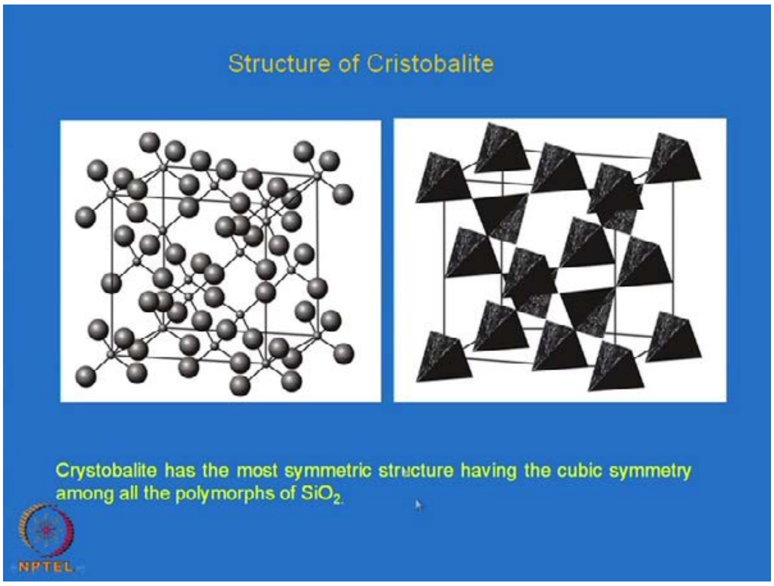

Structure of Cristobalite

Crystobalite has the most symmetric structure having the cubic symmetry among all the polymorphs of SiO_2

And as you can see the change in the structure is only nominal, this is the cristobalite structure. Cristobalite is a most symmetric structure, as you can see it is a highest temperature, cristobalite is available in the highest temperature and normally higher is the temperature or higher is the temperature of stability of any particular phase, that has a more symmetric structure, then the lower temperature phases. So, the cristobalite is the highest temperature phase in the system crystalline phase particularly, and it has the most symmetric structure have been the cubic symmetric.

So, co-accident has a cubic symmetric it is very complex structure, whereas if you talk about cristobalite it has a cubic symmetric. However, one has to find one difference between whatever structures we have discuss so far, whatever whenever you are talking about the symmetry, it is the position of one particular atom either the cation or the anion that dominates that determines the symmetric. Here, the symmetric are the motif here, what we call motif the units are actually tetrahedrons, silicon oxygen tetrahedron those are the motif of this symmetric.

And the corners ideal of the discussing many structures, we are the atoms or positions in the corners of the cube, here is a group of atoms, group of atoms is position adjacent corner of the cube. So, each corner is occupied by silicon oxygen tetrahedrons, not by silicon or not by only silicon only oxygen, it is a tetrahedron cubes which is occupied sitting at each of the corners, as well as the phase centers. So, this is the phase center, this is another phase center, so in all there are the 8 and 6, 16 14, 14 tetrahedral forms the face central cubic structure.

So, this is an unique situation so for as the structure of compounds, inorganic compounds are consider whereas at least whatever we will discuss under this course. So, cristobalite has a close packed cubic structure, FCC structure, but the motif here is not single atoms, but it is the tetrahedron, so these are the details of the atoms here. Once again if the frame work of a cubic structure, so at each corner we have a four different ions, four different ions, one is silicon ion and surrounding it there are four oxygen ions, so that becomes repeating force, a repeating in the structure; so, that is the description of the cristobalite form of silicon.

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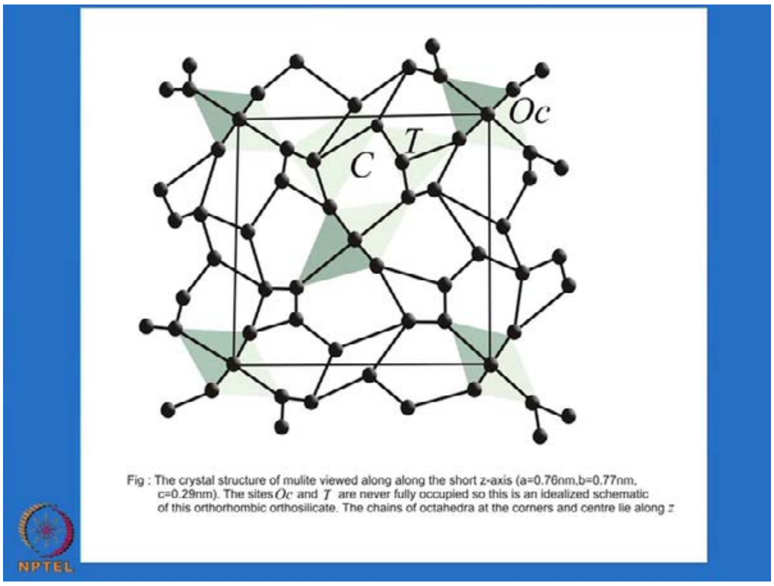

Fig : The crystal structure of mulite viewed along along the short z-axis (a=0.76nm,b=0.77nm, c=0.29nm). The sites *Oc* and *T* are never fully occupied so this is an idealized schematic of this orthorhombic orthosilicate. The chains of octahedra at the corners and centre lie along *z*

This is the not a pure silica of course, it is a another structure, it is mullite, mullite is the chemical formula of mullite is 3 A i 2 O 3, 2 SiO 2, this is a silicate and it has all sides one structure, this is not related to 3 A i 2 O 3 structure not 2 SiO 2 structure, but it is a completely different structure we distribution of silicon and oxygen, as well as silicon and aluminum. And this is what is the structure, this is also a you can see the crystal structure of mullite viewed along their is mistake over the two (()), the short z axis. These are the lattice parameters a, b, c we can see here, a and b are same more or less almost same where as c is different, so it is a kind of tetragonal symmetric.

The sides OC and T are never fully occupied, so this is an idealized systemic, a schematic of this orthorhombic or orthosilicate, this orthorhombic ortho silicate, so these are a orthorhombic structure and changes of the octahedron, at the corners and centers lie along z axis. So, this is again the symmetric is a through a group of atoms, tetrahedron and the octahedron also there. So, this is the mullite structure which is a very important compound, whenever we are talking about any aluminum silicate, heated to any aluminum silicate when heated to high temperature.

For example, kaolin structure, kaolin is a hydrated aluminum silicate, so at high temperature hydroxo alien goes away, and what is remain, what is remain is about is alumina and SiO 2, and they forms some compounds silicates of this nature. So, mullite is one of the very important phases, whenever in silicate structure is heated to high temperature mullite is normally formed, and it has (()).

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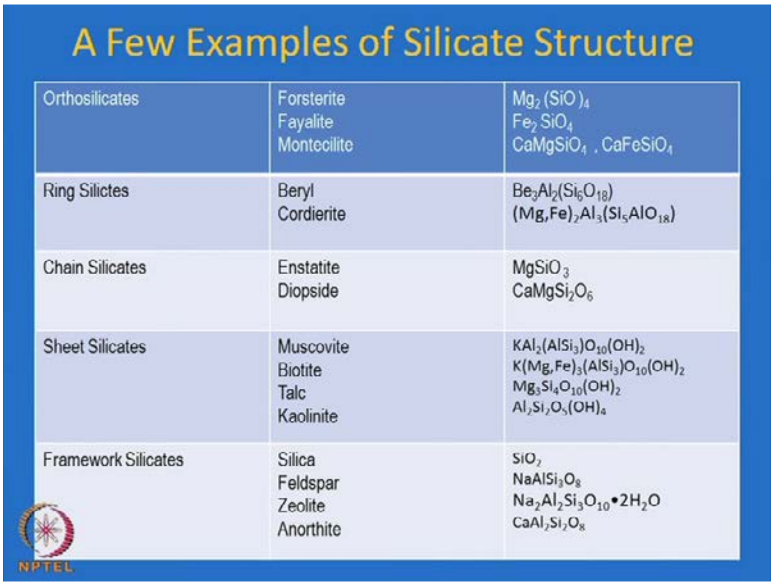

A Few Examples of Silicate Structure

Orthosilicates	Forsterite Fayalite Montecilite	$Mg_2\,(SiO)_4$ $Fe_2\,SiO_4$ $CaMgSiO_4$, $CaFeSiO_4$
Ring Silictes	Beryl Cordierite	$Be_3Al_2(Si_6O_{18})$ $(Mg,Fe)_2Al_3(Si_5AlO_{18})$
Chain Silicates	Enstatite Diopside	$MgSiO_3$ $CaMgSi_2O_6$
Sheet Silicates	Muscovite Biotite Talc Kaolinite	$KAl_2(AlSi_3)O_{10}(OH)_2$ $K(Mg,Fe)_3(AlSi_3)O_{10}(OH)_2$ $Mg_3Si_4O_{10}(OH)_2$ $Al_2Si_2O_5(OH)_4$
Framework Silicates	Silica Feldspar Zeolite Anorthite	SiO_2 $NaAlSi_3O_8$ $Na_2Al_2Si_3O_{10}\bullet 2H_2O$ $CaAl_2Si_2O_8$

Well, so far we have discussed different kind of silicates, let us try to look at it in a (( )) here, we have the left the different kind of silicates, different type of silicates whatever we have discussed so far. The orthosilicates that is the, that is the isolated silicon oxygen tetrahedra that is octal silicate, and then we have ring silicates, chain silicates, sheet silicates and finally, framework silicates, frame work silicate structure. Now, these are some of the examples of orthosilicate, forsterite mean logical name of is forsterite and formula is this Mg 2 SiO 4, this is the unit of SiO 4, and it has 4 minus, so Mg 2, 2 cations added to satisfy the charges.

Similarly, the other silicates like fayalite in these are the logical names of all the silicate listed here. So, fayalite is Fe SiO 4 is again a very important compound, there a low melting compound many of the refectories, do have this particular mineral and impact the presence of such minerals is always documental to the in factory property of the industrial refractorys; because, it has a relating demo low melting point. Montecilite is another kind of silicate is a complex silicate, as you can see here 2 Mg O, 2 Mg is satisfying 4 charges whereas, here one calcium and another magnesium, two together satisfies the 4 negative charges of SiO 4.

So, this is another kind of mixed silicate calcium magnesium silicate, another mixed silicate is here calcium iron silicate, both of them has two charges are bivalent the in this case Fe is ferrous Fe 2 plus, it is not a Fe 3 plus. So, these are the examples of orthosilicates and many of them we appear in association with other phases, in fact forsterite as such is a very good magnesium silicate, so very good compound which are the very important insulating property. And many of the insulators, good insulators do have a forsterite and part of forsterite Mg is added, so that is the particular phases is found and they have a would (()) property also.

Ring silicate, the examples are beryl that is again the numerological name, and formula is beryllium, aluminum, silicate beryllium, aluminum, silicate Si 6 member ring, because you have Si 6, Si 6 O 18. So, it is a 6 member ring and beryllium is very important group of 6 member of the member methane family of silicates; and cordierite, and the next one is cordierite once again beryl silicate. And here we can see there are aluminum part of the silica Si 6 O 18 in that we see again 6 member ring, and part of it has been replace by aluminum, and than it has been other cations been added.

So, it has become Si 5, Si 5 so one silicon have been replaced by aluminum, and in fact aluminum is one of the cation, although most of the time it has octahedral correlation that we have seen earlier. Even the co-random, in co-random structure aluminum has a 6 for coordination, but in silicates, many of the silicates when the association with the silicon and oxygen network, aluminum actually part of the aluminum goes to the tetrahedral side as well replace in silica silica. So, aluminum has a kind of dual character, it can go to the octahedral side also it can go to the tetrahedral side, and that is one of the important features of many of the silicate structures.

So, here that is what is happening, so that is the cordierite structure, now cordierite once again a very, very important compound in the family of ceramics, you know in whenever ceramics are used mostly in high temperatures. So, if you are heating a ceramics from room temperature to high temperature, it will always go through some thermal expansion, because most all materials have some kind of thermal expansion property, some of the high thermal expansion coefficient, others may not have that kind of coefficient.

So, if you are talking about high temperature material, in most of the applications one would like that the thermal expansion coefficient is low, so that there is no much of volume change or geometric change, change of geometric, the volume change during its heating or cooling. Because, during heating or cooling and there is a sufficient amount of volume change, then there is a possibility of brackets, there is the possibility of crack, formation, and the material will use its integrity. Therefore, many applications were, the materials have been heated several times, cool several times for example, in pharmacies many products where all impact, all ceramics have to be heated high temperature.

And it has to be supported on some material and somehow we call kill furnaces, so inside a large scale we have some kind of a supporting system on each of the actual products are kept. And if, so they have to be use large number of times, repeatedly use a inside the furnace, so they have to be heated and cool several times. If the material has a high thermal expansion co-efficient, than there is a possibility of crack, and the life of the material will, and the light of the supporting system will very poor or very low, and therefore, it involves a lot of expenditure.

So, this clean furnaces are all made of, mostly clean furnaces made up of cordierite service, cordierite is a phase which has very, very low thermal expansion co-efficient, compared to many other materials cordierite has very low thermal expansion co-efficient. And therefore, it very ideally suited for what we call furnace, clean furnaces which is actually used to support the others ceramic products which are interest to us. So, cordierite that is why is a very important, a ceramics and needs to know its structure as well as properties, may be time five minutes is discuss how, why the cordierite have the mixed do you have a very low thermal expansion co-efficient.

Now, we have when chain silicates, ring silicate, and then enstatite chain silicate, this is another magnesium silicate, it is this one postulate was 2 Mg SiO 2 here it is that means, two molecules of Mg O is is forming a compound with one molecular SiO 2. Whereas, here one Mg O and one SiO 2 that is Mg O SiO 2, so that is enstatite and that is different structure that is different structure compared to forsterite, both of them basically magnesium silicate, but they have different structure. This is also another one, here also we have a montecilite, we can see the montecilite here which is calcium magnesium silicate, this is also calcium magnesium silicate, but the formula is different, and neurological name is also different and the structure is also different.

So, we can see the kind of the variation one can have in the silicate range of products, and their composition, their structures are quite different although, silica is the main building block of all the silicon materials. Then they have a sheet silica, sheet silicates your mix that little bit about the structure, muscovite that is the potassium mica, and the structure and we have AlSi OH and their. OH and you would be major constituents of all these sheet silica, any sheet silica we have all there is would be a OH, why that is muscovite, kaolinite, then talc, talc is another very important mineral, which is SOP structure is a fine form, where from the name talcum powder came.

So, the talc is a main basically a national layer locked mineral, and is a silicate structure and this silicates or either have, what we call a symmetric structure or asymmetric structure, like kaolinite as a in this place asymmetric structure, one layer of silica and one layer of aluminum hydroxide. Whereas, the muscovite is basically a symmetric structure with one layer of silicon oxygen, another layer of, two layers of silicon oxygen and in between we have a layer of aluminum hydroxide. So, these are talc, magnesium basically hydrated magnesium silicate that is talc, kaolinite is hydrated aluminum silicate.

And the, this is symmetric structure one layer of silicon, one layer of aluminum hydroxide, here two layer of silica and one layer of magnesium instead of aluminum, if we put magnesium in a very similar structure. So, just replace aluminum by magnesium we will get talc, and then these are biotitic, and (( )) is actually mica. Framework silicates when we talk about framework silicates, you know in a sheet silicate if you added clearly, you can when you go from ortho silicate to sheet silicate the basic difference is here there is no breezing oxygen that means, there is no oxygen which is connected between two silicates, two silicon ions.

Here, the silicon two of them is connected, and then if you have chain silicates you have two or three both are possible, and then a sheet silicates three of the oxygen ions are shared by silicon, only one oxygen is available to be connected to bonded with other cations. In this case in a framework all the silicon, all the oxygen are basically which silicon, all the oxygen's have shared between silicon, and that is why you have a pure silicon structure, you have a pure silicon structure, silica structure that is no other cations. However, very similar things also can happen, we other structure, other compounds like feldspar, sodium, aluminum, silicon, oxygen; sodium, aluminum, impact.

In this cases what happens, why the other cations, how the other cations comes in, because silicon a part of the silicon has been replaced by aluminum, silicon has a four tetra valency or four charges, four possible charges as the aluminum has only three positive charges. So, it has one less positive charge, to satisfy that charge another extra positive charge has to come in from the (()), and that is why this sodium and aluminum eclipse sodium and aluminum together is replacing one of the silicon. So, otherwise it is basically a silicon structure, all the oxygen ions, so all the oxygen ions are basically say as by silicon atoms, silicon ions.

But, because one of the silicon ion had been replaced by aluminum, and aluminum in this case goes to the tetra hydroxide, so make compensate for the charge imbalance, once sodium ion has to come in, and that is how a feldspar structure is clear it compound is created; in basically a framework what we called it framework silicates. And as I mentioned earlier feldspar is one of the basic ingredients of y 2 M family of ceramics or (()) family of ceramics, it has a is a low melting point and act as a flux, forms a discuss liquid or discuss glass that oxygen minder for the other ceramic particles, but particularly quartz and mullite, so on.

So, feldspar is very important in gradient of write your familiar course in the ceramic, same with the case with zeolites, zeolites you know is very important for many different purposes, once again because of it is crystal structure, will not be discussing in much about this things. So, I am spending little time on this, once again it has a framework structure and sound is silicon has been replaced by aluminum, sodium has been added, and in addition you have some hydroxyl ion also. So, in the case zeolite forms one of the major characteristics of, important characteristics of zeolite is that it has this structure is such that, it has some histrographic holes, histrographic channels very fine channels, in the level of angstroms.

And that makes use becomes useful for many purposes, including catalyst between many of the zeolites are good catalyst or catalyst carriers, and in very recent times this channels a very fine channels or histrographic channels, are there very uniform channels. And through the channels a one can pass through many different gases, so either they can pass through or they can get absorbed. So, zeolites are some time many times used for absorption purposes this fine force or find histrographic channels, are used for absorption of different order molecule molecules may be some of the gases molecules can be absorbed by this type, there are many different forms of zeolites square, and this channel can be controlled, because of the crystallographic nature.

But, change in the histrographic and therefore, one can absorb different gases for gas separation, one can use them even gas separation can be by two different techniques, one is absorption you will just remove in the gas, and getting absorb in this micro holes or micro (()), micro pores of the zeolites or this is getting absorb their or sometimes it can be used as a membrane, a semi permeable membrane. So, to this channels a particular molecules of gases molecules are passes through the others may not pass through, because it provided they molecular size of those gases are bigger than the channels size.

So, they can be used as a semi permeable membrane, and in the context of new generation of fields or hydrogen economy, where hydrogen separation or hydrogen generation is very, very important, hydrogen separation from hydro carbons, for other gas mixtures are important. This, that is an attempt to make this zeolites, as a to be used as a semi permeable membrane, for hydrogen can pass through, because it has a small molecular size whereas, hydro carbon or some carbon dioxide may not passes through.

So, if you have a mixture of carbon dioxide in hydrogen, made from caking of hydro carbons one can generate either hydrogen, and separate out hydrogen and carbon monoxide, carbon dioxide, so that hydrogen can be separated in this manner. So, zeolites had been a very peculiar, a very important crystal structures having there poor sizes or channel sizes, which can be existed by changing the composition, and the structure one can use it for many different industrial purposes.

So, zeolites is another good important member of the silicate family, and the last one is anorthite is calcium aluminum silicate, all of them as you can see aluminum is one of the ions pressured particular to replace silicon. And accordingly other cations also coming to satisfy this all the balance so this is the, in sort the summery of different kind of silicates and their structures, and also I discussed now the usefulness and many of this compounds, well.

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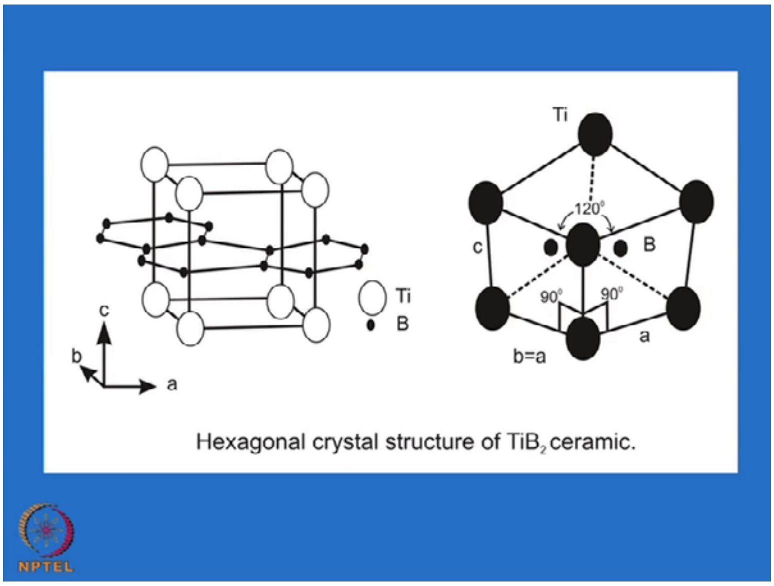

Hexagonal crystal structure of TiB_2 ceramic.

So far you have been discussing about the structures of different oxides, but oxides are not the only group of compounds, which will be useful for our later discussion or further discussion. So, for as their functional properties and their mechanical properties are concerned, so many of them, their particularly the advanced ceramic group compounds are not non-oxides or they may be carbides, nitrides, borides and so on. So, here there are few examples of non-oxide group of family of ceramics, we start with the titanium diborite, it is again useful will come across this compounds later on.

So, let us just have a look at what is the structure of that; this has a hexagonal crystal structure and hexagonal structure, it will remember just now, few minutes back I discuss that one of the angels is 120 degree and that is what shown here. So, the open circles are actually titanium ions, which are larger here compared to the boron, compare to the boron, and in all oxide structures we have seen that cation as a larger, as a smaller size and oxygen with the larger size.

Here actually, both of them in a sensor cations, and they group of compounds, but they are ionicity is very similar and therefore, they do not form ionic compounds, they form mostly covalent compounds. And so the ionic sizes are also different nature, titanium when you are talking about titanettes, titanium is much smaller ion compared to oxygen. And here you find that boron is still finest, still smaller it compared to titanium, so these are the titanium ions in the form of cube, whereas boron ions forms another layer in the form (()).

So, that is the description of titanium diborite, so hexagonal basic symmetric becomes hexagonal crystal, so these are the some of the positions of the boron atoms, how they are distributed and the distribution of the titanium. So, that is the brief description of what we know about the titanium diborite.

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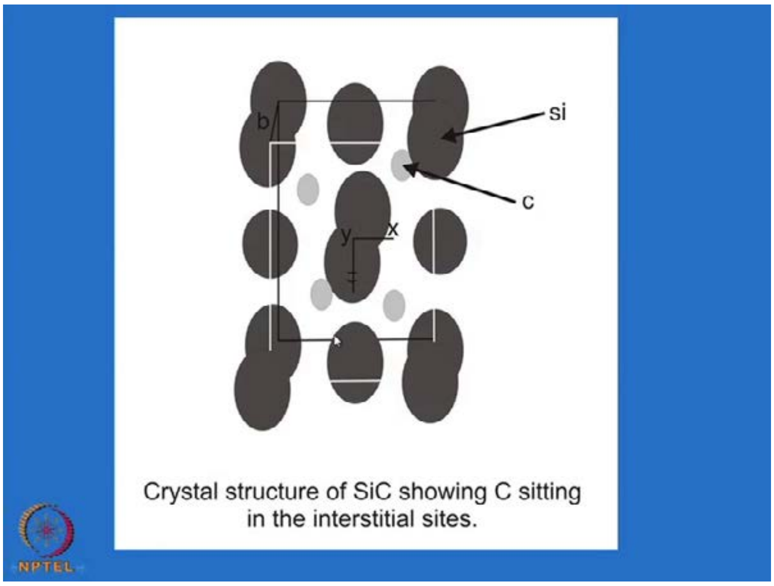

Crystal structure of SiC showing C sitting in the interstitial sites.

Another compound we are discuss, we are mentioned it about, discussing about the desired structure, zinc line structure, so there we have hexagonal structure, as well as cubic structure both are possible. In fact, silicon carbide is a very important group of advanced ceramic materials, and it has a very, very good high temperature mechanical strength, and it has been used extensively for many different purposes, you will discuss them later. But silicon carbide this is typical structure, but one has to remember that silicon carbides has the many different structure types, they are poly types, the different type of poly types we call, we will discuss more, more of them in details.

What are the different kinds of structures available, and what are the relationships between different structures. So, silicon carbide has many different structures are many different atomic arrangements, and accordingly different properties, at least alpha silicon carbide, beta silicon carbide and so on, so we will discuss some of them later on, well and also their properties. But, one thing here you have to remember, carbon atoms most smaller atoms compared to silicon, even compared to silicon carbon atoms are much smaller, and their goes to the interstitial sites. And these are one is the interstitial sites, and this interstitial sites are little or the size in the carbon atom may be slight bigger than the actual interstitial sites available in the silicon arrangement. So, we discuss that later on how exactly the carbon atom goes in to the interstitial sites, and form the silicon carbide structure.

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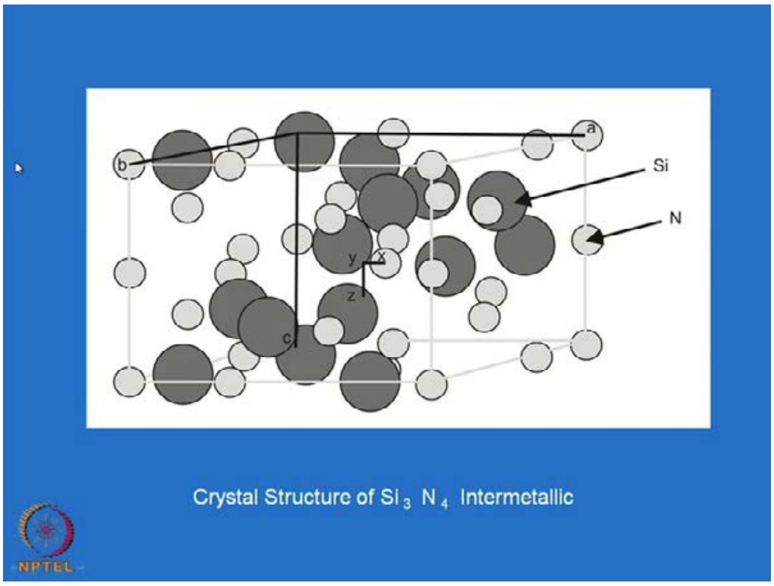

Crystal Structure of Si_3 N_4 Intermetallic

This a little complex structure of silicon nitride Si 2 N 4, once again this is also an inter metallic compound some kind of inter metallic covalent compound in fact, and it has also many different properties is good insulator, (()) and it has good (()). So, this is the sound description in the details are not there, but we can see this is this is a simple description of silicon and nitrogen, the white ions are nitrogen and then bigger ones are silicon. Once again we can see the silicon, this is the metal ion has a larger size than the nitrogen; this is more or lesser cubic symmetric.

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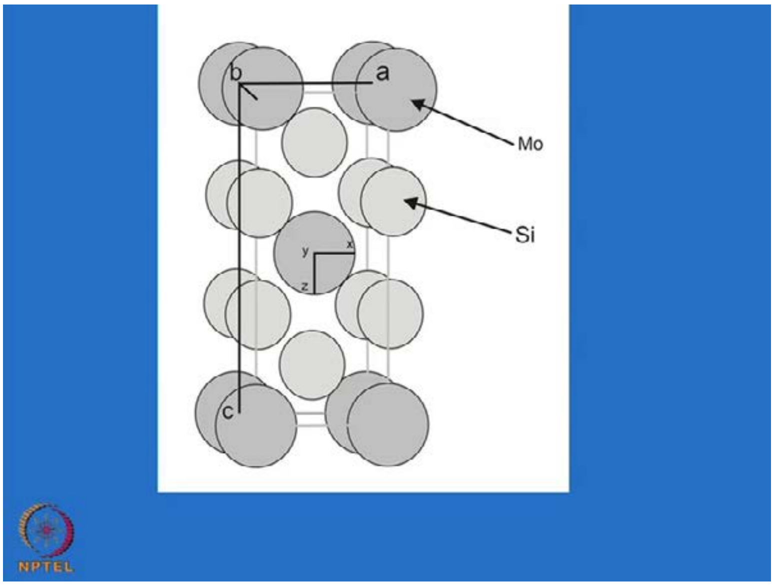

This is another non-oxide ceramics molybdenum disilicide, molybdenum and silicon, here again the size of the size difference is different, molybdenum is the larger size than silicon. So, molybdenum goes to the center of the cube as well as the corner of the cube, and silicon goes in between the interstitial sites, their interstitial sites between their structure of cubic structure of the (()). Molybdenum disilicide is a very important industrial application, this is one material, in fact like silicon carbides; silicon carbide is a semi conducting materials.

Some form of silicon carbide has a good silicon property in fact it has been used as a high temperature semi conductor; so electrical properties of many of these monoxide groups of ceramics are quite interesting. And in that context molybdenum silicide, disilicide a very large conductivity, but not like fully conductors like metallic conductors, but it has some resistance, but (()).

So, both silicon carbides, and molybdenum di silicide may they have similar property in that respect, super is the conductivity concern, and they can be used as in fact, they are extensively used as heating elements, heating elements of different furnaces. Many of the furnace in the basic principle of heating a furnace, is if is basically joule heating that means, you pass some current through this materials, and there is a I r, I square r heating, so current square into resistance. So, these ceramic materials because they have a high melting point and also have a fairly low resistance.

So, you can pass value large current through this, and as a result there will heat here, so this is the heating elements of different furnaces, silicon carbide can be used up to a temperature of about 1400 to 1500 degrees centigrade whereas, it will needs still need have temperature, molybdenum disilicide is the answer. So, most of the (()) furnaces or even in industrial furnaces, if you want to go beyond 1500 degree centigrade up to about 17 up 1800 some cases, so molybdenum disilicide is used as the heating element. So, that is the importance of molybdenum disilicide, so it has very good high temperature mechanical property, as well as electrical property.

So, these are the tetragonal symmetry, and MO Si 2 with molybdenum occupied in the corner and the body lattice positions are occupied by the semi conductor, I think that is completes our discussion on crystal structures. We are discussed fairly large variety of compounds, from oxides to, silicates two, non oxides, some carbide, nitrides, silicates, borides; so all of them had been tested upon, and brief discussion on the crystal structures.

We have gone through that ends our discussed on crystal structure, next time the next class will be discussing about the crystalline importance, because we have discussed, so for about the ideal structures. But impractical or in reality the structures are really not ideal, many positions of the structure are occupied by either vacancies of that or interstitials or impurities. So, we have to understand what is that the, what is their role when there is particular atom is missing, or an extra atom is there will be structured, either or the same material or from the different material. So, that is what we call the atomic (()) or crystal line (()), and we discuss that in the next class.

Thank you.