# Fundamentals and Applications of Dielectric Ceramics Prof. Ashish Garg Department of Materials Science & Engineering Indian Institute of Technology Kanpur

# Lecture No. – 01 Outline of the Course

Okay, so, I welcome you all to this new course on fundamentals and applications of dielectric ceramics. My name is Ashish Garg and I am working here as a professor in the Department of Materials Science and Engineering at IIT Kanpur. So, this is a course basically, primarily, aimed at undergraduates of primarily materials science and ceramics engineering.

It could also be useful for undergraduates of physics, chemistry, electrical engineering, mechanical engineering, or anyone who wants to work in dielectrics or wants to gain knowledge of dielectrics can do this course. As such, there is no prerequisite. If you have understanding of 12th level physics, that should suffice to do this course. So, let me now go to some contents of this course, what you are going to learn over a period of 8 weeks.

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Contents - Bonding and Structure of Ceramics (Iweek) - Defects in Ceramics (week 2) - Linear Dielectrics (week 3 and 4) - Linear Dielectrics (week 3 and 4) - Basic me chanisms, polarization and its mecha-hisms, Polarizability, dielectric constant - Frequency dependence - Impedance analysis - Applications

The contents that we will learn in this course include the bonding and structure of ceramics. So, this will go for about one week. We will not touch too much about bonding and crystallography, we will just straightaway jump to the structure of ceramic materials, but we will have some primer on what is bonding about and what is crystallography about perhaps in today's lecture. And then, we will move on to a very important topic in ceramics which is defects in ceramics. Defects in ceramics are very important to understand, defect chemistry especially. Defects in dielectric ceramics, not in ceramics, so it could be more generic. So, this we will do over a course of week 2.

So, here, we will talk about what kind of defects that prevail in dielectric ceramics, what happens when you add impurities to them, what happens when you change partial pressure of oxygen because most of them happened to be oxides, as a result, when you change oxygen partial pressure there is a tremendous influence on the characteristics or properties of these materials. And then, we will move to what we call as linear dielectrics.

Linear dielectrics are those dielectrics whose polarization behavior as a function of electric field is linear, and here we will first look at the basic mechanisms of dielectric materials. We will look at what is polarization and its mechanisms. Then, we will look at what is polarizability. We will look at the frequency dependence and, of course, dielectric constant here.

That is also important bit. Frequency dependence of above, and then we will look at impedance analysis because it is important to analyze the impedance spectra of dielectric materials to understand their behavior completely, and then we will perhaps look at certain applications. So, this will constitute about two weeks, which is week 3 and 4. There could be some overlap that is possible between weeks, but we will try and stick to our schedule.

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ŮĴHŴ ″<u>Z∙Z∙∕∘</u>≫₩ ″8/∎∎∎∎∎∎∎∎∎∎∎∎∎ - Non-finear dielectrics (week 5-7) - Basics of above - Classes! Piezoelectric, Pyrelectrics e ferroelectrics - Ferroics and Multiferroics : An Introduction (week-8)

And then we will move on to what is called as non-linear dielectrics. We will see what is the meaning of linearity and non-linearity in the subsequent course of time as we learn about it. And in this case, we will learn about what are the basics of above materials, then we will look at the classes of materials, we will discuss each of them. So, we will start from piezoelectrics, then we will go to pyroelectrics, and then we will look at finally ferroelectronics.

All these three materials are technologically extremely important and that is why it is important to understand the fundamentals of these materials, the classes of these materials. So, this will constitute for about two weeks. So, this will go from week 5, 6, and 7, okay? There is a possibility that there is a spillover from the previous weeks a little bit. So, there could be certain overlap.

And then, finally we will move on to ferroics and multiferroics and there we will basically introduce this new topic of multiferroics, looking at the types of multiferroics, what are the materials, what is the importance of these materials and what are the challenges, what is the current status, and this will constitute week 8. So, this is the overall overview of the contents of the course that we will undertake as we progress in this course.

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Bibliography (Essential) - Physical Ceramics: Principles for Geramic Science & Engineering Y.-M. Chiang, D.P. Birnie and W.D. Kingery Wiley- VCH (Structure, bonding and defect Chemistry)

Now, let me go to the bibliography, what are the books that you are going to follow. And here, I would say the first thing is essential bibliography. So, these are the books that you require for yourself. So, first will be Physical Ceramics: Principles for Ceramic Science & Engineering. This is a book written by Y. M. Chiang, D. P. Birnie, and W. D. Kingery. It is

published Wiley – VCH. So, first few chapters especially from the perspective of structure, bonding, and defect chemistry, okay? So, these are the topics which this book covers well. (**Refer Slide Time: 07:45**)

- Principles of Electronic Ceramics by L. L. Hench & J.K. West, Wiley (Linear & non-linear dielectrics) - Elechoce ramics : Materials, Inderties & Applications by J. Moulson & J.M. Herbert, Wiley ( Proferries & Applications) Non-stoichiometry, Diffusion e Electrical Conductivity in binary metal onides by P.K. Kofstad, (John Wiley a Sons) -> (Defect Chemistry)

Then, we will look at another book whose name is Principles of Electronic Ceramics by L. L. Hench and J. K. West. This is published by Wiley. This is a book basically for learning about linear and non-linear dielectrics. This is a very good book for learning the basics of electrical characteristics of linear and non-linear dielectrics. We will also look at Electroceramics: Materials, Properties, & Applications.

This is by J. Moulson and J. M. Herbert. This is again Wiley published book. Again, this is good from the perspective of properties of ceramics and applications. And from the perspective of defect chemistry, there is one very specific book that I would recommend to you; if you have time you can read it, that is Non-stoichiometry, Diffusion & Electrical Conductivity in Binary Metal Oxides by P. K. Kofstad.

This is again basically john Wiley & Sons. This is very good from the perspectives of defect chemistry. So, those who want to improve their knowledge of defect chemistry can read this book. So, these are the books that we will follow. The first book Physical Cera mics by Chiang, Birnie, Kingery from the perspective of structure, bonding and defect chemistry. Then, we will look at Principles of Electronic Ceramics from the perspective of linear and non-linear dielectrics by Hench and West.

And we may also refer to Electroceramics: Materials, Properties, & Applications by Moulson and Herbert from the perspective of properties and applications. If you are interested in defect chemistry, you can look at this book by P. K. Kofstad that is known as Non-stoichiometry, Diffusion & Electrical Conductivity in Binary Metal Oxides.

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And then, there are a host of other books. So, I can just say that supplementary reading. So, supplementary reading could be from the perspective of those who do not know solid-state physics. They can read Solid-State Physics. So, the first book would be by Kittel, this is a very famous book. Then it would be A. J. Dekker. So, this is Charles Kittel, this is A. J. Dekker. And then, one can also look at Ashcroft and Mermin.

These are three books which will provide you good understanding of basic solid-state physics of materials. And then, if you are interested about materials science basics, then I would say Material Science Basics. I would say the first thing would be to read the book of V. Raghavan which is a very nice book giving you complete information to begin for the beginners about materials science. Then, we have W. Callister or W. D. Callister.

This is again similar book to Raghavan but I consider Raghavan a little better in terms of its content. And then, we have WULFF series. So, this is a 4-volume series. We call it WULFF series but basically it is a materials science engineering series from MIT, four volumes. It is a very old book but it is a very nice book to read about. So, these are the books you can read about improving your materials science fundamentals and these are the books you can read about improving your solid-state physics fundamentals.

So, as I said, the prerequisite for this course is basically nothing significant. If you know basics of structure of materials, basics of thermodynamics, basics of solid-state physics, you will do well in this course. So, the supplementary books that I recommended are the ones you can read and improve your knowledge. And this course is suited as I said for final year undergraduate students are third year undergraduate students of most disciplines including materials science engineering, chemical engineering, mechanical engineering, physics, chemistry, electrical engineering, and so on and so forth. And also for fresh graduate students and for like masters and PhD students.

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- Structure & Bonding in dielectric Ceramics - Dielectric Ceramics -> Oxides Panally ionic with & Oxidy -> Cations & anions Collolent character (electro horizonte) (electro negative) Binary Oxides electronegativity

So, now, let us begin with the first lecture, the content of this course. Initially the first module is about, so, the first week that we are going to discuss is going to be on, basically, structure and bonding in dielectric ceramics. Now, essentially, dielectric ceramics are mostly oxides. Oxides are generally a mixture of cations and anions. Cations are generally more electropositive and these are electronegative, okay?

So, cations have tendency to give away electrons, anions have tendency to accept the electrons and the difference in the electronegativity is the driving force to form a bond between the cations and anions. So, you can have binary oxides. So, basically the difference in the electronegativities of two types of elements drives the type of bonding that you will have. So, generally oxides you will find they are either strongly ionic or partially ionic with covalent character. So, generally, this is the bonding scenario in these materials.

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Oxides - Bin ary Oxides (MO), Nac. Nio. - Bin ary Oxides (MO) - Ternary Oxides (MO) (ABOx) - Batios (ABOx) - Batios MI, ML AB - Quarternary Oxides - SrBiz Taz Oq

So, these oxides could be, you can have binary oxides of the form MO, for example, things like, formulas would be MgO, NaCl, NiO, all these are binary oxides. You can have ternary oxides. Binary oxides could be MO, it could be  $M_2O_3$ , it could be  $MO_2$  and so on and so forth. So,  $M_2O_3$  could be something like  $Al_2O_3$ ,  $Cr_2O_3$  and so on and so forth.  $MO_2$  could be  $TiO_2$ ,  $ZrO_2$ , all these are  $MO_2s$ . You can have ternary oxides.

Ternary oxides can be, let us say,  $ABO_x$ . For example, your barium titanate is a ternary oxide, so you have barium as a cation 1, so this is M<sub>1</sub>, titanium that is M<sub>2</sub>, or you can say A B, then of course O which is the anion. You can have quaternary oxides. Examples could be strontium bismuth tantalate, SrBi<sub>2</sub>TaO<sub>9</sub>. So, in this case you have three cations and one anion. So, there are possibilities of multiple kind, but generally we deal with oxides which are binary or at the most ternary in nature.

There are very few examples of quaternary or penternary oxides that we use in literature. Now, given these materials have oxygen in them they are strongly influenced by oxygen content in these and oxidation states of these elements that are present in them. Many of the elements tend to be transition elements which have tendency of balance fluctuations. As a result, there are multiple balances present in the same material. As a result, you may have nonstoichiometry that we will deal in the defect chemistry.

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Atomic Arrangement of cations & Anions - Crystal Structure - Symmetry & Space group

And the cations and anions in these materials are present in sort of, so there is atomic arrangement that is there. So, atomic arrangement of cations and anions gives rise to what we call as, all of them have a certain crystal structure, and they have certain crystallographic symmetry and space group which defines their structure and properties. So, what we will do is that we will first begin with certain fundamentals of crystal structure before we move on to the structure of these materials.

So, these materials as I said, atomic arrangement of cations and anions determines the crystal structure. As a result, they have certain symmetry, certain space groups which is important in imparting certain properties to them.

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Dielectric Materials Applications - Sensors, Actuators, data storage, (transducers providing <u>DRAMS</u> sensing actuation sio<sub>2</sub> - optical devices - Bati 03, PbTi 03 - ...

Now, what are these materials useful for? Dielectric materials are useful for a variety of applications. So, they are used for various applications such as sensors, actuators, data storage, transducers. Sensors means they are used for sensing, okay? So, it could be sensing gases, it could be sensing displacement, this could be sensing stress, so sensing any kind of stimuli. Actuator means providing activation.

Actuators and transducers are the other devices which are based on utilizing the mechanical movement in these materials. So, we will see certain types of dielectric, not all dielectrics, can be used for these purposes, but only certain types of dielectrics are used for actuators and transducers kind of applications. They are also useful for data storage because many of the DRAM materials.

For example, are conventionally made on silicon oxide, but there are a lot of materials which replace silicon oxide such as hafnium oxide, you have tantalum oxide, you have zirconium oxide, yttrium oxides, and here the property that is important in these materials is dielectric constant. So, dielectric constant of the material is exploited to make these thin films in these dynamic random-access memories for storing the data.

They can also be used for optical devices because these electric materials have certain optical properties which can help them work in these devices, but we will not deal with optical properties. And there are materials such as Barium titanate, lead titanate and so on and so forth which are non-linear dielectrics which are used for these sensors and actuators kind of applications as we as we discussed above.

So, there are a lot of applications of these materials, and as we go along the course while describing certain classes of materials we will look at some of the applications in a little bit detail. So, this is what a brief intro of dielectric material is.

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2 0 m 4 Dielectoic Structure of Ceramit S - Electronic Atomic -Micro/Nano Macro

Now, let us go to nitty-gritties of the structure of these materials. We will first discuss the structural aspects of these materials. By structure here I mean, so structure can be defined at various scales. You can have electronic structure which is the structure at the electronic level, you have atomic structure which is the structure at atomic level. And then we have structure at the micro/nano level which is basically micro structure and nano structure, and then we have what we call as macro structure.

So, this is at the electronic level electronic structure; atomic structure is the level of atoms; nano or micro structure is at the level of micro structural features such as grains, grain boundaries, and so on and so forth; and the macro structure is in the form of the shape, the pores, the void, the shape, etc. So, here, when we talk about the structure of ceramics we are mainly concerned with the atomic structure of these materials. So, this is what we are going to talk in the next few slides.

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So, as far as structure is concerned, the first important thing you need to know is what is called a lattice. Lattice is basically you can say periodic array of points in space with identical neighborhood, okay? So, this is basically is point lattice, right? So, any kind of arrangement like this where each point you have a periodic arrangement of points in space and each point, whether you look at this point whether you look at this point whether you look at this point, all of them have identical neighborhood. This is called as point lattice.

You can have this kind of arrangement also. But this will not be a lattice because each point does not have identical neighborhoods. So, this is a lattice. This is not a lattice, okay. So, this is the first concept that a point lattice has regular arrangement of points in space with identical neighborhood. It is periodic, identical neighborhood, and then it has regular arrangement of points in space. This is what is a point lattice.

There are possibilities where you can make lattices which have sort of very nice looking arrangements. So, for example, if I make this arrangement here. I will not draw too many. I will just draw it using a different colour. So, if you just go down one more point here, and another point here may be. So, all these points have equal spacing with respect to each other, sort of hexagonal, it is sort of distorted here, but it is sort of hexagonal. But if you look at this point A and this point B, the neighborhood is not identical.

For A you have one point on the right and two points on the left at certain angles. For B you have two points on the right and one point on the left. This is not a point lattice even though it looks like a regular order arrangement. However, if you have arrangement something like, if

I make this kind of arrangement let us say, and I put points here, here, here, here, here, here, here, and additionally I put points at the center.

Then, whether I look at point A or B all of them have similar neighborhood or identical neighborhood which means this is the point lattice. So, basically, a point lattice is regular, periodic arrangement of points in space with identical neighborhood. This is the definition of point lattice.

ŮŮHV ″∠∙∠・♀・≫⊎ ″₿/∎∎∎∎∎∎∎∎∎∎∎∎∎ Unit-cell smallest repeatable unit choice of  $(a, b, er) \rightarrow 2-D$   $a, b, c and \alpha, \beta, er \rightarrow 3-D$ Symmeby (translation, seflection, trystal systems

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And within the point lattice you can create what we call as unit cell which is the smallest repeatable unit, okay? Within this you can create a unit cell something like that. This is unit cell and unit cell has certain parameters which are called as length and breadth and angles. So, unit cell has unit-cell parameters. We define them as a, b,  $\gamma$  in the case of 2D, and in case of 3D we define them as a, b, c, and  $\alpha$ ,  $\beta$ ,  $\gamma$ .

So, these are called as unit-cell parameters. Now, the choice of the cell is not unique. You can make any shape unit cell. So, for example, in this case, you can make this as a unit cell but this it is also possible to make this as a unit cell. This is also a unit cell, okay? So, this is where the question arises what kind of unit cell shall we choose? This is determined by what we call symmetry considerations.

So, based on the shape and lattice parameters and under symmetry, so if you add symmetry considerations, there are certain symmetry operations which have to be performed. These symmetry operations are translation, rotation, reflection, and inversion. So, if you perform

these symmetry operations, then what we generate is what we call as crystal systems. As I said, choice of unit cell is not unique, okay? You can see from this picture.

This contains one lattice point because you can see that all the four corners have four points which are shared by neighboring unit cells. As a result, we have one point in the unit cell. Similarly, in the neighboring one we again have one point in the unit cell. So, they have same area. They contain one lattice point. If you contain something else, that will also be similar. It is also possible to choose a different shape.

So, you can have multiple shapes, they will be similar in area and they will contain only one lattice point. So, that is why you have to evolve a system which is called as crystal system, but that takes into consideration the aspects of symmetry that we will discuss in the next lecture. Thank you.