Electronic Systems for Cancer Diagnosis Dr. Hardik J. Pandya Department of Electronic Systems Engineering Indian Institute of Science, Bangalore

Lecture – 66 Introduction to COMSOL Multiphysics

Welcome to the session on MEM simulation with COMSOL Multi physics as Dr. Hardik Pandya has already taken a session on how actually you can use the MEMS devices to diagnose for example, some kind of a cancer. In and in addition to that he was also talked about in his other courses that using analog circuits, you can actually control a particular system or a device.

Today, we are going to talk about what is the actual physics that takes place within those devices. So, if you have a kind of a MEMS device, what actually happens within the MEMS device, what is the physics that happens within the MEMS device; if you want to control your MEMS device in different-different type of operation, how can you do that. So, let us begin today's session.

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Agenda

- Why Simulation?
- Introduction to modelling in COMSOL Multiphysics
- MEMS modelling with COMSOL Multiphysics
 - · Piezoelectric devices
 - · Piezoresistive devices
 - · Electromechanical and thermal actuators
 - · Fluid structure interaction
- · Demo on Thermal actuator
- Q&A

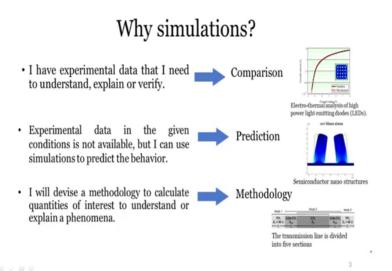
We will start with why simulation, we will try to answer that why people actually are looking for simulation, what are the reasons behind of doing a simulation, why do we need it so much? Then we will talk about we will give a brief introduction of how modelling is possible in a seamless way in COMSOL multiphysics and then we will talk

about different types of different aspects of modelling different devices. For example, as you can see over here, we have a piezoelectric devices. So, how can you model piezoelectric devices, how can you model piezoresistive devices? Or if you are interested to model electro mechanical or thermal actuate actuators, how can you do that? And then finally we will talk about fluid structure interaction.

So, as you can see over here MEMS device is a multiphysics, the MEMS device actually requires a multiphysics analysis. So, it is not just the electrical physics that is going to play a role, but along with the electrical because of the thermal heating of your device how much is the thermal expansion and because of the thermal expansion how much change in the geometry of a structure is. So, all those things needs to be taken into account, and then the electrical physics needs to be taken into the process. So, this is a kind of a fully coupled problem which is going to be solved in today's session. And, we will tell you how to actually proceed with that.

Finally, we will talk about a thermal actuator. We also take a demo on thermal actuators and. So, eventually if you have any questions, you can also post us the questions, and we will try to answer it after the session.

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So, the first question that comes to the picture is why do we need simulation? So, for example, you already have an experimental data with you. And, you want to actually understand the physics behind that experimental data. So, at that time simulation actually

plays a very important role. So, simulation will help you to understand what are the physics behind those results? If you are looking for some other results, so for example, you are looking for a graph, but it is not exactly this graph that you are looking for. There is some something else maybe, you want the device to saturate it further very early as compared to this graph.

So, in simulation you can actually change the input data, you can change the material properties, you can change the geometry of your device and try out many numbers of simulation. And from there you will get many multiple graphs and that is what you will see in the demo how to get different-different graphs for different-different input properties. And from there we can actually choose an optimized solution of performing of making your device.

So, for example, if you want to fabricate a MEMS device, you all know how costly is it to fabricate a MEMS device. But if you use a simulation tool to come up with an optimized design, then you have some basis on which you can say that I can fabricate I can go ahead and fabricate my device. Without a simulation tool, it becomes very challenging. Because if you fabricate a particular device and it does not work, then the complete money that you have invested in fabricating the device is actually gone right, so that is why assimilation plays a very important role before you go ahead and fabricate your optimized design.

The next part is to predict. More or less what happens is that there are some of the cases where you do not know how does your system is going to work in different-different input conditions or it could be a worst case scenario that you want to try out. You are not going to try the worst case scenario on your fabricated device, you are going to use a simulation tool to understand what would be the prediction, what is the maximum displacement as you can see over here.

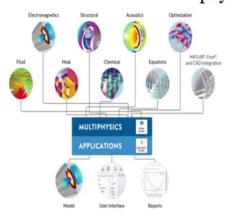
These are two silicon nanostructures and they are kind of we are going to giving a particular load to this and its going to deform at a particular angle. So, we want to know how much angle maximum that it can go before it is going to get it is going to crack right. So, in this kind of simulation plays, in this kind of problem, simulation plays a very important role.

The last part is to come up with a methodology. For example, you already know your physics you are already understand the experimental results, you have all the data, but in the end of the day you need to come up with a mathematical model. The way to come with up with a mathematical model is to do a lot of mathematics right. So, you need to write your own equations and you need to see if those equations are actually matching up with the actual experimental data.

So, COMSOL helps you to come up with this kind of mathematical models. So, it will so COMSOL per say is a software which allows you to write your own equations, , in addition to actually modify the inbuilt equation. So, if you are solving for Maxwell's equations for example, you can actually modify a small part of the equation to start with, and then see how the results are going to change. So, you can actually perform a methodology to verify your analytical results with your experimental results.

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Introduction to COMSOL Multiphysics ${\mathbb R}$



Just to give a brief introduction of COMSOL multiphysics, in COMSOL multi physics if you see the world near yourself, you will find that there are no physics, there are no applications or systems were only single physics is in the application right. So, there are two or more physics that are going into which is actually in application for example, you talk about speaker phones right. So, you give a particular current to your magnet coils and those actually vibrate to vibrate the diaphragm right.

So, here the electrical physics is going to happen when you pump in the current it is going to create the magnetic field, it then it is going to create the forces that is the Lawrence force that is f equal to q into v cross b and that is going to make the diaphragm vibrate. So, this is a complete multiphysics simulation that you can model in COMSOL.

So, we already have many other model files for example, the speaker example that I told we already have those model files. In addition to that, if you see this is a you want if you want to solve a single physics at a time, you can solve it using electromagnetics module. You have structural module where you can solve the deformations.

Then if you want to model acoustics, you can also model that then you have fluid. So, you want to model turbulent flow, laminar flow, you can do that. In heat transfer module you can module convection, conduction and radiation. And then finally, equation sorry we have chemical reaction module, where we can model electro deposition battery and fuel cells, electro chemistry all those can be modeled in chemical reaction modelling.

In addition to it, you can actually write your own equations, let it be in a form of general form or coefficient equation form that is a very simple way to write your own equations. So, in the end of the day, COMSOL is nothing, but solves the prebuilt PDE equations there are a PDE equation for electromagnetic, there are a PDE equations for structural. So, if you talk about multiphysics coupling, then it becomes a coupled PDE equations that you are solving. So, eventually you get a transfer metrics and they then taking a inverse of it, you get the actual the solutions.

So, whatever you do it is using model builder that you can see over here. And then you finally, can create a very simple app out of your model. So, if for example, you are an expert you may be so the people who would be attending this session could be a faculty, you could be a student, you could be also a service engineer, design engineer and R and D engineer, so for all of them what happens is that let me take an example of an R and D engineer.

So, he is a very intelligent or he has a very specific knowledge in electromagnetics for example, ok. So, in electromagnetics he has lot of experience. So, he can actually build a model and then make a very simplified interface of that model in the form of app. And that app he can shared it with his other service engineers who are having a good

knowledge in heat transfer of structural. And in that simplified app, they can actually change the some of the parameters and get the results.

For example, if you talk about speaker, the if some company is creating a new design for a speaker in a mobile phone, so for the electromagnetics part R and D engineer can actually work and create an app out of it. The other person from acoustic field he can share it with the acoustic person and then he just need to change the results and then see how what is the pressure levels across the room within the surrounding the speaker.

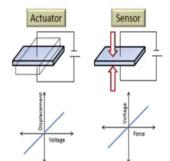
So, the such kind of simple interface are known as apps. So, in the demo also we are going to show that not only R and D engineer, but in addition to it you have faculties who can share this apps to this with the students and they can actually change the parameters and they can get different different results out of it.

At the same time, a student can also make an app a very simplified app and then share it. During a presentation and they can see you can if the professor ask them to change a kind of parameter, they can actually change it and then give show the results at that time itself. So, let us go with the different types of MEMS modelling that is possible with COMSOL multiphysics.

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Piezoelectric Devices

- · Piezoelectric effect
 - Electromechanical interaction between the mechanical and the electrical state in crystalline materials. Common materials are PZT-5H
- Applications
 - Actuators Voltage applied to induce displacement, acoustic transducers
 - Sensors- Displacement applied and voltage measured, measurement devices and sensors



The first type that comes in today's agenda is a piezoelectric effect. There are basically two types of devices that you want to model. The first one is the actuator type that

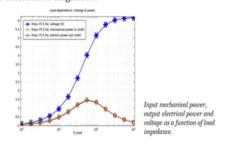
means, you want to have some kind of motion or you want to have some kind of displacement effect. The input that you have is voltage. So, in this particular example, if you give a particular voltage, there would be a particular deformation that is going to take place.

In another kind of application, it could be a sensor. For example, you want to sense how much is the displacement of a particular device, so in that or you want to sense how much is the stress developed within a particular device. So, in that kind of application, you can use the piezoelectric device into it inverse way in the opposite way. In which the force is applied the force is actually an input and then you get a particular voltage as an output.

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Piezoelectric Energy Harvester

This tutorial shows how to analyze a simple, cantilever based, piezoelectric energy harvester using the Piezoelectric Devices interface. A sinusoidal acceleration is applied to the energy harvester and the output power is evaluated as a function of frequency, load impedance, and acceleration magnitude.



So, to begin with one of the example is piezoelectric energy harvester. This is a very interesting example because nowadays people are moving ahead on how to save energy or recover back the energy that we are wasting in day-to-day life. For example, one person is my friend is actually jogging in the morning. So, while he is jogging his shoes are like vibrating and he wants to actually save those vibrational energy in the form of battery that you can use it for his wrist band for example, got it.

So, the way to do that is using harnessing the energy of vibration and then converting back into electrical energy. So, in this kind of example has been modelled in this particular example. So, we also have the application model for it. For example, if you

want to just see this example model, you can go to the COMSOL website. And then you can go to this application models and application files right. And over here, there are a lot of model files over here. And here you can actually search for that particular file.

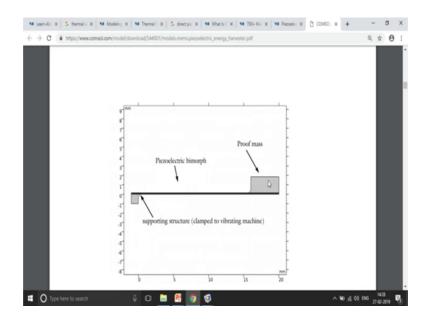
For example, I am looking for piezoelectric energy harvester. So, you know piezoelectric energy I am just searching and there are harvester let me just search for harvester also. So, see this is the example model that I am getting ok. So, you can also download the files. You can see this if you have logged in with your account over here, you can also download this mph file. And you can also see the documentation. So, document is actually has all the datas all the information.

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So, it first talks about the theory part.

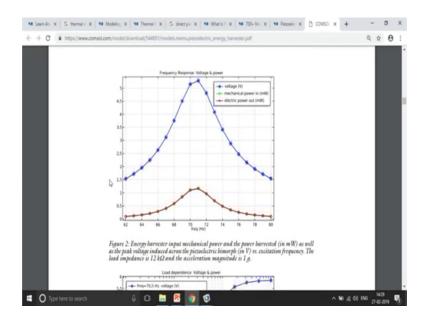
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Then it talks about the setup the problem setup. As you can see over here this is a problem setup, where they have they wanted to understand, they want to take the vibrational energy from a motor for example. So, when the motor are working a lot of vibration is happening right, so any vibrating machine would create a lot of stresses on the surface of the machine right. So, they want to harvest those stresses or the forces, vibrating forces.

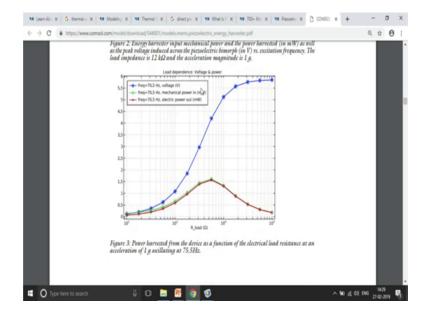
So, in this case I just need to maximize it, I am not sure if you can see it, but this is a bimorph structure. Bimorph structure it means there are two layers of piezoelectric and which is actually coated with a particular metal straight and then we are going to give a vibrational force from proof mass right.

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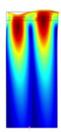
And, then we are going to vibrate it for different-different frequencies that you can see over here ok. And the peak which is available over here is the resonant frequency for that particular device right. So, at that time you will have the highest voltage that you can harness back from your device.

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Surface Acoustic Wave Gas Sensor

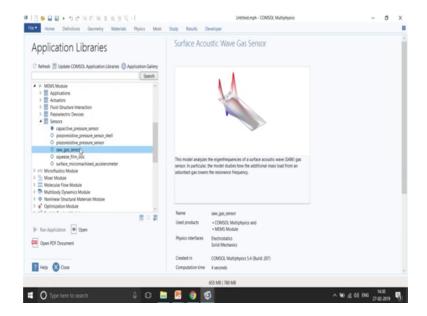
This tutorial analyzes the eigenfrequencies of a surface acoustic wave (SAW) gas sensor. In particular the effect of an additional mass load from an adsorbed gas is investigated. The additional mass loading lowers the resonance frequency.



Another example is surface acoustic wave gas sensor. In this particular kind of an example or this particular kind of an application, what happens is we want to understand the composition of a particular gas. We want to know what is the constituents of the gas and also the concentration of the gas. So, we actually try to model it along with a piezoelectric device. So, let me go ahead and open that particular model. So, what I will do, I will just go to COMSOL. So, this is the first thing that you will see once you open a COMSOL file. And you can go to file, application libraries. Right now I am going to focus on MEMS device.

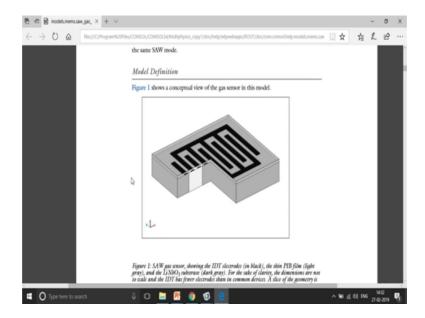
So, you can see there are many modules. You have AC DC module, you have acoustic module, battery and fuel cell, CFD, heat transfer. As of now we are going to focus on MEMS module right. And in this week open, so in the MEMS module also there are many application files, but application models. So, you have many actuators that we will come at a later stage. We have fluid structure interaction. We also have piezoelectric devices. So, right now we are going to talk about surface acoustic wave, so that would be coming in the sensors I guess yes.

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So, this is the saw gas sensors. We also have an example of glucose sensor. So, that is also a part of how you can understand the chemical reactions with the help of an electronic device. So, this is the example model that I was talking about saw gas sensor. You can also open the documentation try to understand what is the theory behind the gas sensor?

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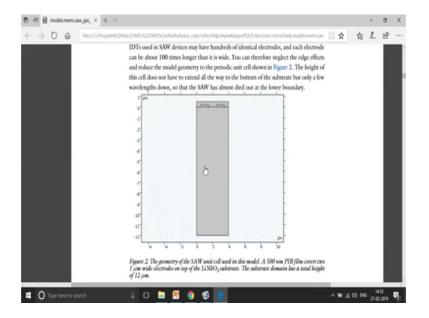
So, any gas sensors micro electromechanic structures has an IDT. So, this is an actual structure as you can see over here and this is the inter digitated electrodes, the black

structures. So, it is like a fingers wrapped on with each other. And once the gas actually passes over this, gas has its own connectivity and its own impedance. So, if you are able to understand that those impedance, we can actually back calculated or do a kind of a reverse engineering to understand what is the composition of the gas, what is the concentration of the gas, what are the different constituents of the gas ok.

So, this is the actual structure ok. But if you are a simulation engineer or you are a student or you are a faculty who is trying to model this surface acoustic wave, you will not go for a complete 3D simulation, because it will take a lot of time. We will a simulation engineer or a person who is trying to do a saw gas sensor; we will come up with a technique with which you can simplify your model. One way to simplify is to use a 2D cross section of your model and then give periodic conditions on the edges for example.

So, in this case, you can see a bright spot over here. So, this is the actual structure go us saw structure surface acoustic wave gas sensor. And it is having IDT in the top and then it has a thin PIB film that you can see over here. And then it has lithium niobate oxide substrate in the bottom right. So, instead of modelling the complete 3D, what we can model is only a 2D structure that you can see over here which I am marking (Refer Time: 20:44) my fingers. So, only 2D structure is being modelled over here.

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So, the 2D structure is now what you can see in your screen. So, this is actually what is modelled in this case, not the complete 3D geometry. This is a more simplified and this is the this is what we should always see or we should also always start with this kind of simulation which is very simple, but it captures the physics which is more important.

So, let me just go into saw gas sensor and open that particular module. So, this is the first thing that you will see once you open that particular module. So, let me just open this component section. So, a COMSOL has a top to down approach. So, the first thing is the geometry part. The next is adding the material. So, once you draw the geometry, you assign the particular materials. Then you add the particular type of physics that is going to happen in this case structural mechanics and electro statics.

And then the multi physics com component where it couples both solid mechanics and the electro statics. And then the machine part because it is a numerical methods, so into device the actual (Refer Time: 21:57) into divide the actual domain into small small parts and then which kind of analysis you want to perform. And then finally, they post processing part that is the results. So, the approach is always top to bottom over here.

One more approach is in the ribbon gain that you can see in the top where you the approach is from left to right. So, you first made the geometry, add the materials, add the physics, then mesh it, then study and then finally, the results. COMSOL has also introduced a new feature of developer, where you can write your own code you can write your own code and also couple it along with the actual model right. So, this is what you can do over here.

So, let me go ahead and talk about the materials. So, as you can see the top structure IDT structure is modelled with aluminum over here. And the aluminum over here is modelled with a particular density Young's modulus and Poisson's ratio. Then we have the PIB domain which is modelled with a particular Young's modulus.

Now you can see E underscore PIB and let me just open this model. And you cannot send e underscore PIB would be defined somewhere else. So, I just go to my parameters, and try to see how my e underscore PIB has been modelled. So, has been introduced in my model. So, e underscore PIB which is the Young's modulus is been modulus 10 GPa. So, similar to this all the other material properties would be defined somewhere over here in the parameter section. So, PIB is the top thin layer that you can see over here.

And then finally, you have the lithium niobate domain over here. And this is the actual piezoelectric domain and that is why you can see and ill or tensor which is defining this particular domain right.

So, you can see a matrix of I believe it will be 6 by 6 matrix of the elasticity of matrix which couples and the coupling matrix with actually couples the structural mechanics with the electrostatic physics. And the relative permittivity as also you can see which is not isotropic material, but here and an isotropic material has been used to model the piezoelectric relative permittivity ok.

So, let me just go to the physics. So, in this case, you can see that the piezoelectric material. So, if this is the something new that was introduced is that you have to introduce once you make the model. Linear elastic material is for all the other domains, but for piezoelectric materials you need to introduce this material model. So, over here you need to write whether it is a stretched stress charge form or strain charge form. And then you give a particular fixed constant.

So, here you can see that I have given a fixed constant in the bottom. Fix constant means that this is the boundary where it cannot move. And then finally, we give the periodic boundary condition this is very important because we claimed that we are going to do a simulation which is very much similar to a 3D simulation right, but we have taken only a very small part.

How do we claim that we are doing the actual IDT structure which is a complete 3D structure? The way that we claim is using the periodic boundary conditions as you can see over here. So, you use a periodic boundary condition that this structure is repeating on the left and right for infinite times. So, this is again a assumption, but it makes our life easy and that is why we use it ok. So, this is how these solid mechanics structure has been modeled.

With a electrostatics we have we need to definitely give a particular ground at somewhere. So, this is the ground that we have given. So, this is the IDT structure. So, one would be the ground and another would be that the electrode where I need to gather the voltage back right. So, to gather the voltage back, I am using something known as floating potential. This is very important. So, if you want to give the voltage you can use the electric potential boundary condition or a terminal boundary condition to give the

potential to give a particular current. But if you want to withdraw a particular voltage you need to use a floating potential boundary condition is very important.

And then again we are using a piezoelectric material model for the lithium niobate oxide. And the next part is the piezoelectric coupling. So, this is what you need to add means this is what needs to be added that there is a coupling between solid mechanics with the electrostatics ok, so just to add it just rightly multiplex and add this electromagnetic piezoelectric effect.

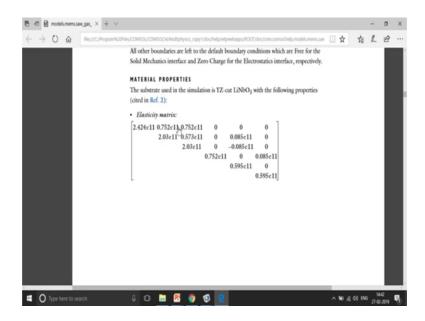
Then the machine part this is also an interesting machine. So, COMSOL allows you to mesh based upon your requirement. So, based upon how the forces are moving you can use those particular type of mesh which is suitable for such kind of forces. For example, here the forces are more or less going to be lateral which is going to move from bottom to top up, top to bottom. So, we have used a map mesh right.

So, we first tried to use the edge mesh and then copy to the right side. So, you can see this is first I have meshed then I copied it to the other side, then a free quad meshed in the top and then I map it to the bottom ok. So, this is such a structured mesh that you are seeing right now.

The next step is the study node. So, an Eigen frequency analysis figures out what are the resonant modes of your structure. So, we will tell you about resonant and p resonant modes, over here what I have done I know a particular frequencies where the resonant frequency may lie. So, I have written is f naught which I have defined in the parameter section. So, I go to my f naught and you can see that this is the estimated saw frequency.

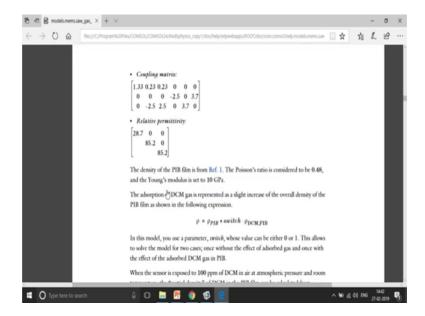
So, it is not that you do not need to know anything; you need to know something about your system of what orders of frequencies would it actually the acoustic the way should be existing. Why? So, this is the basic setup and then we also do a parametric sweep of switch that is 0 and 1 that is with and without the gas.

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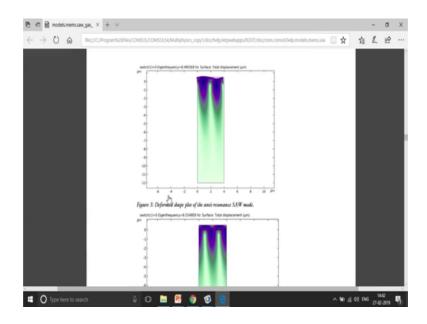
To showcase the results, so this is the actual elasticity matrix that I was talking about this is an upper triangular elasticity matrix.

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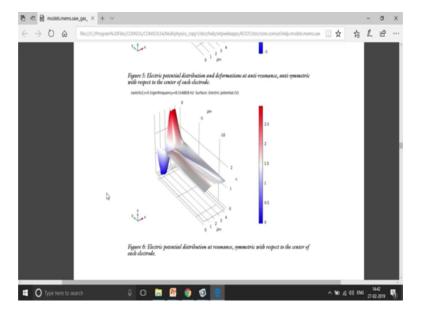
And this is a coupling matrix of 6 by 6 and then the relative permittivity. This is again very important, because here we have assumed that the relative permittivity is not isotropic. We have assumed it as a diagonal matrix first of all and it is also having node in x direction as compared to the y and z direction ok.

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And then we go to the results. So, you can see that this is an empty resonant mode saw mode and this one is a resonant saw mode. So, both of them have been captured using Eigen frequency analysis. It is that type of an analysis.

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You will see many other types of analysis throughout the day, the eigenfrequency analysis figures out the resonant modes of your structure.

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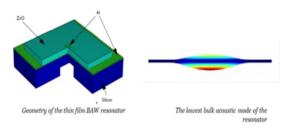


There also references with which the results have been come compared. So, if you want you can also go through the references along with the results that you are getting in COMSOL and then you can proceed with your own gas sensor design.

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Thin-Film BAW Composite Resonator

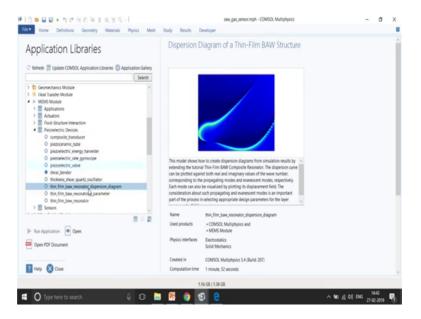
Bulk acoustic wave (BAW) resonators are useful components for many radio-frequency applications, where they can operate as narrow band filters. This example shows how you can perform eigenfrequency and frequency-response analyses of a composite thin-film BAW resonator.



The next structure is the bulk acoustic wave composite resonator. In this particular structure again we have an aluminum domain in the top, then we have zinc oxide a piezoelectric material in the second layer and then the third layer is of aluminum again that is a metal contact layer. And, in the final layer is made up of silicon that is like a

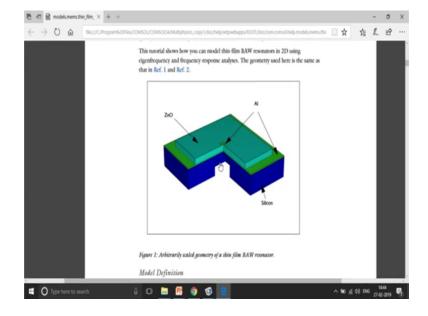
huge part of is made up of silicon. Again interesting deviation from the 3D simulation would be a doing a very small 2D simulation. So, let us see how in COMSOL we have done this simulation.

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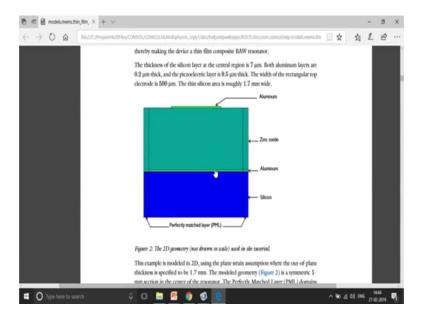
So, I go to my file application library. And again search for bulk acoustic wave. So, in bulk acoustic wave there are many different types of analysis that has been performed. We perform the dispersion diagram. We perform the as parameters and we also perform resonate, this is simple the most simple bulk acoustic wave resonated model.

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So, I will just open the PDF document to showcase how does the modelling has been performed. This is the same diagram that we saw in the presentation.

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However, the way that we have model is not the complete 3D domain, but we have modelled only a 2D structure ok. And in addition to it, as we saw in the earlier example periodic structure where modelled right, but in this case there is no case of periodicity. It is not the above structure of aluminum is not actually getting repeated. In this case hence we have used PMLs on the left and right.

So, the forces that are going to go for the electric currents that are going to flow are not going to get reflected back from these boundaries. We should not forget that this whatever we are doing is a mathematical approach of actually solving the physical problem. So, we need to terminate the boundaries very effectively. One way to terminate those boundaries is using a PML domain. And, as you will see that there is a very particular type of meshing which is required for PML that is a map mesh or sweep mesh.