

Hi, good morning, everyone. Thank you for coming. I'm presenting on behalf of Dr. Mandal and his group, their work on perovskites. Our lab is doing something very similar. And we collaborate on a lot of work as we'll present in a few minutes. So why are we doing this? What's the interest in perovskites? Well, there's this continuous demand for the miniaturization of all electronic devices.

We want all of our cell phones, digital devices, we all want them to be small. We want them to run fast and be able to hold a lot of energy. So we want to develop faster materials that have a very high dielectric constant with a very low loss. And we can use those for applications in microelectronics, memory devices, storage, things like that.

One very commonly studied perovskite is CCTO, calcium copper oxide. That does meet those requirements. But we're trying to expand, build upon those characteristics to see if we can produce something that's low cost and maybe even works a little bit better. So the objectives of the study were to really determine the effect that different dopants have when we substitute on the well-studied CCTO and NCTO compounds.

And we want to measure the dielectric constant and the loss at varying temperatures and frequency to really see if we can get something that's constant across a wide array of variables. So our compounds of CCTO and NCTO were doped with yttrium, nickel, zinc, and germanium. And we'll go through some of the results that we got from that data.

So what do we want out of an ideal capacitor material? We want something with a very high dielectric constant, something in the range of 10^4 to the power of 6. And we want it to maintain a low dielectric loss. So we want something in the range 10^{-2} to the 10^{-4} , so it doesn't lose any of its capacitor capabilities over time.

We want something with high thermal stability that you can maintain its properties at high temperatures and low temperatures. And something that's not variable across frequency. So if it has a high loss, we want it to perform the same as if it were at 130, for example. So perovskites of oxide family are

are very well studied. They have this general formula of a copper titanium oxide, where A can be any sort of metal you want to substitute, like a calcium, for example, for the very well-studied CCTO.

This is the general structure of a perovskite oxide. You can see the cubic structure, where all these elements are placed. So perhaps, new materials have been studied over a wide range of electrical and materials applications, like in sensors, capacitors, resistors. So we're really trying to add to this list to see if we can build upon this knowledge that we already know.

So to go over some of the properties of dielectric constant. So dielectric constant is the ratio of the capacitance of a capacitor, in which a particular insulating material is the dielectric to its capacity in which the dielectric is a vacuum or the vacuum is a dielectric. And then the loss is how quickly we lose that dielectric capability. And we were able to calculate these values based on known capacitance values that we measured.

So if we already know about these perovskite materials, why do we want to develop new ones? If we have CCTO or NCTO, what's the purpose of setting any further? So we really want something that has a low dielectric loss. We've seen that CCTO, its loss is pretty high. And it's not stable across a range of temperatures or frequencies.

We know that when temperature is really low, the dielectric drops off considerably. And when we load a high frequency onto it, the dielectric drops off as well. And we know that if we use something like lead oxide, it's a very toxic environment, so we don't want to use that. So we want to try and develop something that is stable through all these conditions.

And so just to go over some more about CCTO's since it's pretty well studied. It's been demonstrated to have a very high dielectric constant. 10 to the power of 4. It's the highest we've been able to study consistently. And it has a pretty stable range of about 100 to 600 Kelvin. But we know below that temperature, it drops off considerably.

And unlike barium titanate oxide, we know that CCTO has been observed using a high resolution X-ray and neutron powder directions. So it's a material with thermally stable high dielectric constant. And we want to see if this is a characteristic of the family. And if we can really build upon what we already know and make it apply to this wider range. And we have our pick.

So this is the form of CCTO. We can see this cubic structure. This is a two formula unit cell. So we can see that here, as well as in this picture. I've labelled out where the couplers are. Calcium, you can just see the overall structure of this. So this is a list of perovskite materials with their listed dopants. And we can see the dielectric constant on the right.

And we see that CCTO has the highest demonstrated dielectric. And when we do any substitution to it, we know that the dielectric drops off considerably. And so we want to see, why is this the case? Can we change this about the materials using something new, new techniques, maybe? So dielectric constant is a property of a material.

It's controversial about where exactly the property arises from. We think it has to do both with intrinsic and extrinsic properties. Like it being a polar material or something to do with the crystalline structure of the material. But nothing certain is known about that at this time. So to make these products, we have to produce them ourselves in the lab. We can either do this the dry method with all our powder materials or we can do a wet method way.

But wet method not suitable for bulk synthesis. But the dry method can also be tedious. So there's benefits to both, which is why we decided to employ a semi-

wet method to develop our materials. So we formed our solution using the metal nitrates, titanium oxide, and glycine. We heated this continuously with magnetic stirring until we were able to get it into its dry form.

We were able to grind the compound to a very fine powder and calcined it at 1,200 Kelvin for eight hours in our furnace. After this, we were able to form pellets that we would use for testing. We were able to apply constant pre

ssure and form them into the size and shape that we wanted. And then we were able to anneal these pellets, again, at 1,200 Kelvin for eight hours.

And then after this, we were able to achieve-- pellets are doped, calcium pellets and bismuth pellets. We characterized the pellets using four different ways. X-ray diffraction, SEM, dielectric studies, and impedance studies. So I'll go through our preliminary results with those. So we were using X-ray diffraction to verify the composition of our pellets. Make sure that we had phase formation and formed correctly.

So for our yttrium-containing calcium pellet, you can see that we verified the secondary phase of the Y_2O_3 and the copper titanium oxide. Our X-ray diffraction pattern for the nickel-doped bismuth pellets, we can see that we also confirmed a single phase formation of these ceramics as well using our X-ray diffraction. And these are for our germanium-doped bismuth pellets. See, we also confirmed the single phase here as well.

So using the Debye-Scherrer's formula, we were able to calculate the average crystalline sizes of our doped pellets and our nickel at different concentrations of doping as well. So that was our characterization using X-ray diffraction. And then we looked at their morphology through SEM. So we were able to look at it on this one micrometer scale.

And we were able to investigate what these different pellets looked like at this scale. So these are our nickel-doped bismuth pellets. We can see the structure here. And these are our germanium-doped bismuth pellets at this scale. So we can see in the SEM images that there was a lot of porosity and voids in our pellets. You can see here, we have these grains here, a lot of voids in them.

We see that they have a polygonal shape to them. And they're well parted by their grain boundaries. And from these SEM images, we were also able to determine their average grain sizes for the different dopants of the pellets. So next, we're moving into our dielectric studies, which is really where we wanted to focus for this. Because we're looking for something to demonstrate a high dielectric and low loss.

So for our yttrium-doped calcium pellet, we have our dielectric graph on the left. We measured these as a function of frequency at a variety of temperatures. We can see that our dielectric was highest at 1.2×10^4 at 100 Hertz and 500 Kelvin. So at a very moderate temperature and moderate frequency, we were able to achieve in the range that we wanted to for an ideal capacitor material.

And then we see on the right side is our dielectric loss. Graph is also as a function of frequency. And we were able to achieve our lowest tangent loss at 10,000 Hertz and 400 Kelvin at 0.75. This is a bit higher than we would have liked. As I said in the beginning, we want something that's 10^{-3} about for loss. And so we have the right range of dielectric, but not the right range of loss for this material.

These are our nickel-doped bismuth pellets at different concentrations of doping. So we can see that we were able to achieve our highest dielectric for this bismuth at only about 2,000. So it's a big drop off from our calcium pellet. But we were able to achieve a significantly lower dielectric loss in these pellets. So we can see that at 300 Kelvin and 10,000 Hertz, we were able to achieve a delta loss of about 0.07, which is an order of magnitude lower than our calcium pellets were.

So we weren't able to achieve a high dielectric. But we were able to see a low loss in this material. And these are our graphs for our germanium-doped pellets at different temperatures. And we can see that even lower-- our dielectrics are even lower this time. Only about as high as 500 for these pellets. And our dielectric losses were arranged. For one of them, we were

able to see about 0.18. It's still not great, but it is lower than our calcium pellet as well.

So our last way to characterize these we used was a measure of impedance. So we looked at these as a function of frequency as well. And we can see for our calcium ceramic, that we see the appearance of relaxation peaks at these temperatures. We think that these may be due to the grain boundary effects. And these peaks were shifted towards higher frequency regions with increasing temperature. And this shows the existence of temperature dependent Maxwell-Wagner effect.

This is our impedance as a function of frequency for our nickel-containing bismuth pellets. You can see this trend here at the level of different dopants. We can see different [INAUDIBLE]. This is the Nyquist plot for our real and imaginary impedance for the nickel-containing systems, as well as a-- so you can see at the different concentrations, what this looks like.

And then we have our Nyquist plots again for the germanium-containing and the nickel-containing ceramics at varying temperatures as well. So to summarize everything that we talked about today, we were able to demonstrate the atrium-doped calcium pellet with a dielectric in the range that we wanted of 1.2 times 10 to the fourth at this moderate frequency. And we were able to demonstrate a loss about in the range of what we wanted for our bismuth-containing pellets at about-- my next slide-- 0.07.

But for our other pellets at low loss, we weren't able to replicate the high dielectric. So as our loss got lower, our dielectric got lower as well. And at higher dielectrics, our loss got higher. So we're still trying to work out how we can get both in the same material, which is what we want to apply for ideal capacitor materials to be used in industry and things like that.

So our impedance, we saw two major contributions associated with the grain boundaries and our grain effect. We saw the grain boundary appears as a major contribution at higher temperatures. And the grain effects appear at

lower temperatures. We think that's due to the electron polarization. And our impedance studies confirm the presence of our Maxwell-Wigner temperature-dependent. Thank you all for listening.