CERAMIC TECH CHAT

Episode 53

Title – "Driving energy conversion progress through diffraction: Scott Misture"

INTRO

McDonald: "I'm Lisa McDonald, and this is Ceramic Tech Chat.

Research is a community endeavor, but finding your place within that community can be a bit nerve wracking when first starting out. Sometimes simply talking to people, though, will set you on the path to success."

Misture: "You know, we have a career fair here on campus. And we tell all our students, 'You know, it would be great if you go to this thing and just talk to people. Even if you already have a job, just talk to folks.' And very often they come back and they say, 'You know, thanks for that suggestion because everybody wanted to talk to me. I couldn't believe it.' I say, 'Well, yeah, right? You have something they want, and that is a skillset that might fit with their company.' And so, exactly what you said: It can be hard to get started, but then you get started."

McDonald: "That's Scott Misture, Inamori Professor of materials science and engineering at Alfred University in New York. Scott is a characterization specialist who, through the use of diffraction techniques, studies the dynamic behavior of ceramics and glasses related to energy conversion devices.

In today's episode, Scott gives us an overview of his research and demonstrates the personal and broader benefits of being involved in the materials science community."

(music)

SECTION 1

McDonald: "Introduction to section 1."

Misture: "My physics teacher in high school was fantastic. He was like, 'Try this out,' right? And so, it turns out that I made this bridge out of toothpicks of all things. And I won the state competition with this bridge for weight-to-strength ratios. So anyway, looking for colleges, I discovered that ceramics were being used in engine components, and I thought that was pretty interesting. I was interested in cars and this sort of thing as a teenage boy, right? But at any rate, so I landed in Alfred, and here we are. I was very much interested in aviation as well as automotive and got a pilot's license when I was 17 years old. And so that really inspired me to do something with the technology. So, here we are, right?"

McDonald: “So, do you still get to fly planes?”

Misture: “Ah, occasionally, only occasionally. Love to do it some more, but only occasionally these days. I sit on planes quite a lot.”

McDonald: “True, don’t we all?”

Misture: “Right, right. Yeah, so anyway, my journey from there switched during my first four years here at Alfred as a student from being interested more in the mechanical end of things to being interested more in the electrical end of things. When I discovered that ceramics conduct electrons and ions and do all these interesting things functionally, I became really fascinated with that, and that launched me into my graduate studies, which were on the brand new and totally next generation area of high-temperature superconductors. So, that’s what I did as a graduate student. And so then I continued studying conductive ceramics since then, and I look forward to doing it for a while longer anyway.”

McDonald: “So after you finished your schooling, where did you end up first?”

Misture: “So, I actually ended up at Siemens Corporate Research in Munich before I finished my degree. That was an unusual situation but really fantastic experience. So, I was working in the research labs in one of the biggest companies in the world. It was in Munich, in Germany.

And from there I took a postdoc at Oak Ridge Lab in Tennessee, really focused on characterizing materials using neutrons and using X-rays and especially doing that under high temperature or under mechanical loads and trying to understand why materials behave the way they do by looking at how the atoms fit together. And that really sort of became a passion after two or three years there at Oak Ridge.

So, from there, I was interested in academics. I thought that was a fun and flexible and interesting place where you could sort of, you know, be creative and define your own path and build your own playground to play in. So, I did that and landed back at Alfred University, which was my starting point as an undergraduate.”

McDonald: “So it kind of went full circle for you.”

Misture: “Sure did. Yep, sure did. Yes, indeed.”

McDonald: “So, I know you mentioned that you worked a lot with conductive ceramics, and those types of materials can be used in various different fields. But the field that you’ve kind of landed on a lot for your research is the energy conversion field. So, can you talk to us about how you became interested in really focusing your research within the energy fields?”

Mistura: "Sure. So, the idea of having a ceramic do some useful work in energy conversion or sort of, you know, making electricity, in sort of a broader picture, that led me to thinking about how do we improve the materials themselves, right? And so, I was always interested in like engines, propulsion, power generation, and that shifted over to electricity.

And so, the idea of a solid oxide fuel cell is that it can be a very high-efficiency device. So, we have our fossil fuels—or even hydrogen if we're able to make renewable green hydrogen, which we're getting better at these days—how do we take those fuels and make better use of them? Like get more power from the fuel rather than wasting a lot of power from the fuel. And so a typical heat generation power plant takes the fuel, burns it, creates steam, the steam turns a turban, and there's a thermodynamically defined limit to the efficiency of that process. So, the fuel cell gives us a totally different angle with direct electron transfer during the fuel burning process, quote unquote burning process, and that gives us a much higher efficiency device so we can extend our fossil fuels or we can just immediately switch over to hydrogen, which is really the end goal, right, is to switch over to hydrogen fuels.

And then that spills over into photocatalysis. So to make hydrogen, you can use electricity and a chemical electrode to split water to make hydrogen and oxygen, and then you separate the hydrogen and oxygen and you can fuel your fuel cell, right? I mean, there are cars on the road that are running hydrogen fuel cells, and buses in cities, and etcetera. Even airplanes these days, by the way, with ranges of sort of six and seven and eight hundred miles, which is pretty fantastic.

So, the photocatalyst captures sunlight, uses the energy from the sun effectively to break a chemical bond, and then that electron–hole pair can induce useful work, for example, to break down a water molecule to make hydrogen and oxygen. So, if we can use sunlight and a ceramic to make hydrogen, now we can store the hydrogen and use it later, right? And so, we're hopefully aiming toward a zero-carbon footprint energy cycle. And the only exhaust out of a hydrogen—you know, idealized, right?—the only exhaust out of a hydrogen fuel cell is water.

So, that's how those pieces fit together, and we're still working on those topics using somewhat different materials. We're using layered materials that we can pillar and stretch out in one direction or we can peel the crystal structures apart and make super high-surface-area electrodes for doing some of these kinds of reactions that in general work better if there's more contact of the ceramic to the environment. So, that's what we're currently really focused on in my group."

McDonald: "I know you mentioned that these solid oxide fuel cells and photocatalysts to make the hydrogen that could power the SOFC [solid oxide fuel cell], one of the big things with them is they could maybe power some of these larger transportation vehicles, like airplanes and stuff. A lot of people hear about electric vehicles, or using electricity to power vehicles, but what would you say for our listeners is a benefit of maybe using fuel cells versus electricity for powering different types of vehicles, especially maybe some of the larger ones?"

Misture: "Yeah, right. So, I think there's this sort of traditional internal combustion engine and there's the jet engine, of course. And then from there the question is do we go all electric? So, now we have a battery that's powered by the plug in your garage maybe, right? But we have this opportunity to equip the vehicle with a battery or we can equip the vehicle with a fuel cell.

And so the idea with the fuel cell is if you have a large enough fuel tank, you can define the range that you can go, right? So if you had, for example, an ocean-going vessel or an aircraft, you can size the fuel tank to the work you need to do, right? And so it's kind of like designing a modern airliner, which has a lot of fuel tanks hidden, sort of in and about, in the wings and in the fuselage. And the volume of those fuel tanks is defined to the range of the aircraft, right?

So, the fuel cell is sort of an in between. The fuel cell generates electricity, so the propulsion source is generally electric motor anyway. So, we toss this fuel cell in the mix and a fuel tank and then we can be really flexible in that respect. And I think there's a lot of applications for some heavier vehicles with the fuel cells."

McDonald: "So it sounds like a really nice compromise, like you said, between maybe those traditional fossil fuels and going all electric, that can kind of help straddle some of the benefits you get from both worlds."

Misture: "Yeah, that's the intention, right? And, you know, making a huge leap in technology is certainly possible, but smaller steps in technology are generally adopted more easily. If you just look around, there's electric cars, but there's not a huge network of electric car chargers yet. So, that's sort of a just a simple obvious example, right? So, we're hoping that we can have stopgap high efficiency as we move toward high efficiency and even toward fully green electrical energy sources and power sources for vehicles."

McDonald: "So, I know a lot of people have heard about electric vehicles, but it sounds like these fuel cells have a really great potential to equal or maybe even surpass electric-powered cars. But why is it that I feel like it's not as common to hear about fuel cells currently? Are there some challenges that are preventing them from being industrialized as quickly as the electric vehicles?"

Misture: "Yeah, I think that's the case. I think that the electric grid is everywhere in the developed world. But a fuel cell requires a fuel, right? And so, if it's hydrogen, which is the sort of standard fuel that's being deployed in general, you need now a series of gas stations that sell hydrogen. So, we don't have that yet.

But as I understand it, you can drive from far northern Japan all the way to far western Japan on a fuel cell with hydrogen fuel. There's been a big investment in being able to do that in Japan, and they are leaders I think in that idea of having distributed hydrogen sources. And, of course, lots of other folks are doing that in the world today.

But the challenge is exactly what you said, right? The technology is not widely available just yet, and so we have to make a decision: Are we going to think about having hydrogen fuel available in some form? It might be in the form of ammonia instead of hydrogen or whatever, but you make that available to the public in general. And if we do that, then the fuel cell can be much more widely implemented."

McDonald: "So with your research, what are some of the specific questions that you're hoping to provide answers to that maybe bring this technology closer to commercialization?"

Misture: "Yeah, good question. So, we're working on a very fundamental side of understanding the materials. And so what we want to do is we want to see how the atoms fit together and how they behave when they're in, as I mentioned earlier, layered phases, right? So, they're sort of constrained to being sort of two dimensional in nature. And these two-dimensional materials very often have properties that are kind of surprising, and we like that.

So, the sort of two-dimensional material has a big face on one side, a big face on the opposite side, and then it has edges, right? And so all those faces and edges both presumably can be tuned in some way, shape, or form, and we can control the sizes of those to some extent. We can control how densely packed they are: Do we want them really sort of fluffy like a snowflake or do we want them really sort of compressed, you know, like a crumpled newspaper, for example. And not only what's the sort of physical state from a structure standpoint but chemically how do they behave and how do we modify perhaps the surfaces or even modify the chemical composition, right?

These are mostly oxide ceramics we're working on, some oxynitrides, but we're mainly interested in using sort of traditional electroceramics logic, where we can take a different element and replace one of the elements in the sort of baseline material to adjust the properties.

And so we're really focused on trying to understand what's the electrical conductivity, what's perhaps the ionic conductivity, what are the charge transfer resistances when we make a device, and these sorts of things. And that helps us understand a little better how the material itself conducts electrons. And if we can understand that better, then maybe we can tune it to our advantage. That's what we're after ultimately."

McDonald: "With these layered oxides, are you using layered oxides in both the SOFCs [solid oxide fuel cells] and the photocatalysts?"

Misture: "Yeah, so it turns out that we're using layered oxides in their layered sort of 2D form for the photocatalysis primarily. But interestingly, layered oxides are really useful in the fuel cell arena as well for catalysts on both the anode and cathode sides. So, those are really useful, but we don't peel those apart to 2D materials. So, we use sort of the base layered oxide in the fuel cell application, and then in the photocatalyst application, we try to really peel these things apart, adjust the properties, really increase the surface areas really dramatically. That gets us a toehold on understanding the behavior of electrons in those materials."

McDonald: “And as our listeners may know, photocatalysts, one of the key things with them is the exposed surface area: The more surface area, the more things can react. So, that 2D layering probably really helps with that.”

Misture: “You bet. Absolutely. That’s really a key parameter. So, we’re getting better and better at tuning that, right? So, hopefully we’ll continue to get better at that. Yeah, no, that’s absolutely right.”

McDonald: “Yes, exactly.”

(music)

SECTION 2

McDonald: “So, we have a really good understanding now of what the final applications are and why this research is being done, how it’s going to help improve energy conversion in these solid oxide fuel cells and the photocatalysts. But now we have the fun of learning how exactly do you go about learning more about these materials? So, the characterization techniques that you use.”

Misture: “Sure, sure. So, if you ask anybody what do they think I do in my research, they’re going to say, ‘Well, I mean, diffraction of some sort’ because that’s sort of my niche area. And I’ve enjoyed working on diffraction studies and X-ray scattering studies and also X-ray absorption studies as well for many years.

Really important to that is doing the studies under what we call in-situ conditions. In other words, with an applied electric field or with high temperature or with a controlled environment gas around the sample or combinations of those three things. And so that’s really what we’ve spent really a long time and a lot of effort to build up lab facilities that can do these experiments, and they tell us really quite a lot in a short period of time. They also tell us that we’re wrong. In many cases, we predict something will happen when we do the experiments, and we scratch our heads and go, ‘Well, that’s interesting.’ So, we’re constantly learning new things by doing these experiments at high temperature.

And for the photocatalysts, we can watch the thing work, right? So, we can look at their strain responses or how atoms sort of shift or adjust while they’re operating. And there are many times when that gives us the ability to do two things. One is to sort of build a quantitative model that we can then perhaps make into a predictive model. And secondly, we can get an intuitive feel of how the thing works. And with that, you know, sort of chemical intuition, very often we can make educated guesses as to what’s happening, even if we haven’t quite yet built a quantitative physical model, and that can be really very useful.

So, what’s great about it, though, I would say is that it’s not just useful for the active materials but for other components. For example, glass-ceramic seals are needed in these devices. Metal manifolding is needed in these devices, and the metals oxidize at high temperature. So, the nature of the oxide coating, the function of the oxide coating is a question we can address.

So anyway, we have a lot of angles when we use this diffraction technique. That's what I spend my time doing."

McDonald: "So, can we give our listeners a brief overview of how diffraction works and some of the main diffraction techniques and how they differ from each other?"

Misture: "Yeah, sure. So, the diffraction tool works by using an X-ray wavelength or neutron wavelength, if you like, that's on the order of the spacing between the atoms. And when we do that, we get a scattering pattern that is unique to each phase on the planet. So, we have a database of around 700,000 known materials, pure materials. And so, from the point of view, if you're a mineralogist, for example, and you have a mineral sample or an ore sample, you do this analysis and you can tell what phases are present. Maybe there's hematite—iron oxide is hematite—and quartz and crystal and etcetera.

So, we can use it as a sort of fingerprinting tool, but we're more interested in understanding how the atoms respond to some stimulus, right? Temperature, electric field, etcetera. And so we see these more subtle effects in the diffraction patterns, where the scattering pattern changes maybe only a little bit as we have, for example, apply an electric field, but that can give us a direct quantitative measurement of what really happened, right? So, instead of making a measurement, you know, electrical measurement and looking at the data and trying to build the model, we do that part but then we do a match experiment under the same conditions, and then we look at the response of the atoms themselves. So, diffraction gives us the basic linear arrangements of the atoms, which creates this sort of fingerprint.

So that's a piece of it, right? We can do this on bulk materials, which is the typical thing that we do. But we can also, which is really important, we can do this on thin film materials and single crystalline thin film materials. And we can really learn a lot from model systems that are single crystalline thin films. As difficult as it might be to make those, we can really learn a lot.

So, we do that as well, and we can also do these diffraction measurements on things like entire battery cells or functioning photocatalysts, which is submerged in water with ultraviolet light or visible light shining on it. So, we have a lot of angles in terms of the sampling, right? And that gives us really a very big playground to work in, yeah."

McDonald: "It's always nice to have a big playground."

Misture: "Indeed. Yep, yep."

McDonald: “So, I know your deep experience and expertise in diffraction has expanded beyond the university, and you are currently the chair of the International Center for Diffraction Data. So, can you tell us a little bit about where the center’s based, what its history is?”

Misture: “Yeah, sure. So, this database I mentioned of 700,000 or so known pure phases, or the diffraction data for those phases, that is, that’s what the organization does. And so it’s not terribly exciting, but it’s really exciting because people come from all over the world to help support this. It’s a not-for-profit company, and the company does a lot of workshops and training for people who are getting into the field, maybe they have a background in some other area. They also sponsor conferences in addition to their workshops.

But the idea is that they have a staff located outside of Philadelphia that takes data from the literature and takes data from contract sort of data miners, and they put the data together into the database and they checked the data and make sure it’s self-consistent, it’s consistent with other known materials, and they try to produce a really high-quality product that enables, you know, labs like mine that have maybe 20 MSE [materials science and engineering] professors making new things all year long. We want to have the latest updated databases, and so that’s what this company does: It makes these databases.

But there’s really, it’s kind of funny how much is involved, right? So we have a Board of Directors that’s a very international Board of Directors, people from all over the world who are experts in diffraction. And they provide, as a group, guidance to the company of what’s next, what does the community need, where might the next growth area be. If there’s a huge explosion in batteries like there has been, then we need to make sure the database has as many materials related to batteries as possible, just for example. So, that’s what it does, yeah.”

McDonald: “And that’s one thing that’s kind of cool is, like you said, if you identify a new area you want to expand out to get more data to add the database, once it’s added, it’s there. So over time, this database is just getting more varied, more diverse, more options of all the different things people might want to access it for.”

Misture: “For sure. That really becomes important, right, because people might make a material that’s relevant to batteries today, and in four or five years, discover it’s a high-temperature superconductor, right, or whatever else. And so we see that over and over, that sort of known crystal structure types maybe take on very different functions and they’re used in multiple different fields and, so yeah, becomes a really useful tool and one that we can rely on to know that the data is of high quality and that we can look back at something from early on, right? Let’s just say that. Post-World War Two sort of scientists working on something, that data is still good, right? And so that’s a really important point, yep.”

(music)

BREAK

McDonald: "For decades, ACerS and the National Institute of Standards and Technology have collaborated on the Phase Equilibria Diagrams Database, which provides a comprehensive collection of critically evaluated phase diagrams for ceramic and inorganic systems. The current Version 5.2 contains more than 33,000 diagrams as well as expert commentaries focusing on sustainability and clean energy generation. Learn more about the ACerS-NIST Phase Equilibria Diagrams at ceramics.org/PHASE."

SECTION 3

McDonald: "You've been so involved with the Society. You've been past chair of the Basic Science Division, of the ACerS Membership Committee, and you're also an associate editor for *Journal of the American Ceramic Society*. So, with your long experience, how is it that you first came to know about The American Ceramic Society and become involved?"

Misture: "So, when I was an undergraduate student, I got involved in our local branch of the Ceramic Society, student branch, it was called student branch then, I think. And I was also involved in Keramos. And so, I had an invitation to go to one of the Annual Meetings, and it was in Dallas, Texas. And I was really, actually, really surprised at how tightly knit the ceramics community is, and I decided I wanted to stay part of that even if I did other things in my career.

So, I've learned over the years that my first impression was absolutely correct, and it's an incredibly tight-knit community. I try to get to as many meetings as I can and bring my students and postdocs and undergraduate students in particular to these meetings if we can manage that.

So, I think that was the start of that. There was student chapter, and everybody knew about it, so we did it, right? Yeah, it was good, it was good."

McDonald: "So, I guess, you know, in addition to the opportunity to bring your students to meetings, are there any other aspects that you found really personally and professionally enriching when engaging with this tight-knit community?"

Misture: "I would say that the networking is really important. And so, the ceramics community is on one hand small, but on the other hand it's really big and really sprinkled all over the world, right? So, The American Ceramic Society, you know, like the PACRIM meeting, for example, the attendance at that is really spectacularly diverse.

So, I think for me that's a really important piece because I get to know folks, for example, who might be experts in atomic force microscopy or piezoelectrics or whatever it might be. So when I have some challenge that I'm working on in my group, I can reach out to these folks and just say, 'Hey, can you give us a hand with this?' Whatever it might be. And we do a little bit of horse trading. So maybe I do measurements for somebody or help with some sort of analysis that I know how to do. To be able to do that is, you know, you can't really even put a price on that. That's fantastic, yeah."

McDonald: "And I think it's one of those things, the more of an expert you become, the more you realize how much you don't know. And so knowing who you can reach out to the help you fill in those gaps really makes it a diverse, effective research team."

Misture: "Absolutely true. There's so many things that people are doing with materials these days, right? And, you know, as sort of a characterization specialist, I really need to rely on folks who know how to do electron microscopy, for example, really well, or NMR spectroscopy or whatever it might be. And so you need the professional network to be able to do that effectively, I think."

McDonald: "So with all of those experiences, do you have any experiences in particular that are a lot of fun or very serendipitous that you'd like to share with our audience today?"

Misture: "So, I thought one really very funny thing was related to our study abroad program here. So, I was the director of the study abroad program, and we had students in from Germany and France and the U.K., probably Spain also that semester. And a whole lot of our students were overseas as well in the partner institutions that we have in Europe.

So, I went to a conference maybe in August after the school year was over, and I was traveling by car with colleagues on one of the autobahns in Germany on the way back to Frankfurt to get our flight back home. And we stopped in a gas station, and somebody says, 'Hey, Doctor Misture, how's it going?' And that was kind of strange, but it turns out it was one of the German foreign exchange students who had come to Alfred. And I bumped into him, actually the second student who was here from Germany as well. So I bumped into these two students at a gas station in Germany. It's great, right? I mean, small world.

But anyway, that happens all the time. There's ceramics folks everywhere, right? So, it's great."

McDonald: "It might be a small community, but once you start seeing them, they're everywhere, they're everywhere."

Misture: "Yeah, we love it, right? Yeah, we love it. That's great, that's great."

(music)

CONCLUSION

McDonald: "The materials science community is a diverse field, but by combining our knowledge and expertise through nonprofits such as ACerS and the International Center for Diffraction Data, we can collectively advance a more sustainable future.

I'm Lisa McDonald, and this is Ceramic Tech Chat."

(music)

“Visit our website at ceramics.org for this episode’s show notes and to learn more about Scott Misture and his research. Ceramic Tech Chat is produced by Lisa McDonald and copyrighted by The American Ceramic Society.

Until next time, I’m Lisa McDonald, and thank you for joining us.”