CERAMIC TECH CHAT

Episode 47

Title – "Modeling materials and meetings engagement: Jessica Rimsza"

INTRO

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

> In science, it can be frustrating when experiments do not pan out as expected. But it is the ability to embrace accidents and potentially harebrained ideas that can help make your career."

Rimsza: "I heard once that in the lab, you don't want someone to say, 'Eureka!' You want someone to say, 'Hmm, that funny.' That's how all science actually is, right? Something unexpected that occurs. And sometimes when you sort of go after that bit of data, you find something amazing."

McDonald: "That's Jessica Rimsza, staff scientist at Sandia National Laboratories. She is also the current chair of ACerS Meetings Committee.

> In today's episode, Jessica shares the unexpected moments she's had in both the lab and at conferences and demonstrates the importance of embracing spontaneity in both settings."
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> (music)

SECTION 1

Rimsza: "I've always been really interested in materials science in general, and when I'm talking to folks, I say it's because I want to know something about everything. Everything is made of a material, and so really, I was drawn to materials science as a field because if you know something about the material that something's made of, you actually have a lot to say about it.

> And then in terms of ceramic and glass specifically, that really started when I joined grad school. Because I had this broad interest, I didn't have a very specific material that I was working on. And I went to graduate school at the University of North Texas, and my advisor was doctor Jincheng Du, who's still heavily involved with The American Ceramic Society. And he had some projects that were working on ceramics and glasses. And once I understood that glass had this really sort of unique structure, that it wasn't crystalline, it really spoke to me in the fact that it was so disordered. I felt like that was something, you know, you can understand the chaos, I guess if you will, and that's what really spoke to me in terms of working in glass science.

And even now as I branch out into other materials, I'm still really drawn to systems that are disordered, that don't have well-known crystal structures or that have a lot of complex interfaces just because I feel like there's a lot that we don't know there, and that's the area that I like to explore."

McDonald: "That is definitely a very fun area to explore. And the way that you explore this system is a lot through modeling. So, when you first started getting into ceramic and glass research, was it with modeling or was it more experiment and you transitioned into modeling later?"

Rimsza: "I've actually always been using different sorts of modeling techniques to understand these systems. I ran my first simulation, actually, when I was a sophomore at the University of Arizona, and so I sort of started right out by working in simulations. And it's important to me that the simulations provide clearly practical insight into a material. So I don't really develop simulation methods myself so much as use them to ask specific engineering or science questions about a material. And that can be really small-scale molecular simulations that only have a few hundred atoms up to even larger with tens of thousands of atoms, and I've even done some work on an even larger scale where we're looking at centimeter-sized structures, for example. More recently I have started doing a little bit of experimental work as well, just to sort of round out the skillset I have to understand the structure and properties of ceramic materials."

McDonald: "So why is modeling so beneficial to materials science research and development?"

Rimsza: "I like using modeling, and I think it's a really valuable tool because it provides insight into materials that can't be sort of obtained any other way. At the end of the day, all of the materials that we're talking about are made of atoms, right? And so why not just look at the atoms specifically to understand what's going on.

So, obviously there's value in all sorts of different characterization methods. But for me, that sort of fundamental insight where you can actually see the individual atoms move is one of my favorite parts because it gives you sort of a feeling of how the material is responding and you start to get an intuition.

One of the things that I will say, though, is when I'm doing my modeling, each atom has a different color. And so a lot of times what that means is when I see the material in real life, I'm surprised by what color it is. So in the post-processing scripts, silicon is always yellow and oxygen is always red. So I'm looking at red and yellow spheres. Of course, silica is not a mixture of red and yellow, right? So I've always found that to be fun. What do you mean boron isn't blue? Because that's the way that they tend to be colored. So, I find that very interesting and fun as well."

McDonald: "If only they actually were colored red and yellow and blue. It'd make it so much easier."

Rimsza: “It might, it might. Exactly, yeah. So somebody will be like, ‘Oh, we can’t see that,’ or, ‘Oh, that doesn’t show up,’ or ‘Oh, we can’t differentiate those phases in, you know, SEM, scanning electron microscopy.’ and I’m like, ‘How is that? They are such different colors.’ So many good conversations have been had about that.”

McDonald: “Yes, definitely. So currently you’re doing modeling in the context of your job at Sandia National Laboratories. So, how did you end up at Sandia? What was your journey to your current career?”

Rimsza: “Yeah, absolutely. So as I’ve mentioned, I did my undergraduate at the University of Arizona and then I got my Ph.D. at the University of North Texas working with doctor Du. And while it was there, I was actually funded partially on a DOE NEUP project, which is a nuclear energy university partnership. And that’s a specific type of grant that connects researchers at the national laboratories with those at different universities. And through that sort of relationship, I met doctor Louis Karsenti, who was a staff member here at Sandia. And so, she eventually had a new project that was starting up and she was hiring a postdoc, and so she had sent out sort of an announcement. And so I applied that way, and that was my start. So, I got hired here as a postdoc. I’ve been at Sandia for about seven years. Five of those as a staff, and two years as a postdoc before that.

In general, my work here has been focused primarily on atomistic and molecular-scale modeling of different types of like oxide-based materials. So, I’ve had projects related to the fracture of ceramics and glasses, projects related to the fracture and aging of cement. Currently I have projects related to different sorts of materials for carbon capture and also carbon separation and catalysis as well because that follows underneath some of the Department of Energy mission space as well. So in general, a lot of work on interfaces, a lot of interesting applications that are related to sort of the reliability and aging and carbon footprint of different sorts of materials.”

McDonald: “And that is a really hot topic right now. I know a ton of our listeners and especially some of our emerging professionals, our younger students and the people in our Young Professionals Network, are very interested in all of those topics. So it’s really great to hear that you’re getting to dive into this topic that so many people are interested in.”

Rimsza: “Yeah. It’s been an interesting space to work in because when I first started working in glasses, it was really more of we were trying to expand the use of glasses because their brittle behavior can often limit their applications. And so we were doing a lot of work looking at sort of aging and reliability so we could have brittle materials that we would have confidence in, right? If they were used in some sort of high-fidelity applications.

But now we’re starting to have more concern about the carbon footprint of these materials related to processing of glasses. You know, there’s a lot of high temperatures related there, and if you could use other heat sources, like hydrogen, or if there’s ways to produce and synthesize these materials at lower sort of temperatures and conditions. And that’s also really transferable to some of the work I’ve been doing on cement, which has a pretty big

carbon footprint per ton of cement binder produced and different synthesis pathways or different ways to use less of that material while getting the same performance.

So, there's a lot of different aspects of the material, how it's produced, and what it can do for us that we can sort of start tweaking to lower the carbon footprint of the different materials."

McDonald: "So I know one thing that sometimes students are, when they start getting into modeling, are thinking about using these computer-based systems. Would you say that students should get either a minor or just take a few classes in computer science? Or is modeling, it depends on what type of modeling you're doing? You don't maybe necessarily have to be a computer expert to make use of these techniques and tools in your research."

Rimsza: "So for those of you who are interested in doing modeling, I always give the advice that don't be intimidated necessarily by the fact that you're using a computer. I think that strong knowledge of computing isn't necessarily required. It's more that you would have an interest in what's happening sort of deep into the material structure and that you have the willingness to learn the different tools.

So for me, learning modeling doesn't seem like it would be any more difficult than learning how to run an X-ray diffraction, collect an X-ray diffraction pattern, or do any other sorts of analysis. It's just where and how you want to spend your time, and perhaps more importantly, what information you want to pull out of it.

I can say that most of the different scientists I know that do modeling, very few have a specific degree in computer science. I would say it's more common to have a chemistry or material sciences or physics and then move into modeling specifically.

Now there is a whole interesting field of sort of computational modeling that's related to things like efficiency and developing new hardware and architectures and a lot of questions about parallelization to get the most efficiency out of the different simulations. And at that point, when you're getting into that algorithm development, if that's something you're interested in, then I do think having a deeper understanding of computing and how to make those algorithms and stuff starts to become more important.

But for most of the computational materials scientists that I deal with, I would say that it's not strictly necessary. So, if that's your big worry about whether or not you can be a computational materials scientist, I would say don't worry."

McDonald: "Since you've been working with tons of different modeling systems, do you have a favorite type of modeling that you like to do and why?"

Rimsza: "Oh, I don't know if you can have a favorite. I'm sure people do. It tends to be just what you want to know most about the material, right? For me, when I'm presented with a material problem, I like to think of what is the concern, what is our hypothesis, and how

are we going to test it. Just classic scientific method question, right? And what you might find is that a specific type of modeling is the most well suited to answer that question. For example, some simulation methods specifically include electronic effects. So if you have questions about whether or not your material, for example, is going to fluoresce, then you're really restricted in what type of modeling you can do.

And so, I think you might have heard the analogy before that if you're holding a hammer, every problem looks like a nail. And so I think if someone has a favorite type of modeling, you run the risk of being surrounded by a lot of nails and then finding yourself in trouble. So for me, I think it's better to say, 'Okay, what is the question?' first and then pick the best technique to solve it later."

McDonald: "That sounds like a really great and wise approach to tackling the questions that are put before you. So, is there anything surprising about modeling that maybe you didn't realize until you got into modeling? Like 'Oh, wow, I didn't realize this aspect of it.' That might be interesting for students to learn about."

Rimsza: "I've been really impressed with the size and scope of the different questions that we can answer using modeling and how that's evolved even just within the last five or ten years. You know, sometimes I go to conferences, and I see the new techniques and the new studies, and I think, 'Oh, I'm a dinosaur now,' right? Like, you know, this was stuff that wasn't even possible when I was in graduate school. And so I think it's a really exciting and sort of continuously evolving field to be a part of."

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SECTION 2

McDonald: "Speaking of conferences, that makes a great transition to our next set of questions, which is that you are currently the chair of ACerS Meetings Committee. And so, what role do meetings play in the science ecosystem? Why are they so important for researchers to go to and attend and participate in?"

Rimsza: "As the Meetings chair, I'm obviously a huge fan of meetings. And I feel like in some ways it almost makes a society. That's how we pull people together, that's how we have that critical exchange of ideas, that's how we have the conversations that really sort of enable some of the new, evolving science. And I know that there's wonderful ways of being connected virtually. But there's still something sort of magical about spontaneously meeting someone when they ask a question at your poster or at your presentation that sort of really brings us together.

And I can certainly say that once you start attending meetings regularly, and you see the same folks over and over again, it's really some of those connections that keep us coming back, and I think also help sort of expand your mind in terms of what's been going on and what could I do next. Sort of like a refresh, right? So every time I go to a conference, when I come back, I sort of have this little list of things that I had thought about or

different approaches to use when I'm analyzing my results or things I hadn't thought of, new ideas for proposals. And so it's really important to me that that's a part of ACerS, and it's certainly part of why I continue to be involved."

McDonald: "And I know whenever I go to conferences and meetings, I'm always just so impressed by the quality of the presentations, the poster sessions. Everything just seems so magically well-put together when you are being the attendee at a conference. But of course, the reason it feels so magical and great and perfect networking opportunities is because of all the work that goes on in the back end that people don't necessarily see to put that conference together. So, as a meeting organizer, what are some of the steps to, you know, we have an idea for a conference, how then do you get that into a real product in real life that people can go to?"

Rimsza: "Well, first of all, I'm delighted to hear that you just feel that the ACerS conferences run delightfully. And I would like to say that I could take credit for that, but I absolutely cannot. Certainly there's the hard work of all the different session organizers and session chairs and certainly all the ACerS staff that pull a lot of that together.

I think, you know, starting with saying, 'Hey, I have an idea for a new conference,' is a pretty big ask, right? So, I would say if you are seeing something that you want to have at an ACerS conference, that you think, 'Oh my field isn't well represented' or 'I want to see more talks on this.' Rather than jumping straight to saying, 'Oh, maybe we could make a new conference,' I think the more achievable way would be to start by saying, 'How can I get that content at the conferences that I go to?' And the easiest way for that is going to be to organize your own symposium, and that's pretty straightforward.

Usually about a year before the conference or a little more, there'll be a call for symposium for those conferences, and then you can write up a symposium proposal and you send it in. And then there's a committee, often someone from ACerS Meetings Committee or the conference chair, that goes through and picks which symposium are going to be there. And if your symposium is picked, then you get to invite your speakers, and that will be advertised for anyone that wants to present in your session. And then you can start growing sort of the community and you can see what you want. So, if you really want to talk to someone and you just think they have the best science, invite them to your symposium. And then you can go ahead and start making those connections that way."

McDonald: "I think that's a really smart thing to point out, is that it's harnessing what's already existing and integrating into the existing platforms. Because people are already attending those conferences, so you'll probably reach a wider audience by presenting at a place where people already are."

Rimsza: "And I would say, if you have the symposium, let's say that it goes fantastic. That would be great. And it gets bigger and bigger, and it becomes sort of its own unique feature within that conference. Then at some point, you could talk about either spinning it off into its own conference if it's large enough or even incorporating it into some other mechanism.

So, at ACerS, we are inclusive. If there's something you want to see, if there are talks you want to hear, if there are topics you want to learn about, let's go ahead and incorporate them. Like we really have an inclusive view of what a material can be. And that's actually something that the current ACerS president, doctor [Rajendra] Bordia, has brought up, is that he would like to see more content that's not sort of typical ceramic and glasses. I guess what I'm trying to say is that if there's content you want to see, we welcome people that want to help us include that in the conferences."

McDonald: "There's one other question that I just wanted to ask quickly to make sure it's clarified for our listeners, is what is the difference between sessions and symposiums at meetings?"

Rimsza: "That is a great question. In general, symposia are composed of sessions. So, if I'm thinking, for example, of the Glass & Optical Materials Division meeting, we usually have five symposiums that have sort of really rough, overarching topics. For example, one might be structural effects. And then under that would be more specific sessions. So, for example, you might have a session that's specifically on oxide defects or a session that's specifically on aging or whatever. So in general, it goes the overall topic of the conference, and then under that you have the symposia, and then under that you have the sessions, and then under that you have individual talks, right? In terms of how things are organized."

McDonald: "That helps a lot to clarify because I know some of our listeners might not be that familiar with the terminology.

So, one of the benefits of ACerS meetings is that they typically are held in person. It's really easy over coffee breaks in between the sessions to just get chatting with people and network and meet them. But in 2020, when the COVID-19 pandemic happened, we all had to pivot very quickly and have a few years of virtual meetings, which of course is a completely different platform, different beast than organizing something that happens in person.

So, I know you were involved in one of our first big meetings that we had to pivot, the 2020 Glass & Optical Materials Division. So, what was it like having to pivot a conference from in person to virtual? But then also, are there any benefits to virtual that you don't maybe necessarily have in person?"

Rimsza: "So, there's a lot of questions there. So, first I will sort of talk about the pivot to virtual. When COVID-19 pandemic started, we were fully in swing to plan the 2020 Glass & Optical Materials Division meeting, which is going to be in New Orleans that year. It's held in May. And so if you can remember back to when COVID-19 started, that was mid-March, and so at first we thought, 'Oh no, this will all be over by then, and we'll have an in-person conference in New Orleans.' Oh, how naive we were. And then eventually it became apparent that we were going to need to switch to a virtual conference instead.

And actually, there's a lot of behind-the-scenes complications that happened with that pivot, especially in terms of the cost. So initially we had contracts with the hotel and the conference centers that we were going to use and things like that. That really made things complicated in terms of doing a pivot sort of late in the game.

So, we actually ended up rebranding that conference as the 2020 Virtual Glass Summit, the ACerS meetings staff was incredible in making sure that we were able to develop a platform, we had to sort of reconfirm everyone's abstract status, and things like that. And ultimately, I think at that point, everyone was really excited to have a conference because it had been sort of a long time. And so we had a lot of really good participation for that and it came off really well, and I was really happy with how we were able to accomplish that.

But there were a lot of interesting benefits to having virtual conferences for sure. And then one is just the fact that you don't have that sort of cost barrier to attend the conferences. It costs money to fly to one location, it costs time. So in that way it can be a lot more inclusive because you could have more folks sort of participate. And we see that actually, that a lot of times when you have the virtual talks, you'll have a lot more people online. Sometimes fewer questions, so I encourage you if you're at a virtual conference to ask more questions. But that can be really good because you can reach sort of a wider audience as well.

I will say that in general, we've had some trouble with hybrid conferences just because it's so difficult to make sure that you have good connectivity and it's hard to balance sort of having an audience in the room and a virtual audience, making sure that you're asking for questions from people online and in person, making sure that everything's working properly. For me, I think that's actually one of the more challenging modes. Fully virtual or fully in person seems to work the most smoothly. I think we're still looking for that hybrid option that might make the most sense. That's a tough one to crack."

McDonald: "Well, one thing that's fortunate for us is this year ACerS is busy doing its next strategic plan, and I know there's a ton of like little committees that are focusing on publications or meetings or awards. And so maybe if we're fortunate a solution to that hybrid challenge will come up during the strategic planning process this year."

Rimsza: "It could. This could be the year that we figure out how to do an efficient hybrid conference."

McDonald: "So, for someone who would be really interested in getting involved with helping to organize a conference, but they don't necessarily have an idea for a symposium, they just want to support what's already happening. How would you suggest that someone kind of starts getting their feet wet and learning how conferences work and supporting them so that they can work towards maybe taking a larger leadership role in the organization?"

Rimsza: "So for me, I always recommend that undergraduate students, graduate students, or even anyone else that feels like they want to be more included in the conferences they're seeing,

start by attending the business meeting. And so almost every single conference is run by a Division of The American Ceramic Society. So, for example, ICACC is, I believe, run by Engineering Ceramics [Division]. And usually at each of these conferences, they're going to have a business meeting that happens in the evening. That is when the Division leadership comes together and they discuss how the conference is going, any new plans for the next year, they talk about who's sort of going to be the program organizer for upcoming conferences, and you really get to meet the folks that are doing most of the heavy lifting in terms of organizing the conferences. And a lot of times that's going to be a great place to start because if you can talk to the Division chair or secretary or you understand who's going to be in charge of these upcoming conferences, and you can say, 'Hey, I want to be involved.'

Another great way if you're not able to go to the business meeting is if you're in a conference and there's a really interesting session that you're in and you think, 'Oh, I want be a part of this,' is you can talk to the session chair. And a lot of times symposium are done multiple years in a row. So you might say, 'Hey, this was a great session. I'd really like to be involved. Can you tell me who this symposium organizer is? Maybe I can be a session chair next year.'

And I would say the easiest way, lowest hanging fruit to be involved is to be a session chair. Because for that you get to attend the session, you get to introduce the speakers, you get to sort of develop some of your technical expertise in an area, and from there it's really easy to step up then to organizing your own symposia once you get a feel for what it's like to be part of the session."

McDonald: "Those are some really great approaches and pathways that people can take and explore. Based on everything that you said, it seems like there's multiple entry points. There's not one right way to start getting yourself involved."

Rimsza: "Absolutely. And then there's even more, right? If you're a graduate student, you could ask your advisor for help with getting involved. I always recommend that students consider being a part of the President's Council of Student Advisors. I was a part of that when I was a graduate student. And that's sort of a community of graduate, undergraduate students, and they're really involved with ACerS. And that can be a nice gateway toward being involved in meetings as well."

(music)

BREAK

McDonald: "Each year ACerS hosts and endorses a number of ceramic and glass related technical conferences and meetings around the world. These events offer attendees the opportunity to share their latest research, meet experts in the field, and network with colleagues who share an interest in ceramics and glass materials. View ACerS meetings calendar by visiting www.ceramics.org/meetings-events."

SECTION 3

McDonald: “So I noticed that you mentioned that you used to be part of the PCSA, the President’s Council of Student Advisors. So how about we talk a little bit about how did you come to learn about The American Ceramic Society and get so involved to the point that you’re now the chair of our Meetings Committee?”

Rimsza: “So when I first started at the University of Arizona, I was a member of the Material Advantage Chapter, and then I was also, they had a Keramos Chapter as well. So I was a part of both of those. And so I had attended a few meetings just to learn more. I didn’t present really any work but just to be a part of the community. And I think mostly we went for the mug drop competition, which is always very fun. And then once I started as a graduate student, I was working more seriously in ceramics and glasses. And so it became clear that being a part of The American Ceramic Society was going to be part of my sort of scientific community.

And so I’d been to a few conferences that way, and at that point, the PCSA was only a few years old, like three or four years. And so it was recommended to me by my advisor, doctor Jincheng Du, to go ahead and submit an application for that. And once I got there, I realized, ‘Oh wait, there are actually tons of people, tons of graduate students and undergraduates at these different universities, like me, working on the stuff I work at.’ And I just didn’t know them because we were all sitting in our offices or our labs doing our own stuff.

And so the PCSA has this business meeting. It runs for like a full nine hours right before MS&T. And I went to the one that was in Montreal, and it was just so great. All of a sudden I was like, ‘Oh no, wait, this is the community that they’re talking about.’ So instead of getting up my courage to walk and talk to someone during coffee breaks, I sort of had the whole day to talk to these other graduate students. And so that’s how I started getting involved. And so I served as the chair of the [PCSA] Programming Committee. And then the next year, I was actually the chair of the PCSA. So I spent two years involved that way. And then of course I graduated and I had to go and get my full scientist job, which is when I joined Sandia.

And I think that is actually when it’s most difficult to continue your involvement with The American Ceramic Society. Because a lot of times what you do for science changes when you make that transition from graduate student to young professional, as you’re sort of making your own way. So, you break off from your advisor and then you have to do your own science. And sometimes that pulls you closer to ACerS, and sometimes that pushes you farther away.

In my case, I was lucky in the fact that a lot of the work I was doing continued to be with glasses and also that some of the work I’m doing on cements and other types of materials still falls under the ACerS umbrella. So I was able to continue my involvement that way. And that’s when I served as the programming chair for the Virtual Glass Summit. And then once you start doing some of these activities, you start thinking, ‘Okay, well, what

can I do next?' So at that point, I'd had experiences as session chair, as symposium organizer, and I'd been the programming chair of the conference. And so it just seemed natural to continue my involvement by being a part of the Meetings Committee."

McDonald: "It's always great when we can work with people who have been involved with us for so long. You know the Society and other people so well. And with all that knowledge and all that experience, you're able to really make the meetings, like you said, what they're supposed to be: a great networking hub, great educational experience for the people who are going to them."

Rimsza: "Well, and I'll say there's a lot of different committees that touch on different aspects of ACerS if you want to be involved, right? So obviously I've been part of the Meetings Committee, but there's also a Diversity, Equity and Inclusion Committee, there's also Publications Committee, there's sort of an Awards Committee. There's lots of different ways depending on sort of your time commitment, what you have to offer ACerS, and then also what your interests are, right? If you're passionate about something specific, then it's a good opportunity to be on that committee so you can influence that aspect of ACerS at a larger scale."

McDonald: "So what has been the most meaningful and impactful thing about being in ACerS for you, both personally and professionally?"

Rimsza: "The most important thing for me about being a part of Acers and the most impactful is that it feels more like a scientific home in that I think I identify more as a glass scientist or as a ceramist than I would if I wasn't a part of the ACerS scientific community. And so that's been really important just because it's place that I keep coming back to, that I keep learning from, that I keep sharing with. And that's a big part of what sort of keeps people being a scientist actually.

I think it can be hard if you're dabbling in a lot of different areas to sort of identify yourself. This is actually something that I ask when I interview folks who could work with me, is I say, 'Who are you? Are you a surface scientist? Are you a ceramist? Are you a coder?' To go back to your earlier question. And it's interesting to see all these different aspects of being a scientist. Who are you? What is your specialty? And so that's what I asked them. And ACerS I think is a great way of helping you sort of define yourself and understand who you want to be as a scientist."

McDonald: "I think that's just a really beautiful way of putting it is who are you. People don't always necessarily think about that. It's like, 'Yes, I got these degrees, but do I actually see them as a piece of paper I hang on my wall or is that something I identify with and the one I really want to put forward as I'm networking and meeting with other people and engaging with our society?'"

(music)

CONCLUSION

McDonald: “Modeling in science, be that simulations on a computer or demonstrating to others how to get involved in their society, often leads to real-world changes that benefit the entire community.

I’m Lisa McDonald, and this is Ceramic Tech Chat.”

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“Visit our website at ceramics.org for this episode’s show notes and to learn more about Jessica Rimsza’s work at Sandia National Laboratories and ACerS meetings. 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.”