CERAMIC TECH CHAT

Episode 49

Title – “Advancing microscopy with machine learning: Sergei Kalinin”

INTRO

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

Computer modeling and automation have become essential parts of today’s manufacturing environment. But as we progress further into the 21st century, the emerging field of machine learning is poised to increase our use of and reliance on digital technologies in industrial operations.”

Kalinin: “For machine learning to become useful, it has to be a part of manufacturing, it has to become a part of the experimental research. And in this case, we don’t have huge trained workforce that knows both domain areas in machine learning, so we can only create it. And I think that this is a unique opportunity to going forward because now we are in position to train domain scientists to use ML and the real-world problems, and that would be the true return on the investment.”

McDonald: “That’s Sergei Kalinin, Weston Fulton Professor of materials science and engineering at the University of Tennessee-Knoxville and chief scientist in artificial intelligence and machine learning for physical sciences at Pacific Northwest National Laboratory. Before his current positions, Sergei spent 20 years at Oak Ridge National Laboratory, pioneering advancements in the field of scanning probe microscopy for materials characterization.

In today’s episode, Sergei will share his experience in microscopy and machine learning and describe the bright future that he sees for both fields.”

(music)

SECTION 1

McDonald: “So, before you ended up at Oak Ridge, there must have been a journey for you to get into materials science.”

Kalinin: “You know, it’s an excellent question. So for me, I actually started as a chemist and I was actually very young, so it was about 10 years old when my parents were leaving me at for at dacha, about 100 kilometers from Moscow, and that was ‘80s that time. There was no internet. There was also obviously a radio and TV, but most of the time you are free to find whatever fun you can. And it turns out that when you’re in the country house, there are certain type of chemical experiments that you can make if you have access even to the high school textbook.

So, one type of experiments is the applied fermentation. So at that time, you probably don't remember, but in the Soviet Union, that was a Gorbachev prohibition time. So, applied fermentation, it's a great science, it's also useful for the family in many ways. The second type of experiments is the applied pyrotechnics. So, you can easily go to the scrap yard and find aluminum and rust and build things like thermite and so on and so forth. So I can say that my quest in chemistry started when I was very young and it was with the thermite reactions and, as I said, applied fermentation. And I was pretty good at it because I still have all my fingers so it takes some skill set.

So, that was the beginning. After that, obviously, I evolved to more serious chemistry studies. So, I was a part of sort of internship programs that allowed middle and high school students to be exposed to their research. So, I got my first paper published when I was still in high school.

I joined the first materials science department in Russia, and I ended up being the second generation of the students there. So, nobody at that time knew what materials science is, but the idea was to build the program based on the combination of solid-state chemistry, electrochemistry, solid-state physics, and mechanics. So, that was six years with some interesting detours to spend half a year as the visiting student at POSTECH [Pohang University of Science and Technology], South Korea.

And the interesting thing about the place where I was is that the research was emphasized from the first year in the undergraduate. So, in some sense, I'm about 48 now, so I probably spend more than 30 years in the lab with the hands-on chemical research. And another interesting part, thing about this program was there was a very heavy emphasis on mathematics. Once you start with the background which spans mathematical sciences and materials science, kind of 20 years in the future, working on machine learning in materials sciences is obvious."

McDonald: "It really is interesting to see how something you might not appreciate when you first learned it comes back around and it's really able to help you greatly when you enter fields and new topics of discovery."

Kalinin: "Absolutely. So, this is the part which I cannot overemphasize because it's in some sense a story of many scientific projects that I had in my life, where something that I learned long time ago allowed to provide the somewhat unusual perspective on the observations in the lab 20 years later. And, you know, there isin the old physics community, there is a joke about the person who finally was able to solve the problem that his advisor gave him for the master thesis but only did it 20 years later.

So interestingly, something like this actually happened to me. So when I started as the first-year undergraduate in Moscow State, our department head was professor [Yuri Dmitrievich] Tretyakov. So full member of the Russian Academy of Science, very visionary person, from at least some perspectives. And his idea was to discover the signatures of chaos and fractals in the solid-state reactions. So when I was a first-year undergraduate, basically I was one of the people who was given this project, and I obviously took it very seriously, right? If the full member of academia gives you this type of problem, you take it seriously, especially if it is the boss of your boss's boss and also your department head. So it's not really a choice.

Then I spent something like two years trying to dig into that, understand what the fractals are, how they're related to chaotic phenomena. And then I came to conclusion that the way that we do solid state reactions, we don't have a chance to observe it. And the reason for that is the system is too complex, too dissipative, so it's not going to happen. That was disappointing. I wrote a few papers about some theoretical models that we made, but generally it was clear that from the big picture perspective, this is dead end.

And interestingly, maybe 15 years ago, so 20 years after we had this first foray in the chaotic phenomena, at the time when I was running the scanning probe microscopy program at Oak Ridge Center for Nanophase Materials, we had a user come in from Russia who was exploring the polarization switching on the lithium niobate. So very simple experiment when you have the scanning probe microscopy tip, you touch the surface of your sample, you apply the bias, and then you form a ferroelectric domain.

And then he told me, 'Hey, I tried to run this experiment, just trying to place the domains close to each other to see how close they can be before they start merging. And I saw a very interesting phenomena that somehow two domains form and the third domains would not form.' Imagine that you're writing a chain of the domains but somehow only first or second would be written and every third one will disappear.

And then I remembered the paper which I read 15 years prior to that, which said that the period three periodicity is a signature of the onset of the chaotic phenomena. And then I told him, 'Look, I think we are up to something very interesting. How about we experiment with this and this and this parameters?' And that was essentially the fastest *Nature* physics paper in my life, because we literally have the experiment which showed the chaotic phenomenon, essentially a solid-state reaction, and we just saw it as the part of the routine experiment from the totally different area."

McDonald: "This story that you gave us is the perfect example of how you can just pull from previous knowledge to solve the current problems."

(music)

SECTION 2

McDonald: "It sounds like it's very experiment heavy, some of the research that you've been doing. And some of these discoveries that you made with the experiments was made possible through imaging, such as the scanning probe microscopy that you specialize in. So, how does this microscopy technique work, and what makes it unique?"

Kalinin: “It’s actually a very, very simple concept. So, imagine that you have a flexible cantilever. So, for simplicity, you can even use the example of the ruler or something like this. And then there is a sharp tip on the end of this cantilever. So once you touch the surface, there is a mechanical force exerted on the end of the cantilever, and then the cantilever deflects. So, you just need to somehow measure the small deflection, but we can do that by having the laser beam, which is reflected off the cantilever and then goes in the photodetector. So, even small bending of the cantilever results in the strong shift of the laser beam. And the longer is your beam path, the stronger is the deflection.

That being said, sensitivity by itself is not enough because you can be very sensitive, but if you cannot differentiate the sources of the useful signals, it’s not going to be particularly useful. So the trick is to come up with the ways to ask the questions to your system. So, to send specially modulated waveforms to the cantilever and then detect the answers. And once you learn how to do that, you can actually separate electrical, topographic, magnetic, and other forces acting on the probe.

So, there are of course a lot of tricks to that, and a lot of instrumentation development, but the basic principle is super easy.”

McDonald: “When did you first become exposed to scanning probe microscopy during your research journey?”

Kalinin: “So, the first time I learned that the scanning probe microscopy exists when I was a visiting student in POSTECH, in South Korea. So that was ’96. So I came there for half a year. It was an interesting experience. I ended up spending a lot of time looking at the microscope, but I never get to run it because the lab was only setting up.

But that was the time when there was a library, and essentially I probably wrote most, or at least a very big fraction of the papers on the scanning probe microscopy that were written by that time. So given that it was ’96, there was not that much, but quite a few were already in place. And after that I decided that SPM is definitely something worth looking into because that’s a unique technique that allows us to explore the functionality of materials on the nanoscale.

I got lucky a second time that I got accepted at UPenn to work in professor Dawn Bonnell group, who was an expert in scanning tunneling microscopy. And I ended up being fairly early on independent. So basically, four years of my research as the graduate student at Penn was working with the SPM being able to explore new configurations and new materials. And just as an additional incentive, so imagine somewhere in Philadelphia, right? So it can be pretty hot and humid outside. So if you rent an apartment, there is no air condition. If you’re in the lab, there is an air condition. So there was a fairly strong incentive to spend weekends in front of the microscope.”

McDonald: “That is a very good reason to spend weekends at the lab. So, how was it that you came to be at Oak Ridge after your graduate studies?”

Kalinin: “At the time when I was graduating and looking for positions, I had a two-body problem. So, we look for a location where I can continue my journey with the scanning probe microscopy. My wife at that time was interested in the electron microscopy. So Oak Ridge was providing the most compelling offer, and there were people at Oak Ridge, the late Ward Plummer, who basically kind of hired me to join Oak Ridge as the [Eugene] Wigner fellow.”

McDonald: “And once you got to Oak Ridge, I know that you helped pioneer some new techniques within the field of scanning probe microscopy. So since we know kind of the basics of how this technique works, what does some of the new techniques that you were able to develop to expand on the basic technique?”

Kalinin: “There were several aspects to that. So, one aspect was the development of the ways to modulate your probe. So, before we started at Oak Ridge, there were two primary paradigms in the detection and scanning probe. One is so-called the contact mode SPM, when the tip just moves along the surface and we measure the static deflection. Another was the modulated techniques, like typing mode and some versions of Kelvin probe microscopy, magnetic force microscopy, and so on. So in those modes, the cantilever is excited somehow, either through the electrical signal or magnetic signal or through the piezo driving the cantilever. And while we are doing that, we measure the cantilever phase and amplitude of the cantilever oscillations.

So, the problem with the sinusoidal excitation modes, so all of them that are out there, is that it is essentially looking at the world through just one wavelength. So it’s almost like having only grayscale vision. Practically, if we want to understand the details of the cantilever interaction with the surface, we need to understand the behavior over some interval of the wavelengths or frequencies.

So, the first technique that we worked on in 2006 was the modification of the scanning probe microscopy engine, where we excited what we call the band excitation, when we excite our system by the multiple frequencies at the same time rather than one frequency at once. Ten years later, we extended it to the full capture of the signal. So we no longer rely on the Fourier transform; we just collect all the signal generated by the probe.

So, the interesting aspect of this band excitation method was that it made scanning probe microscopy quantitative. And that was a big thing because if the technique is qualitative or have some imaging artifacts, then we can get it to make beautiful images, but these images are not giving us high-veracity information. If you want to do solid science, you better get solid numbers. So, band excitation allowed us to get the solid numbers. And then with that in place, we were able to extend the SPM into the broad family of the multifrequency and the multidimensional spectroscopic methods that allowed us to explore things like polarization dynamics on the atomic level, electrochemical reactions on the nanometer skill levels, and so on and so forth.”

McDonald: “I think what your story really helps demonstrate is that all of these techniques for imaging or characterizing materials, we often see as tools to get to product or material development. But the tools themselves and the techniques themselves, they aren’t just static objects that you use to do things to materials, they are objects that you can improve and make better and open up new functionalities for as well.”

Kalinin: “Absolutely. And now is actually the golden time for scanning probe microscopy from one very simple perspective. So, microscopy is done to solve some specific real-world problem. Very often there is a considerable gap between the community that defines the problem and microscopists trying to solve it, but the real outcomes can be achieved only when those two work hand in hand.

The second important thing about any technique is what are the downstream applications? So if I image this object, am I just going to write another paper or is it going to affect the field in a more meaningful fashion? And we know the examples of the field where open data make a big impact. So, anything from proteins to genetics to astronomy to high-energy physics. So in all those cases, if you determine the structure of the new material, you deposit the results of the structural analysis in the crystallographic database. It means that people in the future are going to use it, and that’s how the added value is created.

So for microscopy, until very recently, this was not the case. So we explore some material or some system using the microscopy, we get images. But generally, this is the last thing we do. So in some sense, microscopy is often the most downstream analysis technique.

But, I think that now the situation is changing because if you look around, there is a progressive interest into the rapid discovery of the new materials, right? Using machine learning to predict them, using the automated synthesis, high-throughput fabrication, combinatorial libraries to synthesize them. But it’s not enough to predict and even it is not enough to synthesize. So for materials to be useful, we actually need to close the characterization loop. So we need to find out whether the materials really have the structure that we predicted. And most importantly, we need to find out whether the material really has the properties that we’re interested in.

And now we can talk about what is necessary to close this characterization loop in the automated synthesis. So first of all, we want to be able to characterize very small volumes of materials because if we have 10,000 new materials character synthesized, we definitely want to synthesize them on microgram level but maybe not at the gram level, otherwise it would be too much. The second thing, we want to be able to characterize the materials fast. Again, because if we have 10,000 samples, we probably don’t want to spend a minute per sample because then it becomes forever.

And if you’ll take these two requirements together, so to do things in the small volumes and to do things fast, scanning probe microscopy is a natural technique to actually allow us to do that. We of course need it to be quantitative and be able to give us the data on the true materials properties rather than topography or something else, but that’s exactly why we have quantitative SPMs.”

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BREAK

McDonald: “The Basic Science Division of The American Ceramic Society is dedicated to the development of ceramic science underlying present and future applications of ceramics. The Division co-organizes the Electronic Materials and Applications meeting and also organizes symposia at the ACerS Annual Meeting at MS&T. Learn more about the Basic Science Division at www.ceramics.org/basic-science-division.”

SECTION 3

McDonald: “I think that Oak Ridge helps really to recognize this importance of, as you phrased it, closing the characterization loop and the rising importance of microscopy by establishing the Institute for Functional Imaging of Materials. So, can you tell us a little bit about how you came to be the inaugural director of this Institute?”

Kalinin: “So, Institute for Functional Imaging of Materials, or IFIM, was formed in 2014. This system of institutes was to create a relatively short-term, so five years, program with very clear sunset conditions. So, if you are successful then it would be sunset, and obviously if you’re not successful, it will be sunset.

So, the idea of IFIM was to try to build a bridge between the imaging method, so scanning probe microscopy, electron microscopy, mass spectrometric imaging, and so on, and machine learning. So that was the mission, and as far as things go in the world, we were probably one of the first people to start to work in this direction because the big inflection point about machine learning, when the deep learning appeared was about 2012.

Actually, we started to get into the machine learning before the Institute as a way to respond to the real-world challenges of generating large-dimensional datasets on SPM. So, as I mentioned in 2006, we started to work on the band excitation SPM, which generated three-dimensional datasets. Once we started to combine band excitation with the complex spectroscopies, it has become common for our lab to generate four- and five-dimensional datasets. And once you have these volumes of data, you need methods that are capable to analyze that.

So, the general principle that if you have the large volumes of data, the best way to analyze it, if you have the physical models that allow you to get the physics-based insights. However, in scanning probe microscopy, very often we don’t know the physical models and sometimes we don’t even known them even approximately. So, we realized that if we want to continue this pathway, we need to find ways to take the large dimensional data set and start with at least representing them in the form that the human can understand, meaning the two-dimensional images. And in the year 2006, there were techniques that at that time were called multivariate statistics. So now it’s a part of machine learning family. At that time, it was complex statistical methods. So, we started to work with the things like principal component analysis, nonnegative matrix factorization.

So very early, once you start to dig into these areas, we discovered the existence of the neural networks. I mean at that time, of course, it was not deep networks, it was the fairly shallow networks. But it was already very interesting experience, and particularly the machine learning methods offered a very, very tempting value proposition. They basically said that if you have the examples of your cause and effect or feature target, whatever, you can train the network using these examples and then you would be able to apply this network for the new data.

So, we started with the neural networks and machine learning long before it has become popular. The Imaging Institute basically put it under one umbrella and the focus was to build the connection between the imaging tools available at Oak Ridge at that time and the high-performance computing.

That, by the way, is kind of super difficult because when we talk about machine learning, we almost always have in mind the large volumes of data, right? So it's almost synonymous with big data. The problem is that we can have big data in the areas which are mature. So, for example, we have big data about the cats on the internet. However, when we do science, we almost by definition try to go where no one has gone before and do something new and unusual. So, new things by definition means that we don't have big data. We may have a lot of data, but it's not big data; it's high-dimensional data.

The second problem is that once we do physical sciences, we very often understand the causative chain: this is the cause, this is the effect. We have some hypotheses, we have some prior knowledge. So machine learning, or vast majority of machine learning algorithms are not causal. So you have features and targets, but you can flip targets and features and it still a legitimate machine learning problem. So as the result, the best majority of the machine learning methods that rely on big data can be useful under certain scenarios, but they're no substitute for the human intuition, decisionmaking, and generally planning. So they can help, but they cannot take over the human role for the time being.

And the most important thing is that just living the life, we implicitly or explicitly try to change certain target that we believe is important, right? And therefore, we make tens and thousands of small and big decisions. And we don't necessarily know how these decisions are going to play out, but we have some big picture in mind where we want this decision to bring us.

So, the thing is that machine learning algorithms, they can make decisions, but the goals that they try to change through these decisions have to be defined by the human. So ML agents, at least for the time being, don't have their own goals. They try to change the goals that we communicate to them. And that's not that easy because if the goal is very well defined, for example, win the chess game by playing by the rules, that's reasonable. Solve the global warming problem, that's not reasonable."

McDonald: “I think these provide some really great clarifications for our listeners on the limits and benefits and things to keep in mind when working with these advanced computer systems. And I know you also recently talked about some of these topics in your April course through the ACerS Online Learning Center with automated experiments and materials synthesis and characterization. So can you tell us a little bit how you came to teach this course for the Online Learning Center and the things that you talked about in that course?”

Kalinin: “Absolutely. So for the last five years, my research effort was focused primarily on the automated experiment. And I realized that in order to be able to run that automated experiment, you need to bring two types of experience to the table. So, one experience is the classical ML experience. So, you just need to understand certain foundational concepts in ML and be able to apply them to new problems. And the only way to do it is through the hands-on experimentation. So, ML is the field where purely theoretical knowledge is absolutely not enough. So, you learn only by doing.

But then there is a second part of this, and the second part is the domain expertise. So in other words, if you are familiar with the mathematics and coding, but you don’t know how these concepts can be applied in the real-world environment on the electron microscope, scanning probe microscope, materials synthesis, making the connection is not terribly easy. So you need to speak both languages.

So since I’ve been on both parts of this device, I felt that I can bring value back to the community by sharing this experience. Of course, you are not going to become an expert after participating in the course, but at least you will know what matters, what doesn’t matter, and sort of have the way charted that says, ‘Start here, go through the set of examples, these are the key concept that you need to understand.’ Once you get into that, you will be able to go to the lab and take advantage of this method.”

McDonald: “I know that you’re also planning to teach another course through the Online Learning Center later this year, so can you give us a little bit of a preview of what that course is going to cover?”

Kalinin: “So, we still need to define the exact time scale, but one of the things that fascinated me for 25 years is the applications of scanning probe microscopy for materials characterization. Many of these topics have been around for maybe 10–20 years. But I think that we are now at the inflection point when the scanning probe microscopy stops being a purely discovery sense but becomes a field that has strong downstream applications for materials discovery and optimization.

That basically means that it makes sense to kind of bring up what are the things that enable these SPM applications. What does it take to make SPM signal quantitative? Because if it is not quantitative, then it is much less useful. Basically share my 25-year experience in the SPM for transport and ferroelectric and electrochemical characterization with the community.”

McDonald: "I know our listeners are going to be excited and have to keep their eye out for when this course comes. And we're so thankful that you chose The American Ceramic Society to share your expertise through our platforms."

(music)

CONCLUSION

McDonald: "The advancement of data-driven research methods and models makes this an exciting time to be a materials scientist. We just need to be sure to support educational initiatives that train the next generation of scientists to take advantage of these techniques.

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 Sergei Kalinin 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."