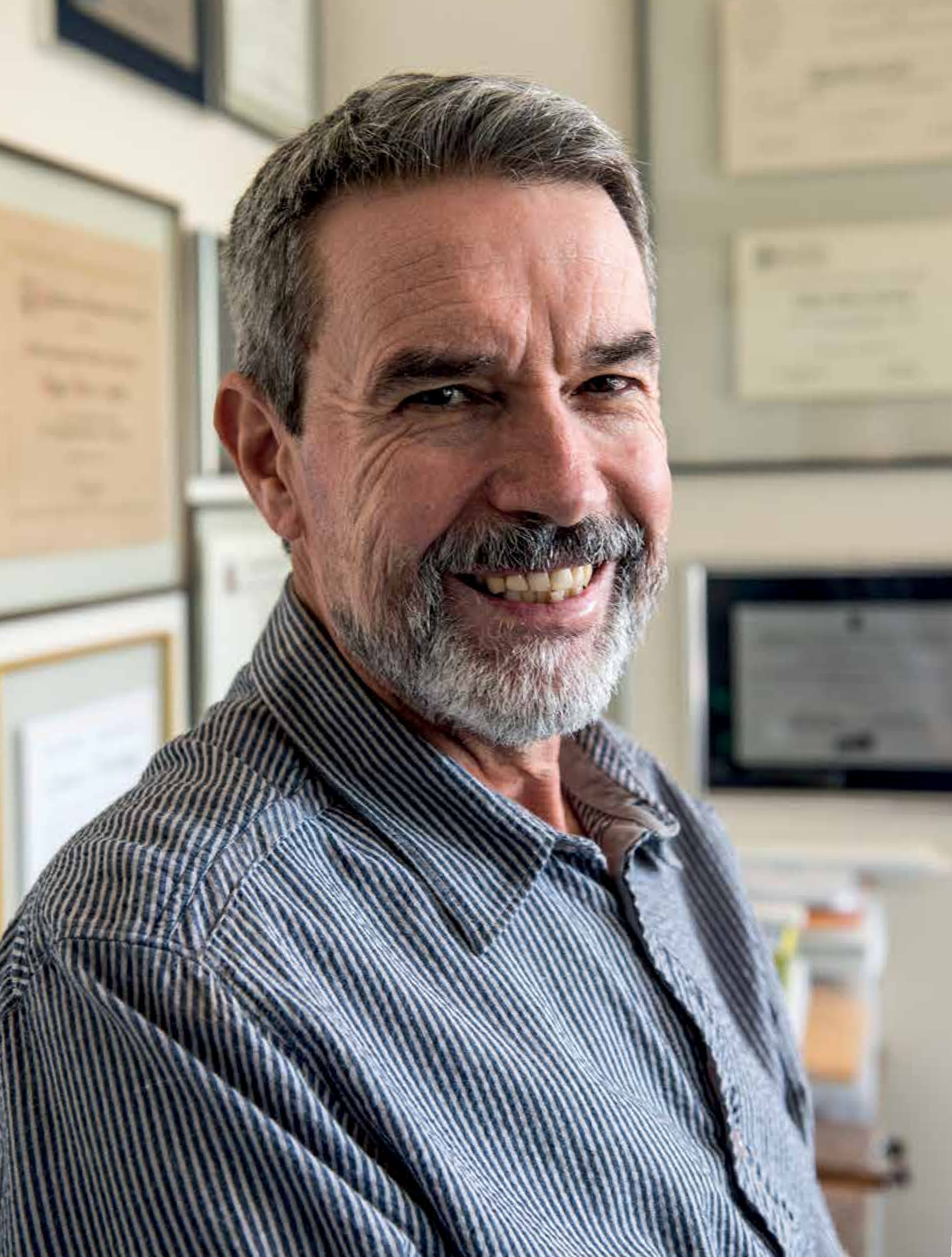

One eye on science, **the other on industry**

An engineer provides insight into how artificial intelligence will help develop novel types of glass and explains his new definition of the material

Neldson Marcolin

PORTRAIT Eduardo Cesar | Published in July 2018

AGE 64

SPECIALTY
Materials science / Glass

INSTITUTION
Federal University of São Carlos (UFSCar)

EDUCATION
Bachelor's degree in Materials Engineering from UFSCar (1976), MSc in Physics from IFSC-USP (1978), PhD in Glass Science and Technology from Sheffield University, UK (1981)

SCIENTIFIC PRODUCTION
3 books, 20 book chapters, 250 articles, and 20 patents

The engineer Edgar Dutra Zanotto likes to cite one of his favorite science articles to show how glass is important to science. "Glass is the eye of science," he says, alluding to the title of a paper ("Glass: The eye of science") by Marvin Bolt, curator of science and technology at the Corning Museum of Glass in New York. In his paper, published in February 2017 in the *International Journal of Applied Glass Science*, Bolt argues that the most important tools in the scientific revolution of the seventeenth century were the microscope and the telescope—both of which have glass lenses as primary components.

When he took an interest in the field in the mid-1970s, Zanotto had not yet come to this realization, but found the subject to be both interesting and under-researched in Brazil. Zanotto earned a degree in materials engineering from the Federal University of São Carlos (UFSCar) in 1976, but it was at the São Carlos Institute of Physics at the University of São Paulo (USP) and at the University of Sheffield in the UK—where he pursued his Master's degree and PhD, respectively – that the then young researcher was exposed to the field that would define his career.

One thing that has marked Zanotto's career is his concurrent interest in both basic and applied science. "I've always worked with one foot in each," he says. His training in both physics and engineering enables him to formulate and test scientific hypotheses and develop special types of glass for use in industry and that has special functionality for use in the human body, such as bioactive glass.

Zanotto was born in Botucatu, São Paulo and was a professor at UFSCar for 42 years. The engineer previously served as a visiting professor at universities in Europe and the US and as a science consultant for companies in Brazil and abroad. He also served as an assistant coordinator of the Scientific Directorate at FAPESP. Since 2013, Zanotto has headed the Center for Research, Education, and Innovation in Vitreous Materials (CeRTEV), one of the 17 Research, Innovation, and Dissemination Centers (RIDC) funded by FAPESP that brings together researchers from UFSCar, USP, and São Paulo State University (UNESP). He is also chairman of the Scientific Advisory Board at Serrapilheira, in Rio de Janeiro. His experience at these organizations has equipped him to actively engage in science outreach.

In the following interview, Zanotto, who is married and is the father of two daughters, discusses his most recent work and a bold proposition published in 2017 describing a new state of matter—the glassy state.

"If our strategy works, we will be able to create novel types of glass in much less time

Could you describe your latest research on the development of artificial intelligence for time savings in the laboratory?
Our focus is on prediction. Science is almost 100% about understanding and describing natural phenomena. Whenever we understand and describe something new, we can publish a paper about it. Making predictions beforehand would be ideal, but is very difficult. If we can accurately predict a phenomenon or trend, we will not have to devote enormous amounts of time, financial resources, and energy to a large number of experiments. We are currently working with students and postdocs—professors Pedro Rino and André Moura from UFSCar and André Ponce de Leon from CeMEAI [Center for Research in Mathematical Sciences Applied to Industry, an RIDC based at USP in São Carlos]—on a computational model to predict phenomena related to the structure, dynamic processes, and properties of glass. If successful, we will be able to create novel types of glass in a significantly reduced length of time. The first two papers are now being drafted and are in the adjustment phase. A postdoc from our group, Daniel Cassar, compiled approximately 55,000 glass transition temperature data points to begin this study.

What is the research about?
Glass is a rigid material made of multiple reactants that are typically melted and rapidly cooled to prevent crystallization. As a result, the atoms get trapped in a state of disorder, forming a temporarily frozen liquid that we call glass. In a crystalline structure, the atoms are perfectly organized, forming a solid. Crystallization is a naturally occurring process in all glasses but can take from seconds to millennia to occur depending on temperature. When heated, all types of glass undergo a phenomenon called the glass transition at Tg—the temperature at which a transformation from rigidity to a high-viscosity liquid occurs—that is dependent on the chemical composition. To develop a glass with a new functionality without spending large amounts of time and energy on experimental tests, it is helpful to know the value of Tg and other properties beforehand. With this idea in mind, Cassar scanned the literature from the last 50 years for papers describing the chemical composition and the relevant Tg of different glasses. Cassar compiled 55,000 different compositions of oxide glasses—there are currently more than 400,000 cataloged glasses. With the help of the artificial intelligence expert André Ponce de Leon, Cassar created an algorithm that was "trained" to correlate Tg with the chemical compositions of 45,000 of these glasses. We used the data for the 10,000 glasses omitted from the training stage to test the ability of the new algorithm to predict Tg values, and we compared them with the reported values to see if they were accurate. There is still room to optimize the resulting neural network, but currently, the maximum error is 6% in 90% of tests, which is good and consistent with the typical errors for the experimental data. With this software, we will be able to predict the Tg of any putative oxide glass. The same logic can be applied to predicting other physicochemical properties of glass.

How will this program save time?
In 2004, I published an article with Chico Coutinho [physicist Francisco Bezerra Coutinho from the USP School of Medicine] in which we calculated how many glass compositions would be possible using 80 "friendly" chemical elements. We used 1% composition increments to combine those elements in different ways. In this prediction exercise, we found that it would be possible to obtain 10^{52} types of glass—an astronomical figure. The 400,000—or 4×10^5—inorganic glasses known today represent only a tiny fraction of that number. We would require an infinite amount of time and resources to produce 10^{52} different types of glass, which is simply impractical. The solution is to perform computational simulations until we find interesting formulas that could have unusual properties. Then, we can go to the lab to test each composition and see if it really delivers the properties that the software predicted.

Last year you proposed a new state of matter—the glassy state—something that is neither a solid nor a liquid. If it is neither of these, what is it then?
I will begin by answering another question: what is the difference between information and knowledge? We begin with one piece of information, then find another, then another; information accumulates over time. By joining and connecting the different pieces of information, we

PERSONAL ARCHIVE

The physicists Robert Weeks, Phillipe Bray, and Nevil Mott (a 1977 Nobel Prize winner) with Zanotto, who had just been handed a Zachariasen Award from JNCS, and engineer David Pye in 1990 *(left to right)*

gain knowledge. It has taken 40 years of studies and research to gather insight, reflect on it, and then write the article on the glassy state, published in the *Journal of Non-Crystalline Solids [JNCS]*.

What are the pieces in the information puzzle?

The first is the atomic structure of glass, which is the same as that of the liquid from which it derives. Glass is a frozen liquid that is temporarily in a noncrystalline state. Next comes the concept of structural relaxation—a spontaneous and partial rearrangement of the molecules in the material—and finally crystallization, when all the atoms and molecules are aligned in a well-defined, three-dimensional structure. This transition happens with all glasses, which will all eventually crystallize over longer or shorter lengths of time. How long? At relatively high temperatures, the change takes just a few hours. At room temperature, the amount of time is very difficult to precisely determine, and we need to perform calculations and simulations. The new definition of glass proposed in our 2017 paper states that the molecular structure of glass is the same as that of the mother liquid, with the atoms frozen in the same position, and is very different from that of a crystal. Over time, glass spontaneously relaxes until it crystallizes. At a temperature close to Tg, glass crystallizes in a matter of minutes or hours; at low temperatures, glass takes much longer to crystallize.

Were these concepts already known?

Researchers in the field have long been considering these concepts, but no one had put it all together like John Mauro [of Pennsylvania State University] and I did. I wrote the first draft of the article, and Mauro joined me later. We combined different information and clarified the nature of glass.

How did this collaboration develop?

I presented these ideas during the Society of Glass Technology (SGT) Centenary Conference in Sheffield in September 2016. The Indian-American professor Arun Varshneya from Alfred University, a well-known "glass guru" and a long-time friend of mine, said straight away: "I do not agree with this package; we need to discuss it." We had a lengthy discussion in Sheffield, and when I returned to Brazil, I decided to write a draft. I sent it to Varshneya, who invited a cousin of his, Prabhat Gupta, a very good theorist from Ohio State University, into the discussion. Varshneya also invited John Mauro, who had been his brightest doctoral student; Mauro was one of the inventors of Gorilla Glass, a special glass for smartphones. After exchanging a dozen emails with these researchers, I invited them to participate as coauthors, but they never responded. I thought the lack of response meant they disagreed with my proposition. That was in October 2016. In December, I was touching up the manuscript when John Mauro sent me a Christmas message and asked me what had become of the article. I replied that it was almost finished, but that I was the sole author as they had not shown interest in joining me. He immediately replied that he was still interested. Between Christmas and New Year, we each took turns spending a day working on the paper until it was finished and submitted for publication. As of a few weeks ago, the paper had already received more than 7,000 views. That is many views for a paper in a small subfield of materials science. To give a quantitative idea of how large that number really is, the JNCS website has 26,000 articles, and all are available to download. From publication to date [6/24/2018], our paper has outranked all these articles in downloads.

How large is the glass research community?

Estimates indicate that there are approximately 3,000 glass researchers globally and only 100 to 120 in Brazil who publish regularly in this field. Of these, 14 professors and 60 students and postdocs are at CeRTEV. Outside Brazil, there are companies with many more researchers, but in an academic setting, there are few large groups. I know of only one that is bigger than ours—a very large group in Rennes, France. In China, there are possibly larger groups because they publish even more prolifically than US researchers in this field. In Japan, the US, and Europe there are typically one to three professors in each group. For these reasons, I believe our team is among the global top five. When Hellmut Eckert [a German chemist, deputy coordinator at CeRTEV, and professor at USP São Carlos] and I formed the RIDC group, the center gained greater visibility on the international scene.

Has visibility increased across both science and technology?

Yes, for both. In fundamental scientific research, we have a group that uses different techniques to characterize the structural features of glass. Structure and chemical composition are what determine the optical, mechanical, thermal, magnetic, chemical, and biological properties of glass. This group also does research on dynamic processes, the mechanisms at play when glass is heated—the atoms begin to move, relax, melt, or crystallize. Crystallization is the area in which I am most actively involved. We study both structure and dynamic processes, and the two subjects combined determine a given glass's properties and potential applications, which are divided into five categories at RIDC: mechanical properties, which we research to develop

Bioactive glass ceramics: an eye implant (*left*) and middle-ear ossicles

EDUARDO CESAR

stronger and more resistant glasses and glass ceramics, a type of material that is currently high in demand in global industry; electrical properties, such as for ionic conducting glasses, with potential applications in new and more efficient batteries; bioactive properties, for glasses made of bioactive materials for use in living organisms; optical properties, for which glass is best known and that we modulate by adding impurities to modify color, absorption, etc.; and last, materials for catalytic processes.

How is research on bioactive glass progressing?

These materials are very promising. Bioactive glass was first invented in the early 1970s with a chemical composition comprising sodium, silicon, calcium, and phosphorus. This composition gives the glass high bioactivity when in contact with body fluids. This type of glass can be used in applications that include bone regeneration, such as prostheses, dental problems, skin wounds and degeneration of nerves and cartilage. As a powder, bioactive glass functions as a kind of glue. Some of these potential applications are already in use. For example, an artificial iliac bone made of bioactive glass ceramics has been developed by Tadashi Kokubo of Chubu University, Japan, for implantation in the hip. According to Kokubo, this glass has already been used in thousands of patients. Here at UFSCar, with the help of two former students who are now professors, Oscar Peitl and Murilo Crovacce; several postdocs, notably Marina Trevellin; and students, we have created a bioactive glass ceramic material similar to the middle ear ossicles that is used as a replacement when the ossicles have been damaged as a result of a severe infection. We conducted successful clinical trials at the USP School of Medicine in Ribeirão Preto led by the physician Eduardo Tanaka Massuda, but further testing is needed to receive approval from Anvisa [Brazilian Health Regulatory Agency]. This [Zanotto shows a specimen] is another example: it is an artificial eye made of a patented bioactive material. Once implanted, the eye attaches to the nerves in the ocular cavity, so it moves naturally in tandem with the good eye. We conducted successful clinical trials at the Botucatu campus of the UNESP School of Medicine led by Silvana Schellini and Simoni Milani Brandão. But again, we need to continue testing.

You publish in the Journal of Non-Crystalline Solids, of which you are also an editor. Doesn't this create a conflict of interest?

I began working as an editor in 2010, but I had already published approximately 70 articles in the journal before then. This journal is my favorite journal because it was established 50 years ago, because it is highly rigorous—it rejects 2/3 of submissions, with an average response time of only six weeks—and especially because it is read and highly respected by the global glass research community. When I was invited, I replied to the Elsevier publisher Karine Van Wetering that I would agree to be an editor only if I could continue to publish in the paper. She replied that there would not be a problem as there would be three editors. My papers would be submitted to ad hoc peer reviewers without my knowing who they were. She wanted me and the other editors to continue publishing there because that would send a message to readers that the editors value the journal they edit.

What made you first take an interest in glass?

I graduated from the third materials engineering class at UFSCar, which created the program—the first in its field in Latin America—in 1970. At the time, there were few professors available in the field, so UFSCar invited visiting professors. The visiting professors came from USP and UNICAMP, and many came from abroad. One of these professors, Osgood James Whittemore [1919–2010] from the University of Washington, invited me to work on a scientific initiation project. The project was an experimental study on the chemical durability of candidate glasses for the encapsulation of radioactive waste. The purpose of the project was to collect waste from nuclear power plants, add reagents, melt everything, and cool it down quickly, forming a large block of glass. The resulting monolith is compact and impermeable and is intended to be buried in an abandoned coal mine many meters underground, encapsulated and separated well from the surface environment, without contaminating the air and groundwater. This method is still in use today. I then began to do research on glass. I picked up books from the library and started reading papers. I was keenly interested. It was also an opportunity to practice my English. These interests landed me a job as an assistant lecturer in the Department of Materials Engineering [DEMa] at UFSCar.

Was that the only reason you were hired at the age of 22?

I was a dedicated student, spoke English, and was performing research on glass. DEMa needed professors in this field, and there were no specialists available. Because I only had an undergraduate degree, I was given an ultimatum from the head of the department, Dyonísio Garcia Pinatti [1946–1986]: "You have two years to get a Master's degree in any subject related to glass, then study abroad for a PhD, then return to head our glass research group." Fortunately, the only researcher doing glass research in Brazil at the time was Aldo Craievich from the Physics department at USP in São Carlos. I owe much of my scientific training to having completed my Master's degree in physics under him. Craievich then recommended me to an acquaintance of his, the famous physicist Peter James [1940–2005] of the University of Sheffield. I was awarded a grant from CAPES [Brazilian Federal Agency for Support and Evaluation of Graduate Education] and went to do my doctorate under Peter from 1979 to 1982. Sheffield had the largest glass research team in the world at that time. The experience was extremely valuable for my training.

In what way does your group collaborate with companies?
At all levels. We might make an interesting discovery and then prospect for companies potentially interested in conducting pilot-scale trials and licensing the invention. Companies might approach us instead. For example, we helped to perfect this material [Zanotto produces a 1 cm2 piece of glass and illuminates it with a laser], which diffracts light. This material has nanometer-sized crystals inside that are spaced one visible-light wavelength apart or approximately 400 nanometers from each other. This is the only material in the world that can be used for high-power laser diffraction gratings. There is a crystal hologram in here. Any high-power system, such as an industrial laser machine, requires several parts like this inside. There are only three companies in the world that produce this material. This tiny part costs US$5,000. The product was already available in the market, and I helped to optimize it. The material was invented at Corning and was then improved and produced by Optigrate at a facility in Orlando, Florida. I spent 10 months there in 2005, on invitation, while taking a sabbatical at the University of Central Florida. Their material performed very poorly; the material was unfit to market because it scattered too much light. Optigrate agreed to allow me to publish certain articles during the course of the collaboration, which is not customary, as companies typically require us to sign a nondisclosure agreement.

You have recorded many of your lectures about glass. Why?
I produce two types of videos: formal lectures and science outreach videos. I record all of my lectures and publish them on the internet. The results have been fantastic. If a student misses a class, the student can just watch the video. If students need to study for a test, the lectures are readily available. We also produce 1- to 5-minute educational videos explaining concepts and experiments with glass, and we have science-themed manga in print and on the CeRTEV webpage. We began to do science outreach due to requirements placed on RIDC. It has been pleasurable as well as a learning experience.

> “I record all of my classes and publish them on the internet. If a student misses a class, they can just watch the video

Serrapilheira, of which you are a member, shares the same interests, doesn't it?
The institute's founders and sponsors, Branca and João Moreira Salles; the Board of Trustees; and the Science and Administration boards all expect researchers and grant holders to engage in science outreach if they have the desire and the skills to do so. This year the institute launched a public call for proposals for its first science outreach support program, called Camp Serrapilheira, to train facilitators and to identify and select outreach projects to be funded.

Do you think the institute can make a difference in funding science?
Yes. Serrapilheira is currently working to organize research groups led by promising young researchers who demonstrate potential for high-level research in relevant fields at the cutting edge of knowledge. An estimated R$16–18 million will be invested annually. The grant model is a dream for researchers as it is much more flexible than that at any public research institution. The project selection system is rigorous, but successful candidates can use their grant money toward any research-related costs, such as hiring other researchers, buying equipment and materials, engaging services, and traveling on research-related business. These researchers can do so without having to resubmit resumes, subproject proposals, cost estimates, or price quotes for review. Moreover, the laborious stage of project accounting is handled by a foundation, not by researchers. We provide full flexibility because we trust researchers and want them to devote most of their time to research, not to project management. This model is in contrast to public agencies, which typically demonstrate mistrust of researchers. For example, I have 42 years of research experience, I am head of a RIDC, and I am a member of the ABC [Brazilian Academy of Science], but when I apply for a scientific initiation grant from any government agency, I have to write a project proposal, submit an updated resume, and submit resumes for my students. There is a large painstaking bureaucracy. At Serrapilheira, we trust our researchers and give them greater freedom.

You like to say you "believe in old-school researchers." Why?
"Old-school" researchers would dedicate 20, 30, 40 or even 50 years not only to collecting data but also—and especially—to connecting all the data to create knowledge. Of course, there are bright young scientists who can make the necessary connections in less time. I have discussed this several times with Fernando Reinach, a biologist and fellow member of the Board of Trustees at Serrapilheira. Reinach is among those who think that only young researchers have a future. I disagree. I believe that senior researchers who are active and remain motivated in tackling the day-to-day challenges of doing research, designing and conducting experiments, testing hypotheses, creating theoretical models, attending conferences, mentoring, publishing, teaching and learning—and receiving criticism—can continually improve. The quality of my current research is better than that of my earlier research 10 and 15 years ago. I hope to continue making progress in the coming decades. ■