Advanced Photon Source upgrade will transform the world of scientific research

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Senior Research Associate Tim Graber tests a monochromator designed for use with the upgraded APS. The monochromator is now operating at the 2-ID beamline. Credit: Rick Fenner / Argonne National Laborator

From chemistry to materials science to COVID-19 research, the APS is one of the most productive X-ray light sources in the world. An upgrade will make it a global leader among the next generation of light sources, opening new frontiers in science.

In the almost 25 years since the Advanced Photon Source (APS), a U.S. Department of Energy (DOE) Office of Science User Facility, first opened at DOE's Argonne National Laboratory, it has played an essential role in some of the most pivotal discoveries and advancements in science.

More than 5,000 researchers from around the world conduct experiments at the APS every year, and their work has, among many other notable successes, paved the way for better renewable batteries; resulted in the development of numerous new drugs; and helped to make vehicles more efficient, infrastructure materials stronger and electronics more powerful.

Research conducted at the APS has also directly led to two Nobel Prizes, and contributed to a third. Most recently, the APS is making significant contributions in the fight against COVID-19. Its beamlines are involved in research to both identify the protein structures of the virus and find potential pharmaceutical treatments and/or vaccines. Such work makes clear the ongoing importance of X-ray light sources, like the APS, in solving critical problems for our world.

Yet while the APS is still one of the preeminent research facilities of its kind, the electron storage ring that is at its heart was designed beginning in the late 1980s and, as groundbreaking as it was at the time, now relies on dated technology.

"After 25 years, the challenge is how do we continue to make the APS an interesting and useful place for researchers?" asked Jim Kerby, chief project officer for the APS Upgrade (APS-U), who came to Argonne to help answer that question. "How do we create a facility that continues to provide opportunities for work that can't be done anywhere else?"

As the APS readies to undergo an $815 million upgrade that will, as early as late-2023, enable science at a completely new and unprecedented scale, the APS team at Argonne and the thousands of researchers it supports are excitedly looking ahead—even if nobody can completely know the full range of scientific opportunities that await.

"The APS Upgrade will allow us to conduct new experiments that we can barely even imagine right now. It will be transformational," said Jonathan Lang, the APS X-ray Science Division (XSD) director.

"From Usain Bolt to an F-15"

The APS works like a giant X-ray microscope. It produces extremely bright X-rays that can peer through dense materials and illuminate the
structure and chemistry of matter at the molecular and atomic level. As part of the upgrade, the existing 1.1-kilometer circular storage ring will be replaced and X-ray beamlines and other equipment will be updated, creating a vastly more powerful X-ray facility and brighter X-ray production.

The brightness of the X-rays will be up to 500 times greater than the current machine, said Kerby, and will significantly improve performance.

"That's hard for anyone to really imagine," Kerby said. "It's like going from Usain Bolt, a world-record holding track and field sprinter known for being one of the fastest men on Earth, to an F-15 fighter aircraft. Both are fast, but it is two very different kinds of speed. Experiments that were previously impossible to perform in a realistic amount of time will now be conducted in minutes to hours."

Another major enhancement involves beam coherence, which relates to how ordered the X-ray light is. Lang said it will go from something like a spotlight that produces a broad wash of light to something much more like a laser.

According to Stephen Streiffer, deputy laboratory director for science and technology, interim associate laboratory director for Photon Sciences, and director of the APS, coherence is especially important: "High-energy X-rays that are ultra-bright with very high coherence will allow us experiments in real environments, not just model environments."

Streiffer said it was essential that the new X-ray source enables measurements across multiple physical and time scales. "Think about exploring the electrochemistry in a battery. It goes from a nanosecond with atoms diffusing in a local environment all the way up to macroscopic changes in the battery over days, weeks or even years. With the increased brightness we will be able to look at the whole picture."

Lang pointed to another angle. "Currently, you can only see one small part of a material, and it takes a long time. With the upgrade we will get both high resolution and a broad field of view. For example, to understand mechanical properties in polycrystalline materials, you want to see how elements are distributed around grain boundaries between crystals, but you also want to see how a large number of grain boundaries compare. This will allow researchers to look at many more cells, in ways that might ultimately dramatically improve structural materials used in the automotive and aerospace industries."

With the higher brightness, Lang said, will also come an immense data load. "But we have high performance computing on campus so that's great synergy. They can crunch the numbers to handle the data. It's a unique source and resource very nearby." And with the new Aurora supercomputer set to debut in 2021, there will be even more opportunities to leverage Argonne's unparalleled resources.

Bob Hettel, the director of the APS-U project, was involved in designing the current APS while at SLAC National Accelerator Laboratory. He said it's a very exciting time for X-ray technology, particularly with advances in storage ring design, and APS has "come up with an aggressive approach that enhances and improves upon what others have been doing the last two decades."

For Hettel, the biggest challenge is that there isn't a single technical hurdle, but rather it's the integration of so many different components. "There are a
Kerby said the earliest the APS would be shut down is June 2022—but not until all the pieces of the new machine have been checked out and are ready to be assembled in the old machine’s place—with the upgraded APS coming back online about a year later. At that point, he said, users will have to completely recalibrate how they think about what scientific experiments are possible.

Changes the whole game

Conal Murray is a research staff member at the IBM Watson Research Center in New York who had his first beam time at the APS more than 20 years ago, and who has been returning almost every year since.

His current research involves strain engineering in future generation transistors. Advances in this field are important to device scaling in applications ranging from smart phones to high-performance computing, where greater transistor density can be achieved while increasing overall functionality.

"The enhanced coherence and brightness will allow us to do measurements of actual devices, not just representative structures. We could only do this with the APS Upgrade," Murray said. "But I'm just as excited about the unexpected results that will come from this upgrade. We won't know the full benefits until it's built and operating."

For Gayle Woloschak, a research scientist at Northwestern University, the APS-U will allow her to "jump ahead to the next level of what we can do. We will be able to do a rapid scan of cells, a significant number in a short time." This will vastly increase how many patients can be tracked and provide a much better understanding of what occurs during treatment.

For researchers like Stephan Hruszkewycz, in Argonne's Materials Science division, the X-rays at the APS are one of the only ways to see how materials behave under extreme conditions, which is essential to meeting a range of energy challenges. "The upgrade is a huge opportunity for materials science. With the improved characteristics and by adopting new methods, we will be able to look at materials in a state that gives us a much richer idea of how they are transforming in extreme environments."

Si Chen, a physicist in Argonne’s X-ray Science Division who works primarily with biological applications, said the APS-U will also involve major equipment enhancements. "One of the most important things is not only the upgrade itself, but all of the new instruments to use the brightness that the upgrade is going to provide."

Chen said the X-ray endstation she currently works with can study a few cells per day; using a new second-generation machine after the upgrade, this will increase to thousands of cells per day. "We will be able to collect data much faster, and that larger population will increase the confidence of the research conclusions."

She added that the new machine will allow researchers to achieve a 10 nanometer focus—which is six to eight thousand times smaller than a single human hair.

The Northeastern Collaborative Access Team (NE-
CAT) runs two beamlines at the APS, funded by the National Institutes of Health and servicing 600-700 unique users. Malcolm Capel, NE-CAT deputy director, agreed that several transitions will need to occur at once. "Our control systems are 20 years old, too. We will have new software and more documentation of our systems for users."

Laurence Lurio is chair of the physics department at Northern Illinois University whose work involves examining biological materials such as proteins and lipids. He said that the improved beam coherence will allow his research team to focus more on science than technique.

"The most exciting thing with the upgrade is that we will go from making very challenging, technique-driven measurements to something that is much easier and convenient to do. The technique has to be easy enough that you can look at the science. If you're trying too hard to make a measurement you can't look at the important applications."

Lurio added that if it weren't for the APS and the support of DOE, such innovative work would not be possible. "Coming from a mid-size university, we don't have a huge budget for research infrastructure. And that's probably true for even larger research universities. But we can all come to APS and suddenly have the best tool in the world to do an experiment. The availability of this facility changes the whole game."

On solid ground for another 25 years

The potential for future pivotal discoveries as a result of the upgrade are virtually limitless. Examples may include revolutionary systems to convert sunlight into energy and store that energy; detailed mechanisms by which pollutants move through soil; cleaner, more efficient biofuels; a transformational understanding of the structure in Earth's inner core; new drugs to treat infections resistant to antibiotics; and a better understanding of how the brain processes and stores information with neurons.

Kerby said he had no doubt that the upgrade would produce many spectacular examples of innovative science. But added, "The really important thing is not the specific examples; it's the opportunity to go in directions that people previously hadn't thought about, or had written off."

And that, said Lang, is ultimately the goal for the upgrade.

"We want to ensure the APS is relevant for another 25 years," Lang said. "In 10 to 15 years, people will start coming up with new ideas. The APS Upgrade will put Argonne on solid ground in the world for another 25 years. You can't predict the future much further out than that."

Provided by Argonne National Laboratory