The Future of PV, Batteries and More – At the Bleeding Edge

By John Benson

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1. Introduction

To the extent that you can invent a new tool like a high-resolution microscope, my sense is that you tend to be surprised by what problem it's applied to solve. People will look at things we can't even imagine now – and solve a problem we're not even sure we have yet.

-- Leslie Thompson, IBM Materials Characterization Expert

They are out there, the tools that Ms. Thompson is talking about. For instance, I was reading a recent issue of Scientific American, and read a brief article about a major breakthrough in electron ptychography (the last word is (maybe) pronounced "tie'kogræfi"). Ptychography is *a computational method of microscopic imaging. It generates images by processing many coherent interference patterns that have been scattered from an object of interest.*[1] The advancement allowed this technique to examine compounds at the atomic-scale in three-dimensions. This will greatly expand our understanding of these materials and allow engineers to better model how they will behave.

This post is about the above new tool and breakthroughs in important renewable technologies that it might hasten.

2. The Blessing & Curse of Silicon

Currently 99% of electronic devices are based on silicon, and a large majority are based on crystalline silicon. For photovoltaic (PV) cells this is mono-crystalline or "mono." Silicon is very plentiful and thus inexpensive. It is also thoroughly developed. The only significant sector in electronics that uses a silicon compound (vs. pure silicon crystals) is power electronics, which is evolving to Silicon Carbide (SiC).

There are literally hundreds of compounds out there that may be more suitable for specific electronic devices than crystalline silicon, but the latter element is well understood, and the tools to better understand other candidates have not been available.

2.1. Electron Ptychography

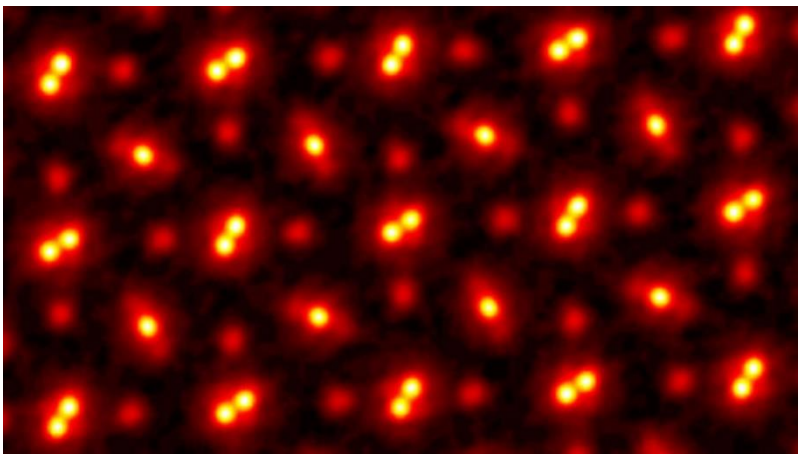
Now a team, again led by David Muller, the Samuel B. Eckert Professor of Engineering, has bested its own record by a factor of two with an electron microscope pixel array detector (EMPAD) that incorporates even more sophisticated 3D reconstruction algorithms.[2]

The resolution is so fine-tuned, the only blurring that remains is the thermal jiggling of the atoms themselves (image below).

[1] Wikipedia article on "Ptychography," https://en.wikipedia.org/wiki/Ptychography

[2] David Nutt, Cornell Chronicles, "Cornell researchers see atoms at record resolution," May 20, 2021, https://news.cornell.edu/stories/2021/05/cornell-researchers-see-atoms-record-resolution

"This doesn't just set a new record," Muller said. "It's reached a regime which is effectively going to be an ultimate limit for resolution. We basically can now figure out where the atoms are in a very easy way. This opens up a whole lot of new measurement possibilities of things we've wanted to do for a very long time. It also solves a long-standing problem – undoing the multiple scattering of the beam in the sample, which Hans Bethe laid out in 1928 – that has blocked us from doing this in the past."



This image shows an electron ptychographic reconstruction of a praseodymium orthoscandate ($PrScO_3$) crystal, zoomed in 100 million times.

Ptychography works by scanning overlapping scattering patterns from a material sample and looking for changes in the overlapping region.

"We're chasing speckle patterns that look a lot like those laser-pointer patterns that cats are equally fascinated by," Muller said. "By seeing how the pattern changes, we are able to compute the shape of the object that caused the pattern."

The detector is slightly defocused, blurring the beam, in order to capture the widest range of data possible. This data is then reconstructed via complex algorithms, resulting in an ultraprecise image with picometer (one-trillionth of a meter) precision.

"With these new algorithms, we're now able to correct for all the blurring of our microscope to the point that the largest blurring factor we have left is the fact that the atoms themselves are wobbling, because that's what happens to atoms at finite temperature," Muller said. "When we talk about temperature, what we're actually measuring is the average speed of how much the atoms are jiggling."

The researchers could possibly top their record again by using a material that consists of heavier atoms, which wobble less, or by cooling down the sample. But even at zero temperature, atoms still have quantum fluctuations, so the improvement would not be very large.

This latest form of electron ptychography will enable scientists to locate individual atoms in all three dimensions when they might be otherwise hidden using other imaging methods. Researchers will also be able to find impurity atoms in unusual configurations and image them and their vibrations, one at a time. This could be particularly helpful in imaging semiconductors, catalysts and quantum materials – including those used in quantum computing – as well as for analyzing atoms at the boundaries where materials are joined together.

The imaging method could also be applied to thick biological cells or tissues, or even the synapse connections in the brain – what Muller refers to as "connectomics on demand."

While the method is time-consuming and computationally demanding, it could be made more efficient with more powerful computers in conjunction with machine learning and faster detectors…

The above described tool will help in the quest to better understand all materials, and the team that developed this technique has opened it to other investigators to hasten this process.[3]

See the link below for important support for this mission that this group has recently received.

https://news.cornell.edu/stories/2021/05/225m-nsf-grant-accelerates-materials-discovery

3. Initial Discoveries

The team is working on several developments. These are based on the original electron ptychography discovery it made in 2018, as well as the more recent one described above.

3.1. A Quantum Development

Cornell scientists have identified a new contender when it comes to quantum materials for computing and low-temperature electronics.[4]

Using nitride-based materials, the researchers created a material structure that simultaneously exhibits superconductivity – in which electrical resistance vanishes completely – and the quantum Hall effect, which produces resistance with extreme precision when a magnetic field is applied.

"This is a beautiful marriage of the two things we know, at the microscale, that give electrons the most startling quantum properties," said Debdeep Jena, the David E. Burr Professor of Engineering in the School of Electrical and Computer Engineering and Department of Materials Science and Engineering…

The two physical properties are rarely seen simultaneously because magnetism is like kryptonite for superconducting materials, according to Jena.

"Magnetic fields destroy superconductivity, but the quantum Hall effect only shows up in semiconductors at large magnetic fields, so you're having to play with these two extremes," Jena said. "Researchers in the past few years have been trying to identify materials which show both properties with mixed success."

The research is the latest validation from the Jena-Xing Lab that nitride materials may have more to offer science than previously thought. Nitrides have traditionally been used for manufacturing LEDs and transistors for products like smartphones and home lighting, giving them a reputation as an industrial class of materials that has been overlooked for quantum computation and cryogenic electronics.

[3] David Muller's Cornell Applied Physics Research Group, see https://muller.research.engineering.cornell.edu/

[4] Syl Kacapyr, Cornell Chronicles, "Researchers create 'beautiful marriage' of quantum enemies," https://news.cornell.edu/stories/2021/02/researchers-create-beautiful-marriage-quantum-enemies

"The material itself is not as perfect as silicon, meaning it has a lot more defects," said co-author Huili Grace Xing, the William L. Quackenbush Professor of Electrical and Computer Engineering and of Materials Science and Engineering. "But because of its robustness, this material has thrown pleasant surprises to the research community more than once despite its extremely large irregularities in structure. There may be a path forward for us to truly integrate different modalities of quantum computing – computation, memory, communication."

Such integration could help to condense the size of quantum computers and other next-generation electronics, just as classical computers have shrunk from warehouse to pocket size.

"We're wondering what this sort of material platform can enable because we see that it's checking off a lot of boxes," said Jena, who added that new physical phenomena and technological applications could emerge with further research. "It has a superconductor, a semiconductor, a filter material – it has all kinds of other components, but we haven't put them all together. We've just discovered they can coexist."

For this research, the Cornell team began engineering epitaxial nitride heterostructures – atomically thin layers of gallium nitride and niobium nitride – and searching for conditions in which magnetic fields and temperatures in the layers would retain their respective quantum Hall and superconducting properties.

They eventually discovered a small window in which the properties were observed simultaneously, thanks to advances in the quality of the materials and structures produced in close collaboration with colleagues at the Naval Research Laboratory…

Potential applications for the material structure include more efficient electronics, such as data centers cooled to extremely low temperatures to eliminate heat waste. And the structure is the first to lay the groundwork for the use of nitride semiconductors and superconductors in topological quantum computing, in which the movement of electrons must be resilient to the material defects typically seen in nitrides…

Other co-authors of the paper include David Muller, the Samuel B. Eckert Professor of Engineering in the School of Applied and Engineering Physics; and researchers from the U.S. Naval Research Laboratory, the National High Magnetic Field Laboratory, and semiconductor company Qorvo.

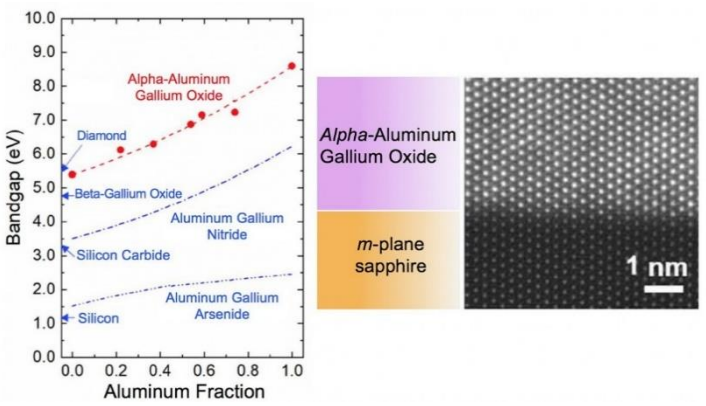
3.2. A Wide Path

The path that leads to the next generation of high-power electronics is not long. But it needs to be wide. Very wide.[5]

A Cornell collaboration has found a way to grow a single crystalline layer of alpha-aluminum gallium oxide that has the widest energy bandgap to date – a discovery that clears the way for new semiconductors that will handle higher voltages, higher power densities and higher frequencies than previously seen.

[5] David Nutt, Cornell Chronicles, "Ultrawide bandgap gives material high-power potential," Jan 19. 2021, https://news.cornell.edu/stories/2021/01/ultrawide-bandgap-gives-material-high-power-potential

The image at left shows the energy bandgap of alpha-aluminum gallium oxide compared to similar materials, and the effect of replacing gallium atoms with aluminum. The image on the right is an overview of alpha-aluminum gallium oxide grown on a substrate of sapphire…



The collaboration was led by co-senior authors Debdeep Jena and Huili Grace Xing, both professors in electrical and computer engineering and in materials science and engineering. The team also included David Muller, the Samuel B. Eckert Professor in Applied and Engineering Physics, who specializes in electron microscopy…

The researchers set about creating a more stable alpha-gallium oxide by growing it on a substrate of sapphire, which has a similar atomic structure. Jinno used molecular beam epitaxy – known informally as "atomic spray-painting" – to create the single layer film. Chang then used scanning transmission electron microscopy to study how its atoms were arranged and detect any defects that may have been created by crystal lattices that weren't perfectly aligned. Those very defects often give materials unique characteristics, but they can sabotage the performance of electronic or photonic devices.

One of the issues Jinno and Chang encountered was that different phases sometimes crept into their samples.

"Sapphire has a lot of facets," Chang said. "If you grow on one facet, and then on the other facet, the quality of the alpha-gallium oxide films will be totally different. It doesn't always result in a good, clean, quality film."

The team eventually identified the right symmetry of the right sapphire facet, called the m-plane, which resulted in a stable alpha-gallium oxide film. They slowly replaced some of the gallium atoms with aluminum as a way to widen its bandgap even more.

Conventional gallium oxide has a bandgap of 3 to 4.7 eV (electron volts); every electron volt represents a huge leap in performance. Beta-gallium oxide reaches up to 4.8 eV. The bandgap of the new alpha-aluminum gallium oxide starts at 5.4 eV and, as more aluminum is swapped in, it expands to 8.6 eV – almost eight times the bandgap of silicon.

Author's Note: Silicon Carbide, the leading new power electronics material, has bandgap of about 3.2 (see the above chart).

"These are actually the widest energy bandgap crystals that have ever been realized by epitaxy. The fact that Riena and Celesta could grow and understand these atomic layers and found the right sort of playground – which is the surface of sapphire – to grow them on is a major breakthrough," said Jena, who connected the current work to the discovery of high-quality crystalline gallium nitride, which over the last two decades has revolutionized LED lighting.

Not only is alpha-aluminum gallium oxide robust enough to handle enormous amounts of energy at high speeds and high temperatures, it is also lightweight and compact – qualities that could make it a crucial component in aeronautical technologies as well as other high-power electronics.

The material is also incredibly efficient, which could reduce the loss of energy in converting and transmitting solar power.

"This is really moving semiconductors into unchartered territory in terms of how much energy they can handle," Jena said. "At the same time, it is forcing us to rethink the materials that we always believed to be insulators, like sapphire. Can we actually change their properties to our own benefit in terms of controlling their energy gaps and electronic properties by doping it as we do with silicon and gallium nitride?"

4. Future Discoveries

I believe in the future there will be new rechargeable battery chemistries developed, as well a further evolution of existing chemistries. Currently lithium-ion chemistries dominate the market for self-contained rechargeable batteries. The two largest (and rapidly growing) markets for these are electric vehicles (EVs) and battery energy storage systems (BESS).

The primary lithium-ion battery chemistries are LFP ($LiFePO_4$ or Lithium Iron Phosphate), NMC ($LiNi_XMn_YCo_ZO_2$ or Lithium Nickel Manganese Cobalt Oxide), and NCA ($LiNi_XCo_YAl_ZO_2$ or Lithium Nickel Cobalt Aluminum Oxide).

There are also various types of flow batteries, which may be useful for long-duration BESS designs. Although the flow battery market is only a tiny fraction the size of the lithium-ion market, it has shown some signs of life lately.

I would guess the tools described in the above sections are already playing a role in future battery development. The following are promising new development for rechargeable batteries, but I found no specific documentation of the use of the new tools described above. This is not surprising as all developments and developmental tools for energy storage tend to be very proprietary.

As I'm final-prepping this paper for posting, I found a potential source for another future paper, a Honeywell Flow Battery. There was just one problem, I could find absolutely no information on the chemistry used for this battery, hmmm. Read the next subsection and we may know why.

4.1. Flow Batteries

When it comes time to design a new battery chemistry, scientists only can try a handful of possibilities experimentally, as it takes time and resources to synthesize and investigate each new molecule. By performing reliable molecular simulations using supercomputers, researchers can speed up the desired materials screening process and expand the breadth of their search, while getting detailed information about the possibilities inherent in different chemistries.[6]

[6] Jared Sagoff, Argonne National Laboratory Joint Center for Energy Storage Research, "Active learning accelerates redox-flow battery discovery," Oct 1, 2020, https://www.jcesr.org/active-learning-accelerates-redox-flow-battery-discovery/

However, even high-throughput simulations run on these supercomputers can only look at a fraction of the possible viable chemistries that exist for certain types of batteries. In a new study from the U.S. Department of Energy's (DOE) Argonne National Laboratory, researchers are taking the next step in accelerating the hunt for the best possible battery components by employing artificial intelligence.

The study team, led by Argonne chemist Rajeev Surendran Assary, investigated the inner workings of redox flow batteries, in which chemical energy is stored in dissolved molecules that interact with electrodes. Flow batteries are promising for applications in the electric grid. They replace solid cathodes and anodes with liquid solutions infused with molecules that store and release energy. Conventional flow batteries are based on molecules that have one charge storing element per molecule, with limited versatility. Researchers at the Joint Center for Energy Storage Research (JCESR), a DOE Energy Innovation Hub led by Argonne, introduced the concept of storing and releasing energy with materials called "redox active polymers," or redoxmers, which are based on larger molecules, each with tens of charge storing elements.

Compared to conventional systems, redoxmers allow much greater flexibility to independently customize many aspects of battery characteristics and performance. Redoxmer flow batteries open a new window on flow battery design because they can provide high functionality at low cost, with little harm to the environment. JCESR's redoxmer flow batteries have the potential to transform how we think about and use flow batteries for the grid.

In the case of the redoxmers under study, Assary and his colleagues noticed that, as the battery charges and discharges, they tend to form an inactive film. To prevent this phenomenon, the Argonne team looked to design a redoxmer that could be electrically cleaved at a particular voltage, freeing it to re-enter the electrolyte solution.

"You can think of it like cleaning a pan that you cook on," said Argonne postdoctoral researcher Hieu Doan, another author of the study. "To remove sticky food residues more easily, you may use high heat, and that's what we're doing with electricity."

The researchers wanted to have the cleaving voltage be just outside the battery's normal operating window, so that it wouldn't interfere with performance, but also wouldn't require a lot of additional energy.

To find a redoxmer that would cleave at the appropriate voltage, Assary and the team turned to Argonne's Bebop supercomputer at the Laboratory Computing Resource Center. First, the researchers ran a set of 1,400 different redoxmers using density functional theory (DFT) calculations, which are highly accurate but computationally expensive. However, these 1,400 redoxmers represented only a tiny slice of the total chemical space that the researchers were interested in…

To find the ideal molecules from a larger dataset consisting of more than 100,000 redoxmers without running extensive DFT calculations, the researchers used a machine learning technique called active learning. This larger dataset included redoxmers that were structurally similar to those in the original DFT dataset of 1,400 molecules…

"The model guarantees that by adding this new data point to the training set, it will become better, and then we can train it again," Doan said. "Whatever maximizes the accuracy of the model, that will be the next data point to pick..."

Indeed, when the same approach was applied to the 100,000+ dataset, it successfully found 42 desired molecules within 100 picks…

4.2. Solid-State Magnesium-Ion Batteries

Magnesium batteries have long been considered a potentially safer and less expensive alternative to lithium-ion batteries, but previous versions have been severely limited in the amount of power they delivered.[7]

Researchers from the University of Houston and the Toyota Research Institute of North America (TRINA) reported in Nature Energy that they have developed a new cathode and electrolyte—previously the limiting factors for a high-energy magnesium battery—to demonstrate a magnesium battery capable of operating at room temperature and delivering a power density comparable to that offered by lithium-ion batteries.

Magnesium ions can hold twice the charge compared to lithium, and have a similar ionic radius. As a result, magnesium dissociation from electrolytes and its diffusion in the electrode, two essential processes that take place in classical intercalation cathodes, are sluggish at room temperature, leading to low power performance.

One of the paper's co-authors, Professor Yan Yao, said the results came from combining both an organic quinone cathode and a newly-tailored boron cluster-based electrolyte solution.

"We demonstrated a … redox chemistry to create a cathode which is not hampered by the ionic dissociation and solid-state diffusion challenges that have prevented magnesium batteries from operating efficiently at room temperature," Yao said. "This new class of redox chemistry bypasses the need for solid-state intercalation while solely storing magnesium, instead of its complex forms, creating a new paradigm in magnesium battery electrode design."

Author's Comment: Intercalation: insert (something) between layers in a crystal lattice.

TRINA researchers have made advancements in magnesium batteries, including the development of highly recognized, efficient electrolytes based on boron cluster anions. However, these electrolytes had limitations in supporting high battery cycling rates.

"We had hints that electrolytes based on these weakly coordinating anions in principle could have the potential to support very high cycling rates, so we worked on tweaking their properties," said Rana Mohtadi, a Principal Scientist at TRINA and another of the paper's co-authors. "We tackled this by turning our attention to the solvent in order to reduce its binding to the magnesium ions and improve the bulk transport kinetics. We were fascinated that the magnesium plated from the modified electrolyte remained smooth even under ultrahigh cycling rates. We believe this unveils a new facet in magnesium battery electrochemistry…"

"The new battery is nearly two orders of magnitude higher than the power density achieved by previous magnesium batteries," said post-doctoral researcher Hui Dong, who also contributed to the paper. "The battery was able to continue operating for over 200 cycles with around 82% capacity retention, showing high stability. We can further improve cycling stability by tailoring the properties of the membrane with enhanced intermediate trapping capability."

[7] Tom Lombardo, Charged Electric Vehicle Magazine, "Discoveries highlight new possibilities for magnesium batteries," Jan 5, 2021, https://chargedevs.com/newswire/discoveries-highlight-new-possibilities-for-magnesium-batteries/

4.3. Iodide Battery

IBM Research has discovered a new battery design that doesn't use heavy metals and may outperform lithium-ion batteries. To expand the promise of these batteries from the lab into reality, IBM Research has signed joint development agreements with Mercedes-Benz Research and Development North America, battery electrolyte supplier Central Glass, and battery manufacturer Sidus.[8]

As battery-powered alternatives for everything from electric vehicles to smart grids are explored, there remain significant concerns around the sustainability of battery materials. Many of these, including nickel and cobalt, pose tremendous environmental and humanitarian risks.

IBM Research's design is built from materials which do not use heavy metals or substances with sourcing concerns.

This new battery design from IBM Research uses iodide as an active cathode material, which is able to be extracted from seawater. The overall combination of this cathode material with a new and proprietary electrolyte formulation, including a reaction mediator, makes this battery system unique from other metal iodide batteries, resulting in its outstanding performance and low flammability. It holds even more promise than lithium-ion batteries across a number of transportation and energy technologies:

For electric vehicles, the battery's low flammability, low cost and fast charging time (less than 5 minutes to reach an 80% charge) — all of which are obstacles with lithium-ion batteries — could enable a widely accessible electric vehicle to become reality.

In the expanding area of flying vehicles and electric aircraft, this battery can be optimized to achieve a high power density that outperforms lithium-ion batteries — critical for uses in which the ability to quickly scale power is key.

Initial tests have also shown this battery can be designed for a long-life cycle — giving it the stability to be a sustainable, low-impact and low-cost option for power grids and energy storage.

This discovery builds on IBM Research's deep foundation of exploratory and breakthrough chemistry and materials science. For example, the research team tapped into atomic force microscopy to better understand the forces within these battery materials at a molecular and atomic level. This same infrastructure is what has powered other transformative IBM discoveries – from semiconductor development to quantum computing.

5. Final Comment

Photovoltaic technology, energy storage technologies, electric vehicles and the underlying technologies: power electronics and computer science have changed the world. As the above suggests, we are nowhere near the end of this path.

[8] Kelly Pickerel, IBM via Solar Power World, "IBM Research discovers new battery design that could outperform lithium-ion," Dec 18, 2018, https://www.solarpowerworldonline.com/2019/12/ibm-research-discovers-new-battery-design-that-could-outperform-lithium-ion/