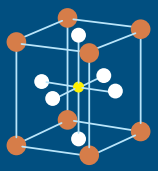


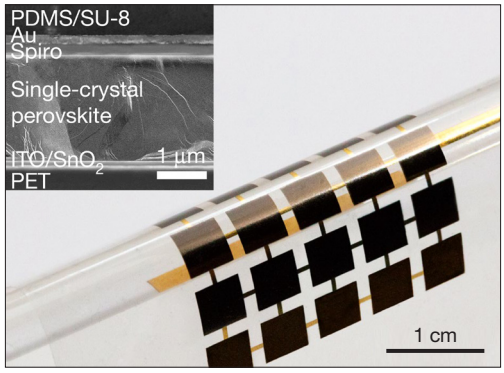
RESEARCH HIGHLIGHTS: Perovskites

By **Pabitra K. Nayak**

Metal halide perovskite materials have revolutionized low-cost processed optoelectronic devices. Efficiency records of perovskite-based devices break at a regular pace. Fundamental understanding of this class of materials is progressing rapidly, leading to better optimization and stability. MRS Bulletin *presents coverage of the most recent impactful advances in the burgeoning field of perovskite research.*

High-efficiency halide perovskite-based optoelectronic devices are mostly comprised of polycrystalline thin films. However, single-crystal materials show better charge-carrier transport, lower density of defects, and better stability in comparison to their polycrystalline counterparts. However, fabrication and mass production of large area devices with single-crystal thin films has been a challenge.

Sheng Xu from the University of California, San Diego, and co-workers have reported in *Nature* (doi:10.1038/s41586-020-2526-z) a solution-based lithography-assisted epitaxial growth and transfer method that enables fabrication of single-crystal perovskites on any arbitrary substrate. The authors describe precise control of the thickness (from 600 nm to about 100 μm) and area (continuous thin films up to about 5.5 cm × 5.5 cm), and compositional gradient in the thickness direction of the single-crystal thin films. These solution-grown and -transferred perovskite single-crystal films have quality comparable to those directly grown on epitaxial substrates and were found to be mechanically flexible. The authors also prepared lead-tin gradient alloying to achieve a graded electronic bandgap. Optoelectronic devices based on the perovskite single crystal show better stability than their polycrystalline counterparts.



An array of single-crystal-based flexible perovskite solar cells. Inset: a cross-sectional scanning electron microscope image of the cell. Credit: *Nature*.

Long-term stability of halide perovskite solar cells has been a major concern and comes in the way of commercial deployment of the technology. Yen-Hung Lin and Henry Snaith from the University of Oxford and co-workers have found a way to address this stability issue. In work published in *Science* (doi:10.1126/science.aba1628), they showed that by incorporating the ionic compound 1-butyl-1-methyl-piperidinium tetrafluoroborate in a formamidinium-cesium lead-trihalide perovskite material, they could achieve highly stable perovskite solar cells. Under simulated sunlight and ambient atmosphere, the encapsulated cells retained 95% of the post-burn-in efficiency (the stabilized efficiency after the initial drop in efficiency that happens in a short timespan) after a period of 1200 hours at 85°C.

The perovskite material used in this work has a mixed-halide composition, which makes it susceptible to light-induced halide segregation, another challenge associated with this class of materials. The authors have reported that the ionic compound additive slows down the compositional segregation in the perovskite film, even during aggressive aging tests. The additive also improved the open-circuit voltage of the solar cells, which generally indicates lower density of electronic defects. The authors postulate that the lower defect density in the perovskite material suppresses the degradation and halide segregation in the solar cell, which are mainly initiated by trapped charge carriers at the defect sites.

The bandgap of the perovskite material reported in this study is well suited for perovskite on Si tandem application. The authors foresee that the combination of this perovskite with Si technology would result in efficient and stable tandem solar cells.

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Electrification of remote areas needs low-cost, off-grid power systems. Solar flow battery (SFB) technology is one such option. However, obtaining both high energy-conversion efficiency and long device lifetime simultaneously for SFB systems has been a challenge.

Work by Anita Ho-Baillie, Song Jin, and co-workers, reported in *Nature Materials* (doi:10.1038/s41563-020-0720-x), showed that a combination of high-efficiency $(FAPbI_3)_{0.83}(MAPbBr_3)_{0.17}$ perovskite/silicon tandem solar cell and redox batteries based on bis-(trimethylammonio)propyl viologen (BTMAP-Vi) and 4-trimethylammonium-TEMPO (NMe-TEMPO) redox couples can provide a high-performance solar flow battery.

The authors have used numerical methods for the rational design of components to achieve an optimal match between the maximum power point voltage (V_{MPP}) of the solar cell and formal cell potential (E^0_{cell}) of the redox flow battery. The authors achieved 20.1% solar to output electricity efficiency. This perovskite on a Si tandem cell is compatible with aqueous organic SFBs while being cost-effective. The Si bottom cell with a gold back-contact comes in contact with the aqueous electrolyte. The performance of the photo-electrode (i.e., the tandem cell with the electrolyte) is similar to the performance of a solid-state tandem solar cell, indicating the compatibility of the tandem cell and electrolytes for flow battery applications. The conceptual design in this work could help in future optimization for storage systems with integrated solar conversion ability.

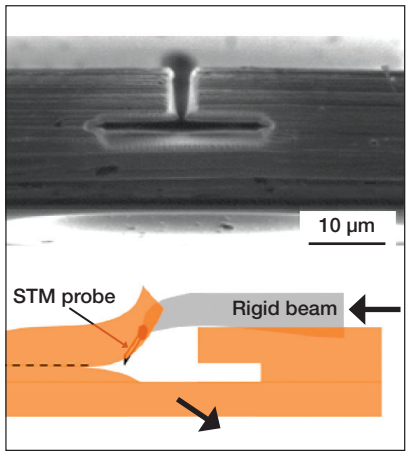
Knowledge of the electronic energy landscape of an electronic material is important for the optimization of its optoelectronic properties, as well as its application in devices. Formamidinium lead triiodide ($FAPbI_3$), a three-dimensional electronic material, shows an intriguing quantum confinement effect, as reported by Laura Herz from the University of Oxford and co-workers in *Nature Materials* (doi:10.1038/s41563-020-0774-9). The authors used temperature-dependent absorption spectroscopy and *ab initio* simulations to confirm the presence of an intrinsic quantum confinement in the nominally bulk semiconductor $FAPbI_3$. They attribute this quantum confinement with a length scale of 10–20 nm to the coexistence of different crystallographic phases or domains in the bulk film of $FAPbI_3$.

The authors consider this discovery to be highly exciting since it obviates expensive top-down nano-processing steps needed to achieve an electronic quantum confinement effect while maintaining an efficient flow of electrical current through the film. They expect that the intrinsically formed nanostructures in bulk perovskite material will enhance radiative recombination, thus lowering the threshold for amplified spontaneous emission and facilitate the realization of an electrically pumped laser using this material.

Nanoindentation on peeled high-performance polymeric fibers reveals failure mechanisms

High-performance fibers are key to many structural and lightweight applications as they are the main reinforcing components of continuous fiber-reinforced composites and fabrics. These fibers are drawn from synthetic polymers such as poly(*p*-phenylene terephthalamide) (PpPTA) or ultrahigh-molecular-weight polyethylene (UHMWPE). During the drawing process, highly oriented and crystalline nanofibrils of 10–50 nm width form and assemble into larger bundles of 100–500 nm width, thereby creating a hierarchical microstructure. Although it is known that hierarchy generally improves the properties of materials, its role in the failure of synthetic fibers has not been studied. In particular, measuring properties at the intermediate submicrometric scale is challenging. To better understand the role of this organization in the mechanical performance of fibers, the research groups of Yuris Dzenis at the University of Nebraska–Lincoln and Kenneth Strawhecker at the US Army Research Laboratory have taken up the challenge and studied the mechanical interactions between the bundles. Their results were published in *ACS Applied Materials and Interfaces* (doi:10.1021/acsami.9b23459).

To measure the properties at the submicrometric scale, they developed a special protocol in which a T-shaped notch was first cut using focused ion beam milling. Then, a scanning tunneling microscope probe was inserted into the notch to peel away a thin layer of the fiber that delaminated at the bundle interface. The uncovered polymeric surface was then probed by nanoindentation to measure the interfacial separation energy absorption between bundles. Taylor Stockdale, the first author of the article, explains that "by performing repeated indents at the same location, we



Electron micrograph showing the T-shaped notch made by focused ion beam and cartoon showing the peeling process using the scanning tunneling microscope (STM) probe. Credit: ACS Publications.

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